SBMLDock

Docker Driven Systems Biology Tool Development and Usage

E. Z. Gnimpieba, M. Thavappiragasam, A. Chango, B. Conn,
C. M. Lushbough

Introduction

- Simplify researchers workflows
- Docker is a new emerging technology
- Work with our SBML tools

SBMLDock

- Collects 7 CLI tools to manipulate SBML files
- We packaged in a special way
  - Each tool has it’s needed libraries
  - We wrap java execution of all tools
  - We provide test data for each tool

Tool specifics

- ParaABioS
- SBMLChecker
- SBMLCompare
- SBMLMerge

Tool specifics

- SBMLSplit
- SBMLModeler
- SBMLAnnotate

Docker specifics

- A self contained system
- Interacts with the kernel of the host system
- Repeatable and shareable
- Runs on Linux
    - Windows and Mac can work

Docker specifics

- Mount volumes in the container

  -v /tmp/sbmldock:/tmp

- Tell the container where to run

  -w /tmp

- Run our image
- Call one of our programs

Run a tool

- We've included test data
- This is what SBMLAnnotate would produce

```
wjconn@ted:/tmp/sbmldock$ docker run -v /tmp/sbmldock:/tmp -w /tmp usdbioinforma
tics/sbmldock SBMLAnnotate /opt/SBMLAnnotate/one.xml out.xml
start..
wjconn@ted:/tmp/sbmldock$ ls
hsperfdata_root  jsbml.log  out.xml
wjconn@ted:/tmp/sbmldock$
```

Tools in a docker container

- Tools run the same on every system
- Docker images have unique numeric ids
- Containers run the same every time you start them

Conclusion

- Collected SBML specific tools
- Docker provides:
  - Usability
  - Reproducibility
  - Unique identification

- **Acknowledgement:** This work has been partially supported by the National Science Foundation/EPSCoR Award No. IIA-1355423 and by the state of South Dakota, through BioSNTR.

- **References.**

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Opinion Paper

Evolutionary Constraint-Based Formulation Requires New Bi-level Solving Techniques

Marko Budinich, Jérémie Bourdon, Abdelhalim Larhlimi, Damien Eveillard
ComBi Team, LINA,UMR 6241 CNRS, EMN, Université de Nantes

Computer Methods in Systems Biology, September 2015

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- Constraint Based Models are a type of metabolic models

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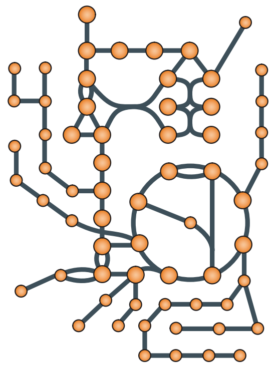

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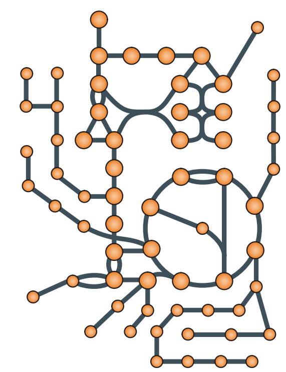
- We are interested into rates of reactions **v** (fluxes)



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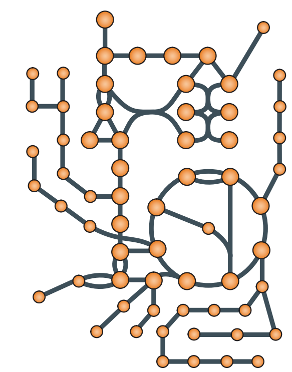

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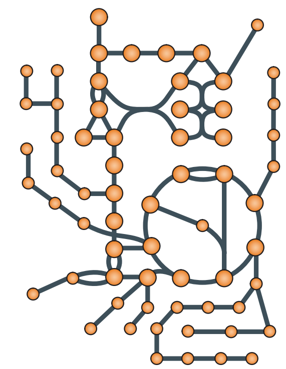

Metabolites

−1	0	0	0	0	1	0	0	0
−1	0	0	0	0	0	1	0	0
0	0	0	−1	−1	0	0	1	0
1	−1	0	1	0	0	0	0	0
0	1	−1	0	0	0	0	0	0
0	0	−1	0	1	0	0	0	0
0	0	1	0	0	0	0	0	−1

Reactions

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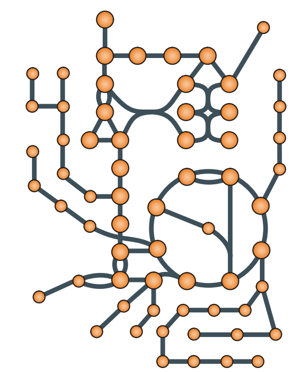

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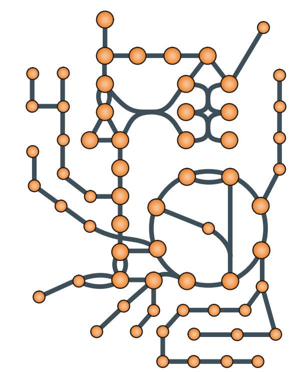

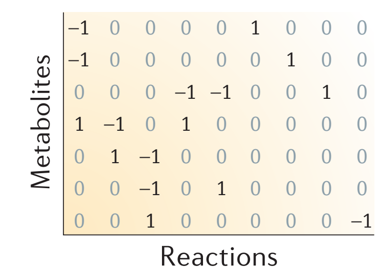

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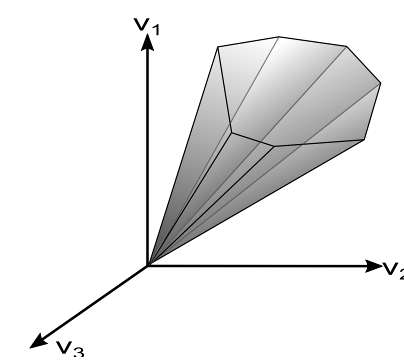
$$lb \leq v \leq ub$$



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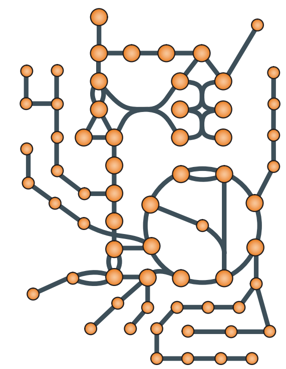

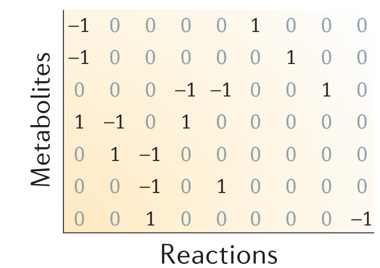

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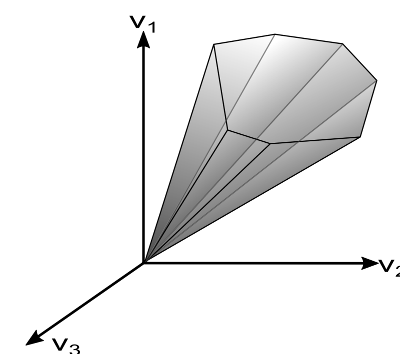

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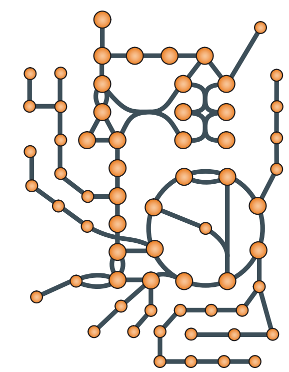

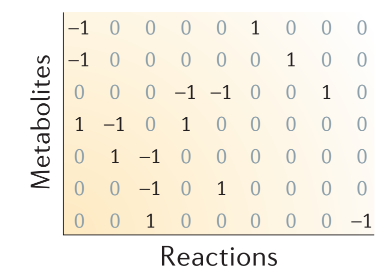

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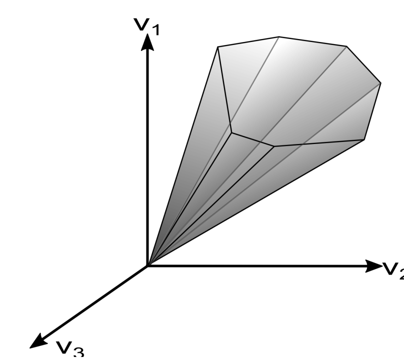

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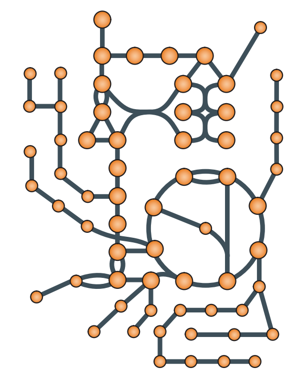

Metabolites × Reactions

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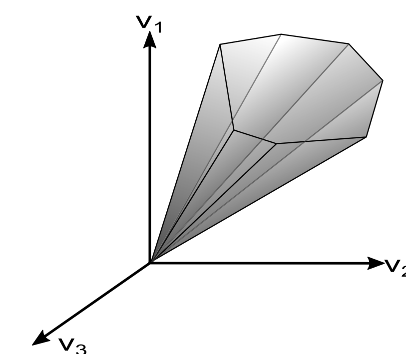

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Evolution

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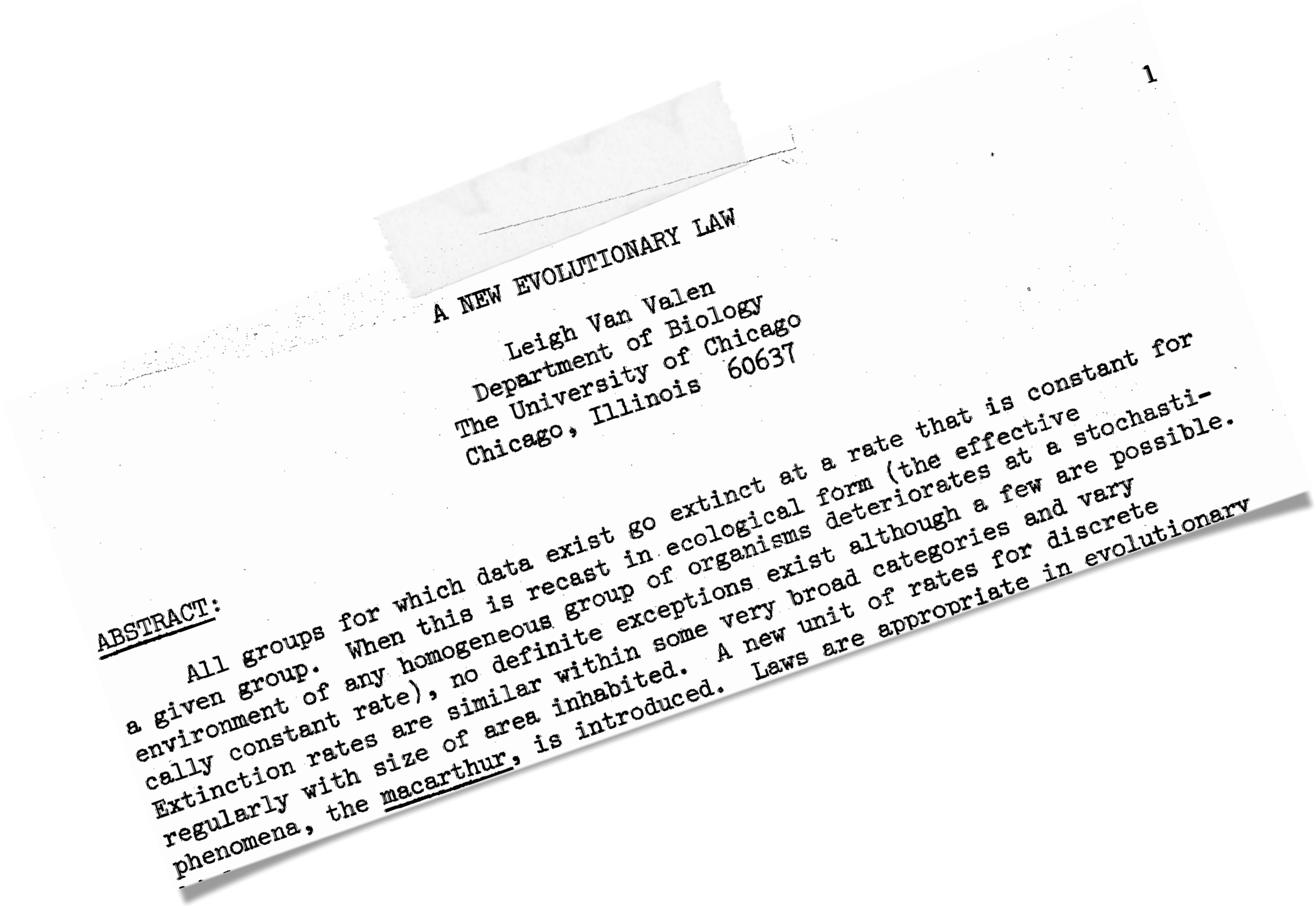

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A NEW EVOLUTIONARY LAW

Leigh Van Valen
Department of Biology
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ABSTRACT:

All groups for which data exist go extinct at a rate that is constant for a given group. When this is recast in ecological form (the effective environment of any homogeneous group of organisms deteriorates at a stochastically constant rate), no definite exceptions exist although a few are possible. Extinction rates are similar within some very broad categories and vary regularly with size of area inhabited. A new unit of rates for discrete phenomena, the macarthur, is introduced. Laws are appropriate in evolutionary

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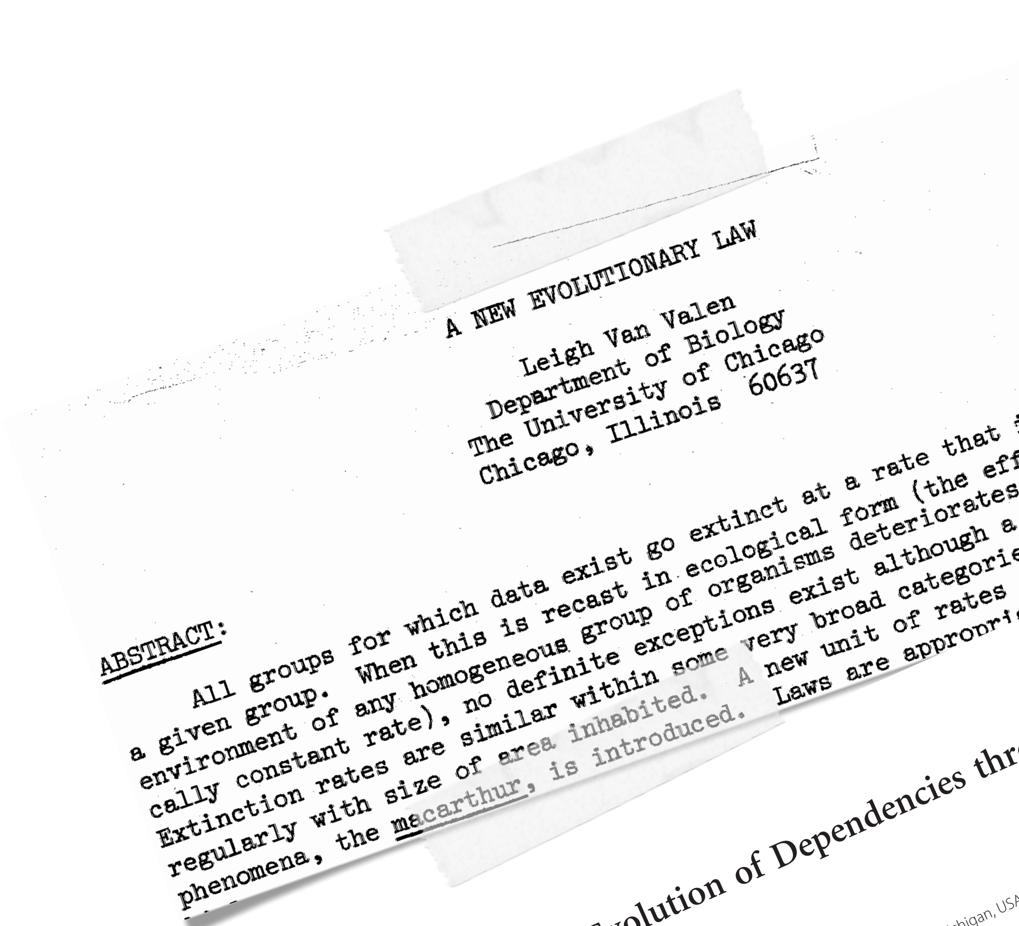

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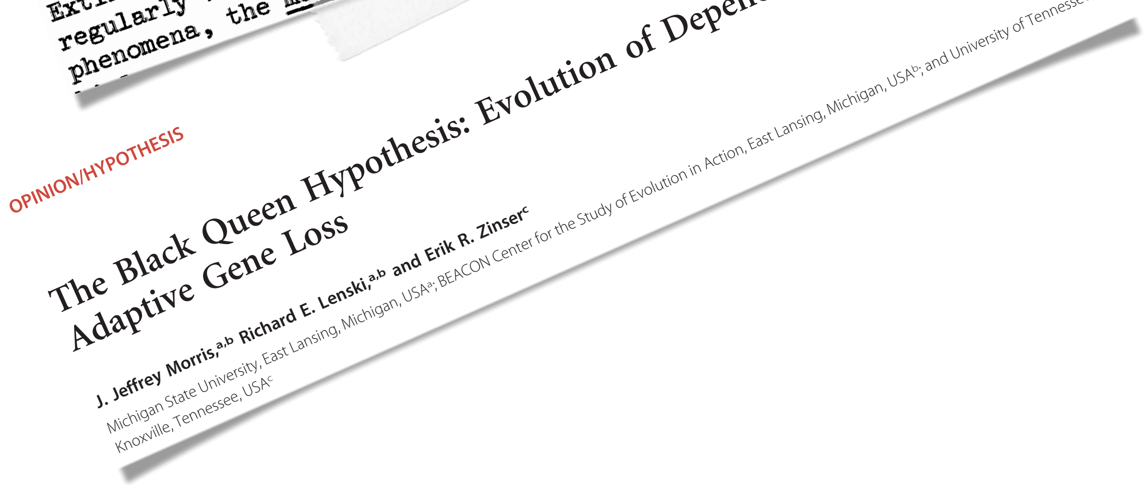

OPINION/HYPOTHESIS

The Black Queen Hypothesis: Evolution of Dependencies through Adaptive Gene Loss

J. Jeffrey Morris,[a,b] Richard E. Lenski,[a,b] and Erik R. Zinser[c]

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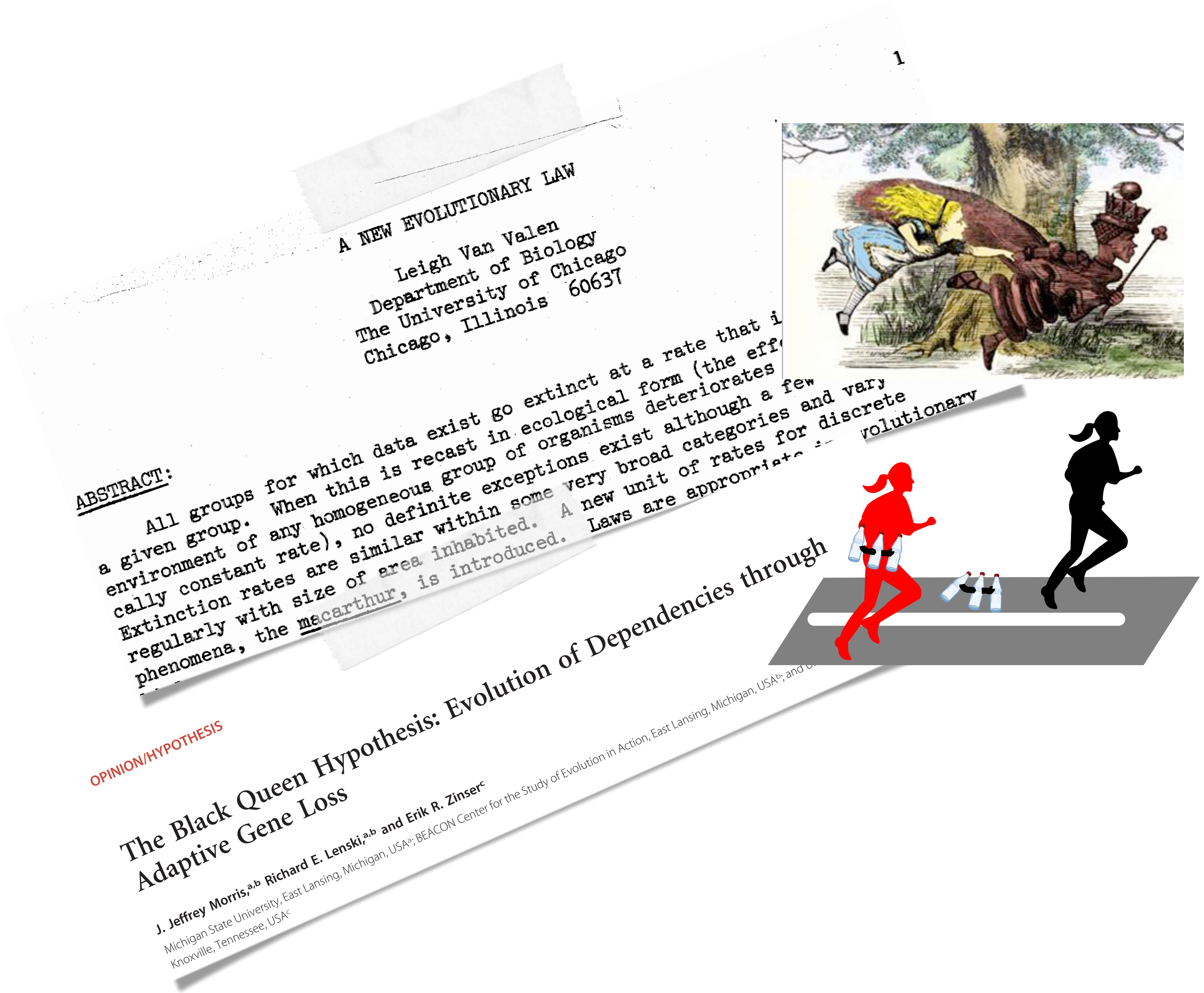

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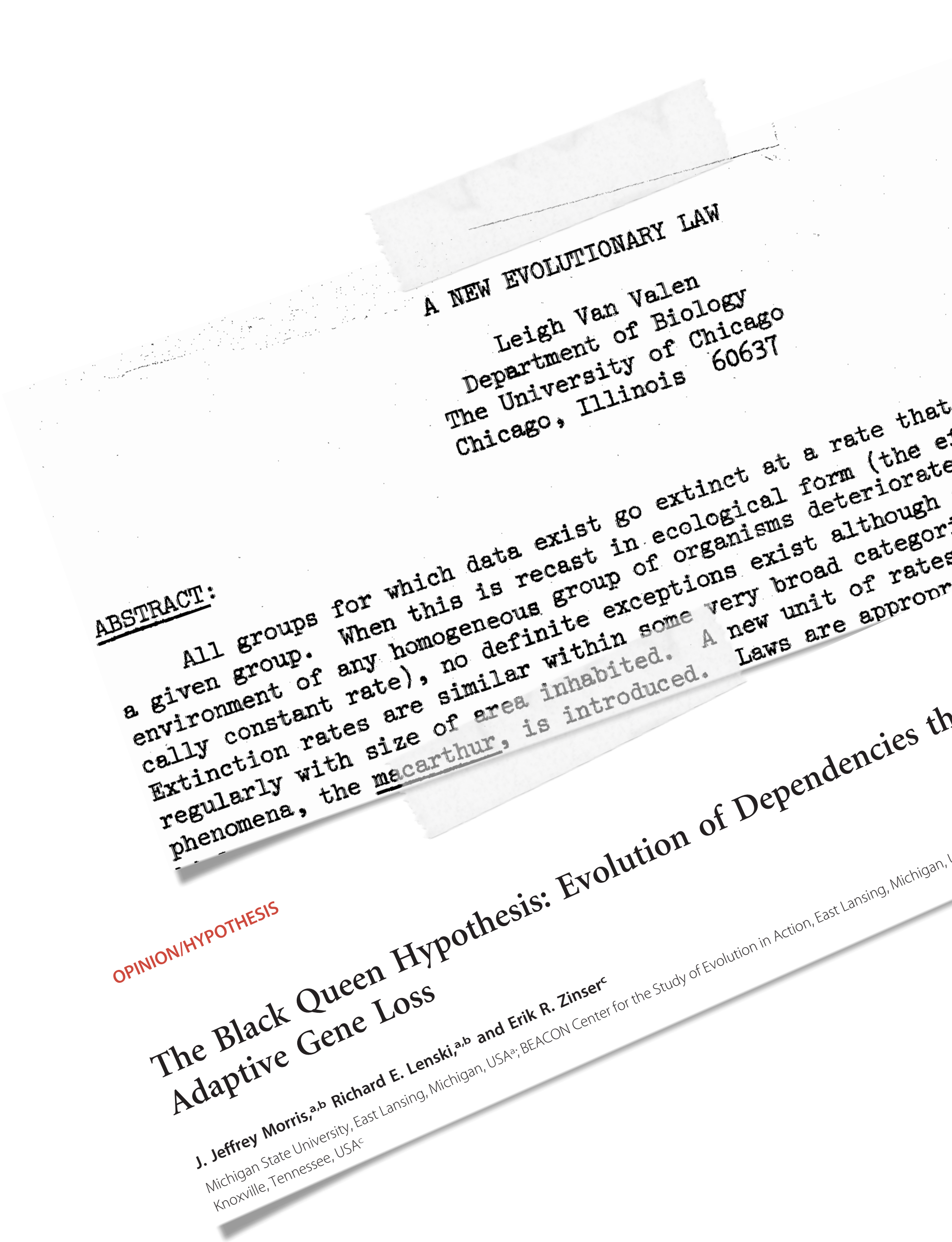

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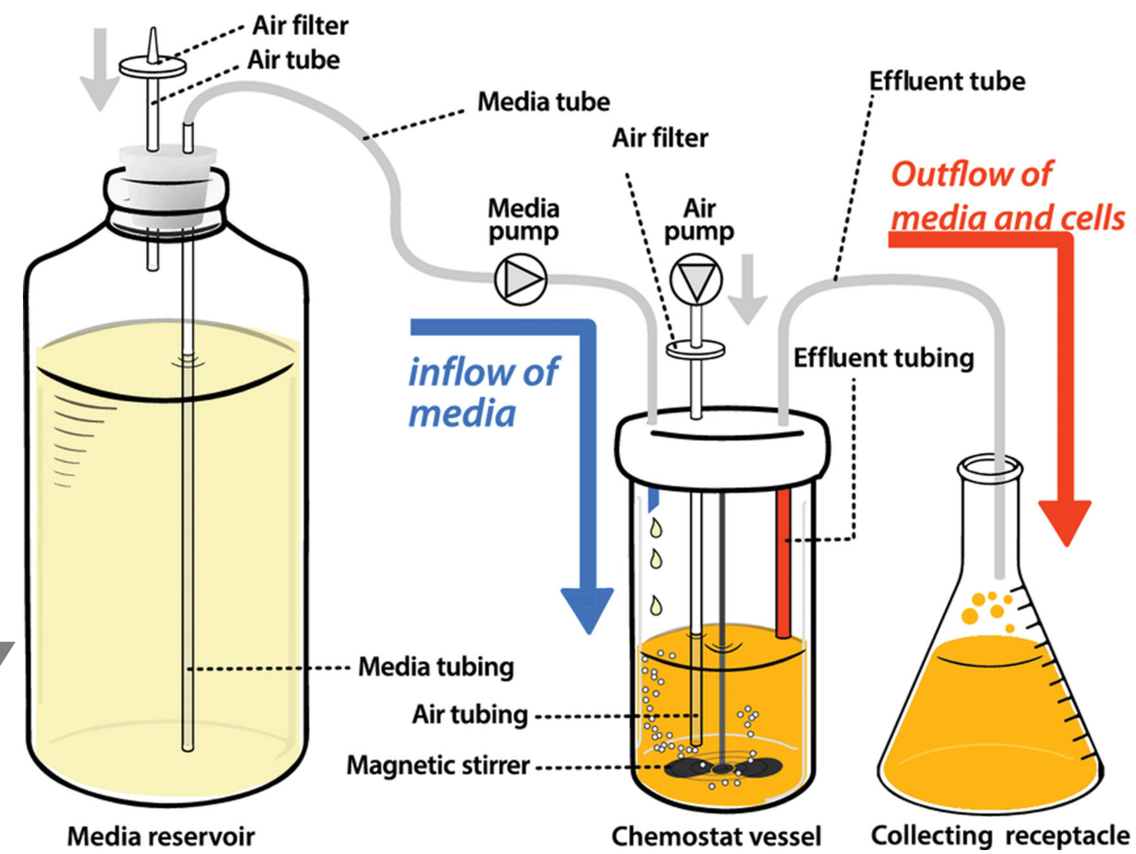

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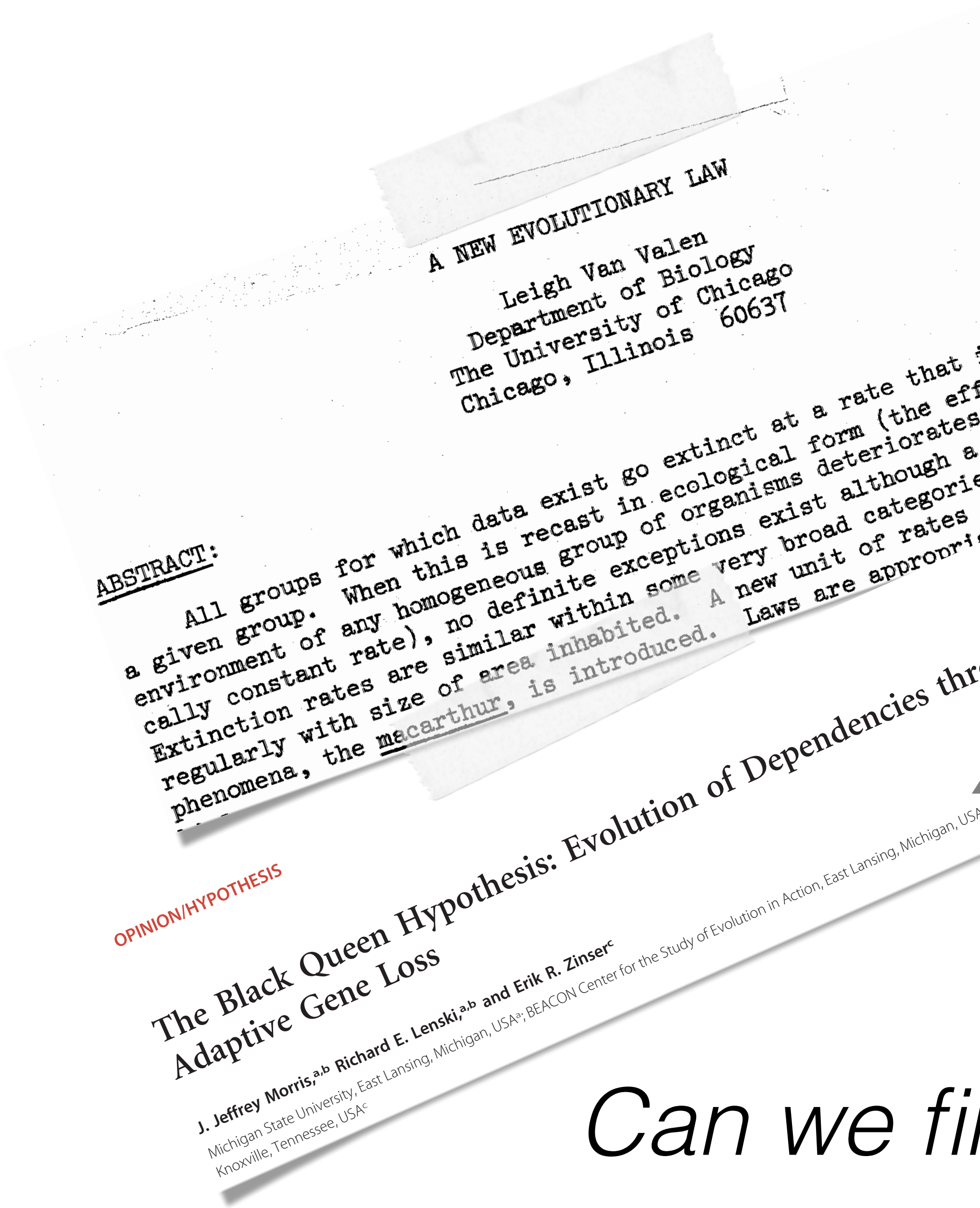

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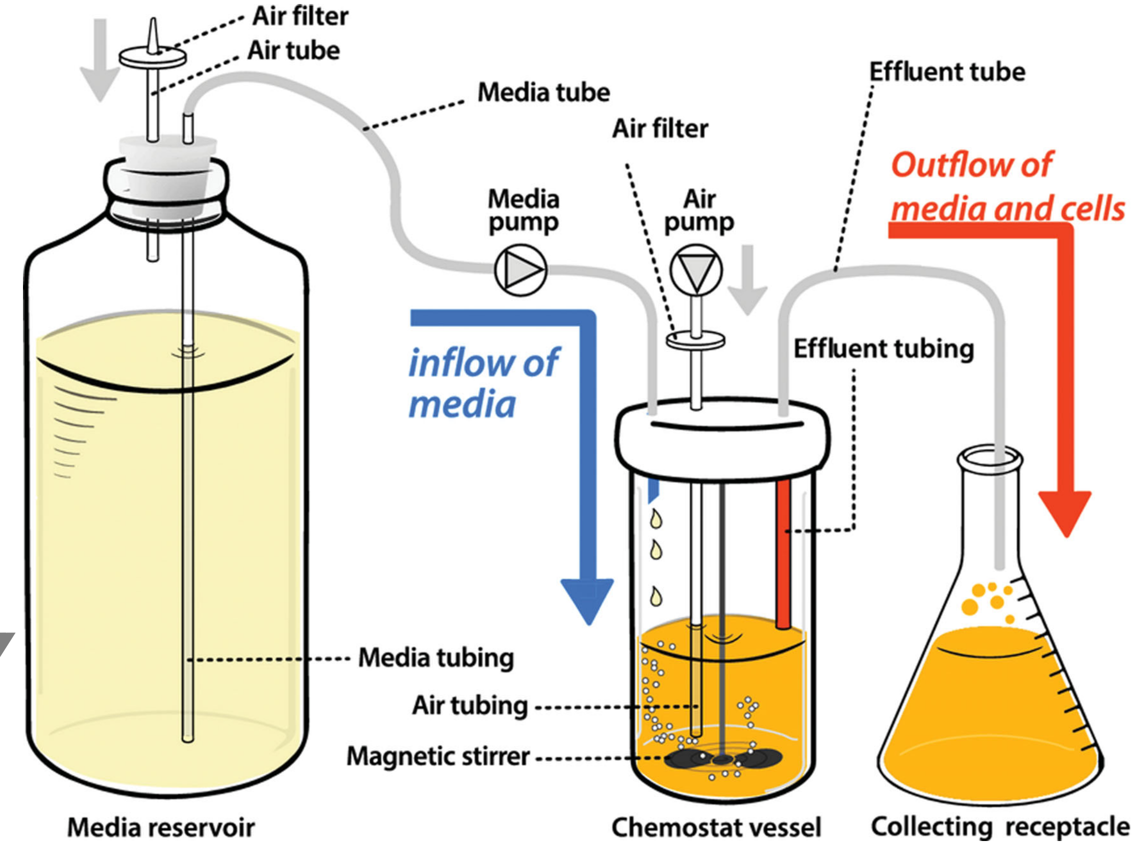

Can we find candidate genes for these theories?

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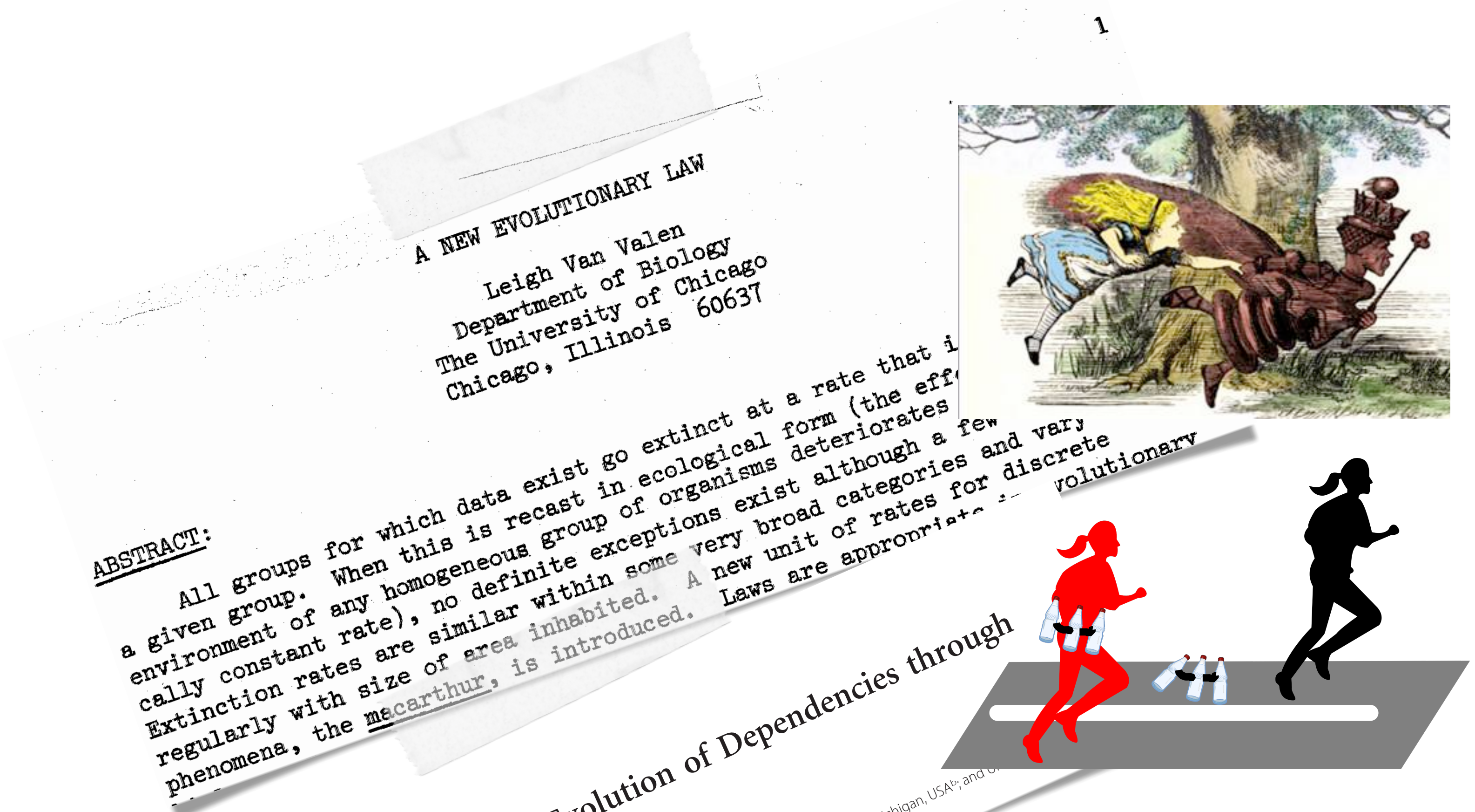

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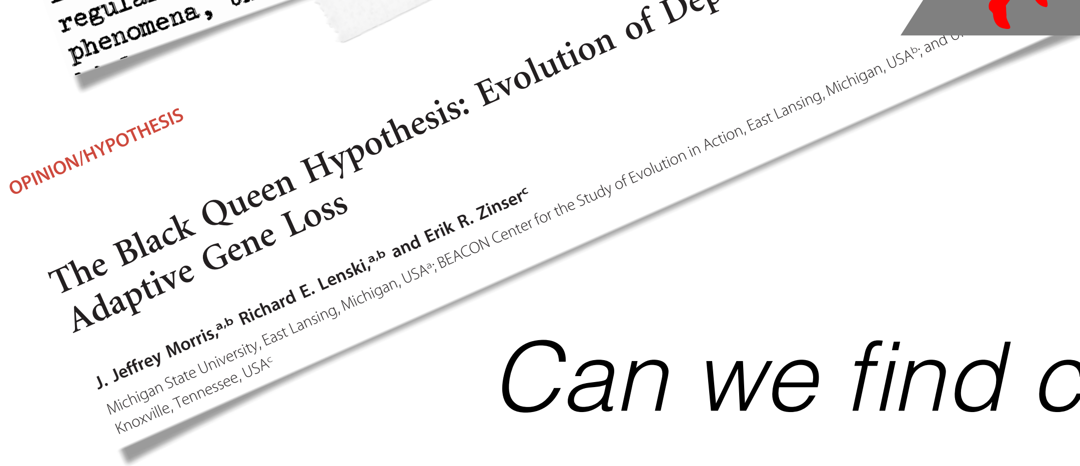

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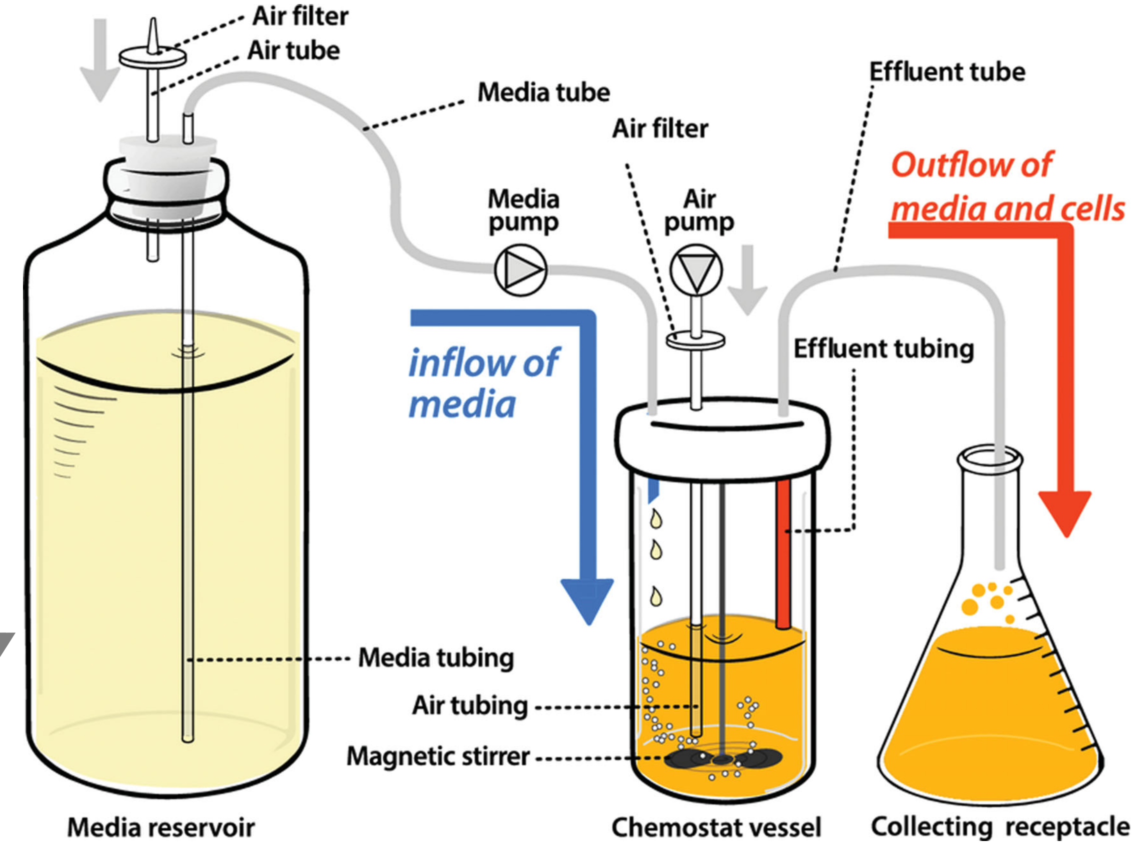

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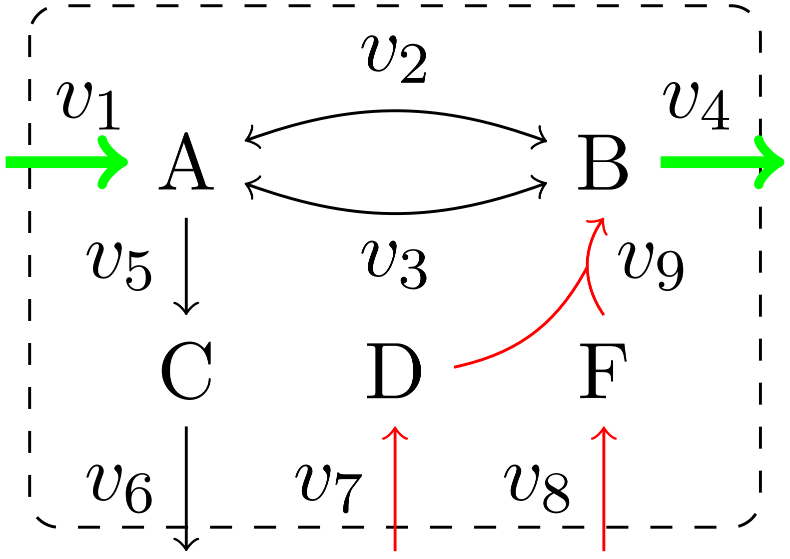

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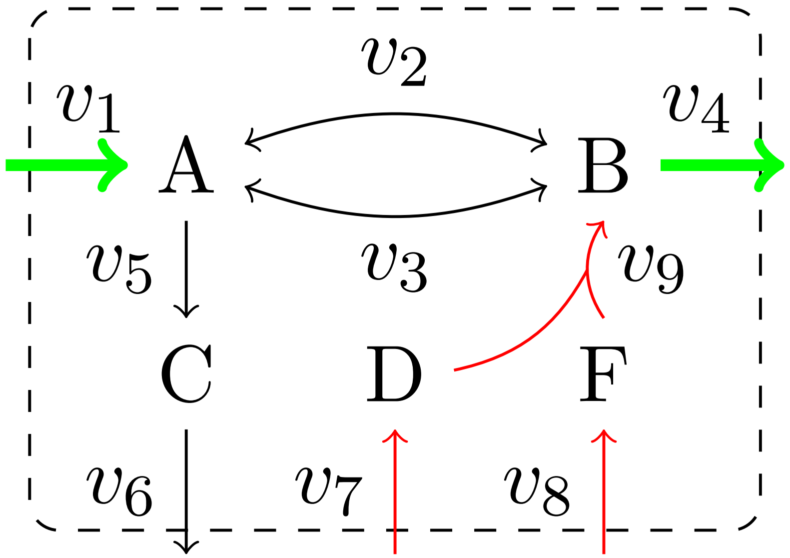

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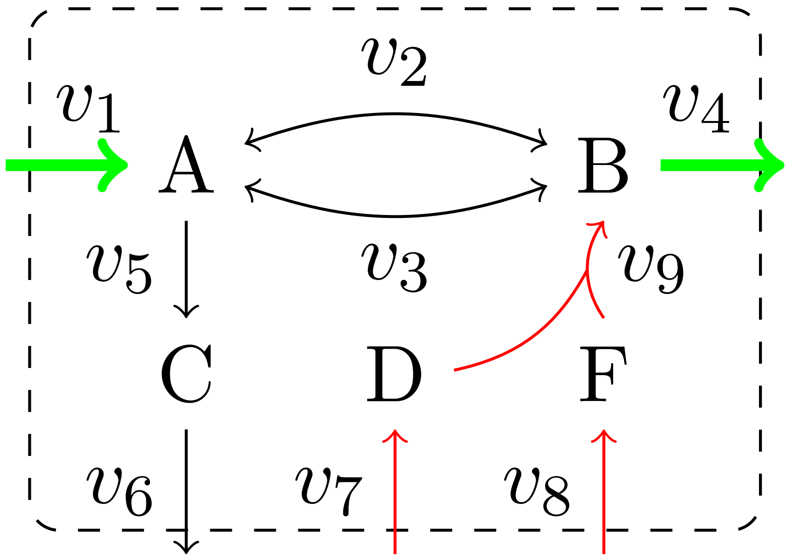

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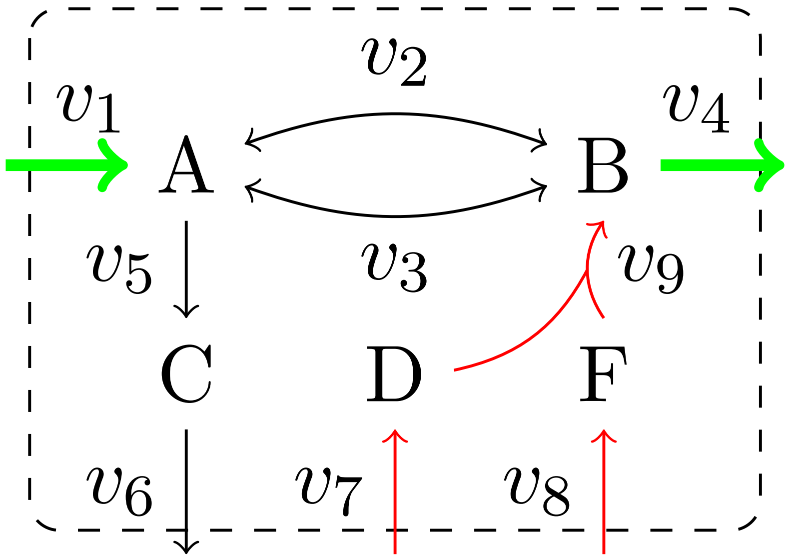

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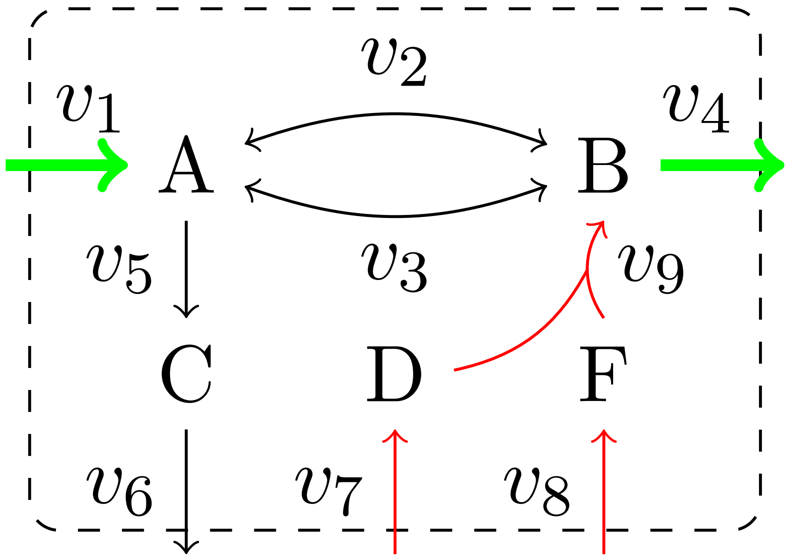

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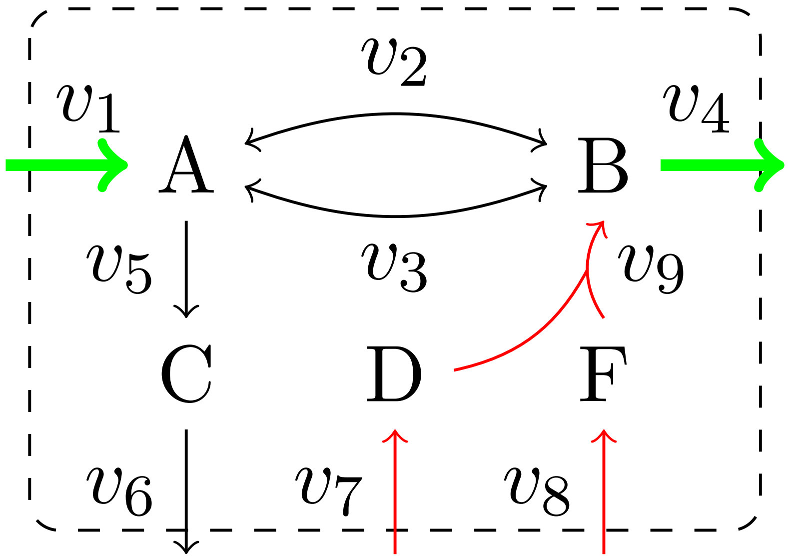

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s.t
Sv=0
lb ≤ v ≤ ub
$v_i = \mathbf{E}_1, i \in \mathcal{L}$
...

...

$\mathit{max}\ c^T v$
s.t
Sv=0
lb ≤ v ≤ ub
$v_i = \mathbf{E}_n, i \in \mathcal{L}$
...

It is possible to determine conditions $\mathbf{E}$ to obtain most of blocked reactions?

A Bi-Level Optimization Approach

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First, we find number of blocked reactions

A Bi-Level Optimization Approach

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$$max \sum_{i=1}^{n} f_i^+ + f_i^-$$

subject to

$$\mathbf{Sv} = 0 \qquad (1)$$

$$\mathbf{lb} \leq \mathbf{v} \leq \mathbf{ub} \qquad (2)$$

$$\mathbf{v}_L = \mathbf{E},\ L \in \mathcal{L} \qquad (3)$$

$$f_i^+,\ f_i^- \in \{0, 1\} \qquad (4)$$

$$f_i^+ + f_i^- \leq 1 \qquad (5)$$

$$v_i \geq \epsilon f_i^+ - M f_i^- \qquad (6)$$

$$v_i \leq -\epsilon f_i^- + M f_i^+ \qquad (7)$$

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Next, we pick settings $\mathbf{E}$ to maximize blocked reactions

$$min\ z$$

subject to

$$\mathbf{lb_L} \leq \mathbf{E} \leq \mathbf{ub_L}$$

$$z = max \sum f_i^+ + f_i^-$$

subject to

$$\mathbf{Sv}=0 \qquad (1)$$

$$\mathbf{lb}\leq\mathbf{v}\leq\mathbf{ub} \qquad (2)$$

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... ...

$$v_i\leq-\epsilon f_i^- + M f_i^+ \qquad (7)$$

What is next?

- In general, Mixed Integer Bi-Level problems are considered as an “still unsolved”
- Links environmental conditions to evolution processes
- Developing algorithms to solve these type of problems are of interest in System Biology

“Nothing in Biology Makes Sense Except in the Light of Evolution”

– Theodosius Dobzhansky (1900-1975)

Thanks for your attention!