Of Walks and Graphs

An Introduction to Walk Theory I

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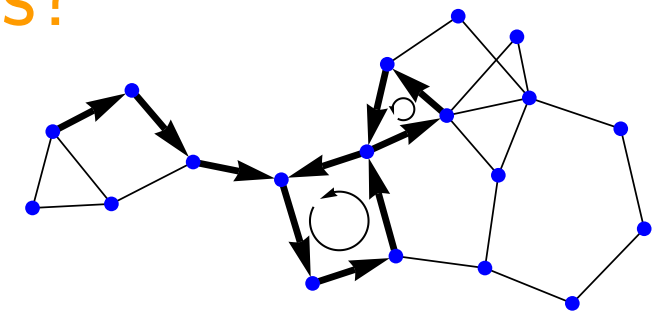
Seminar

September 2014

Outline

Why Walks?

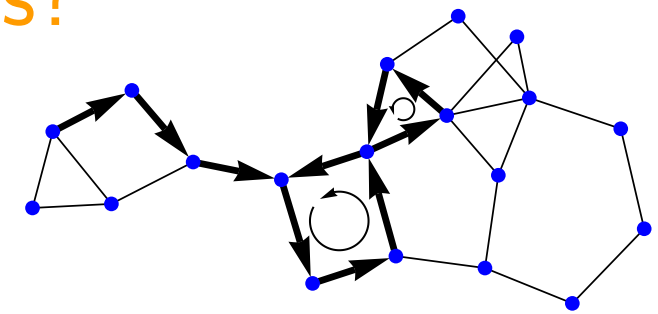
Walk: a *trajectory* on a graph



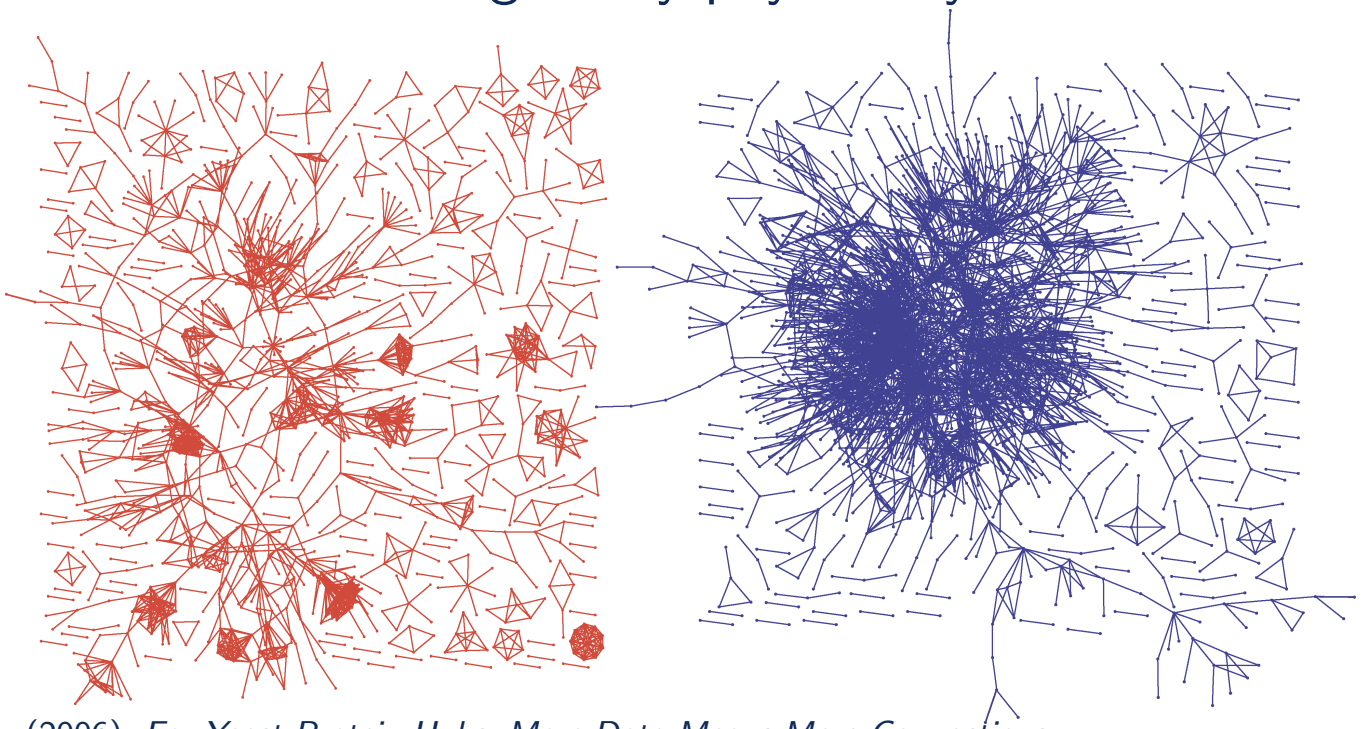
- Why walks?

Why Walks?

Walk: a *trajectory* on a graph



- Why walks?
  - $\hookrightarrow$ Random walks, quantum random walks
  - $\hookrightarrow$ Network analysis is often walk-based
  - $\hookrightarrow$ Processes undergone by physical systems



R. Robinson (2006), *For Yeast Protein Hubs, More Data Means More Connections.* PLoS Biol 4(10): e331. doi:10.1371/journal.pbio.0040331

Why Walks?

Walks are pervasive objects!

- Adjacency matrix $\mathcal{A}^n$ = number of walks on graph

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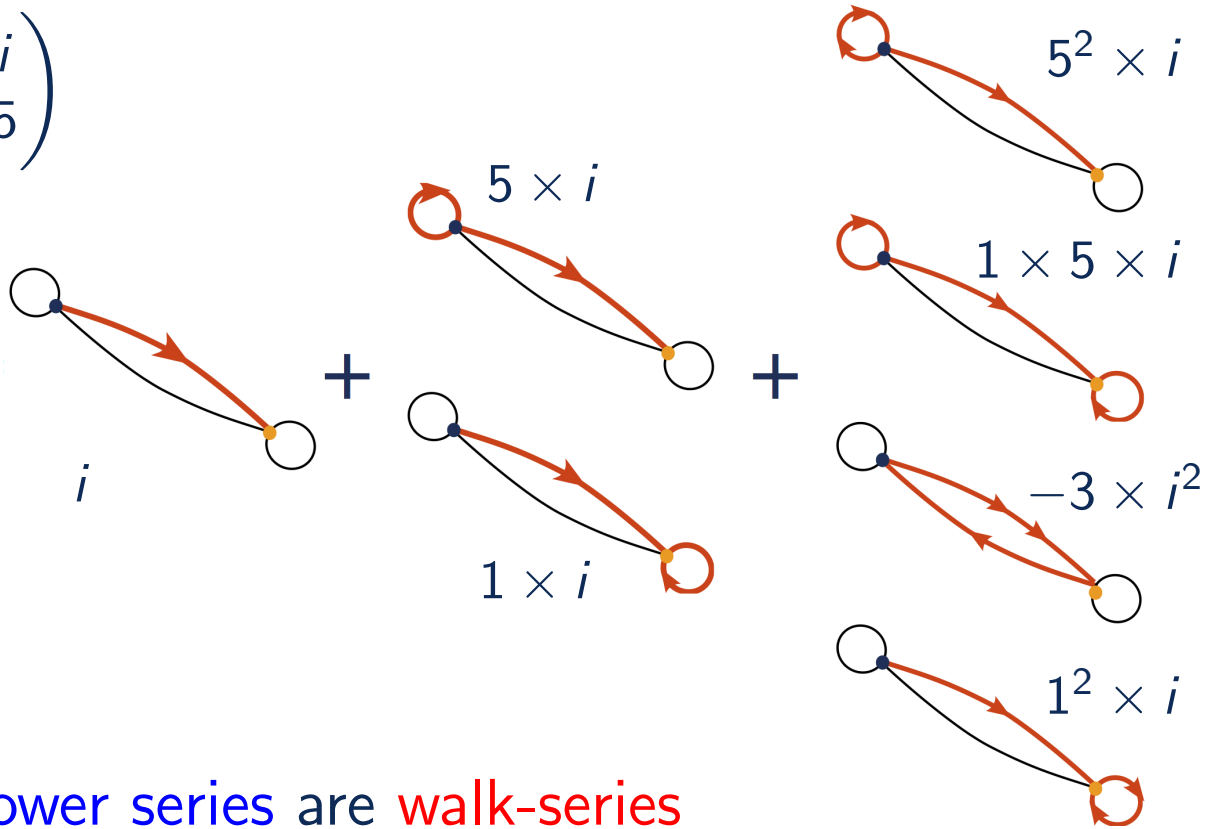
Walks are pervasive objects!

- Adjacency matrix $\mathcal{A}^n$ = number of walks on graph
- Arbitrary matrix $\mathcal{M}^n$ = sum of walk weights

$$\mathcal{M} = \begin{pmatrix} 1 & i \\ -3 & 5 \end{pmatrix}$$

$$\Big(\sum_{n} \mathcal{M}^n\Big)_{\blacksquare \to \blacksquare} =$$

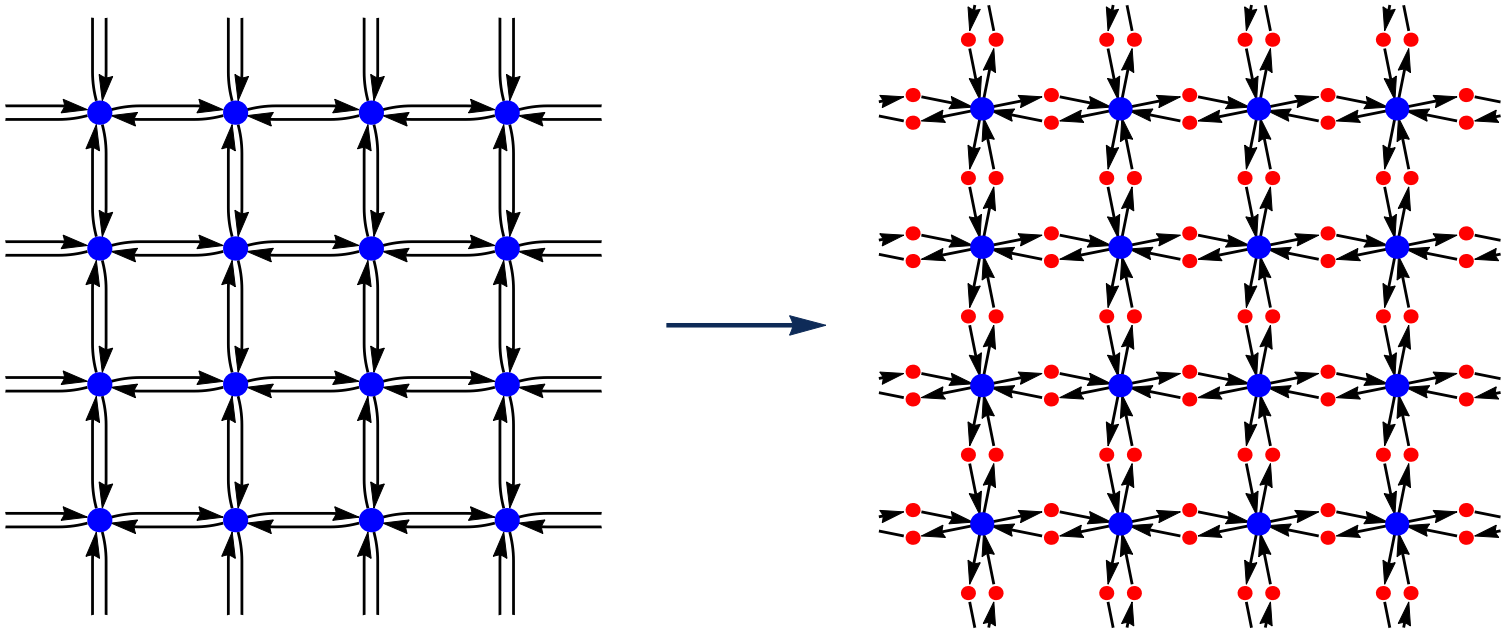


$\longrightarrow$ Matrix power series are walk-series

Analytic matrix function $f(\mathcal{M})$ = series of walk weights

Strange Observation 1

- Changing a square lattice



$$\#W_{\bullet\to\bullet'}(\ell) \longrightarrow \#W_{\bullet\to\bullet'}(2\ell)$$

Strange Observation 1

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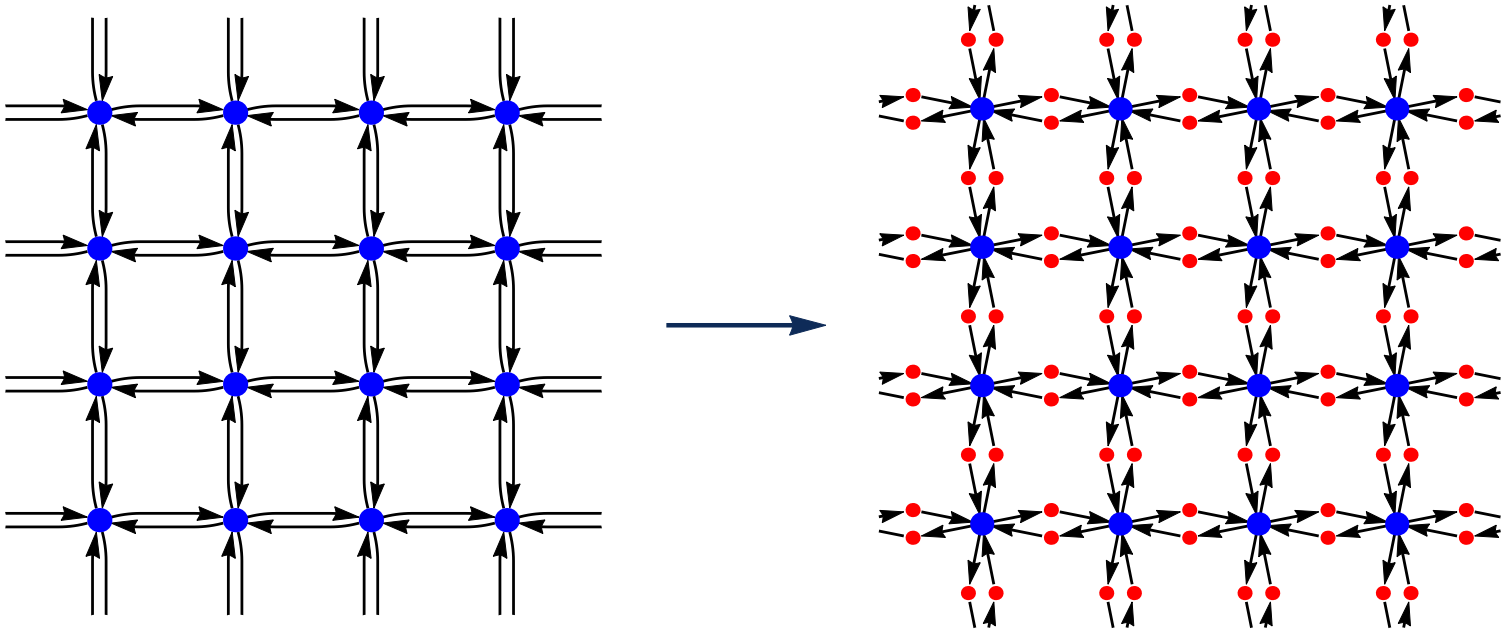


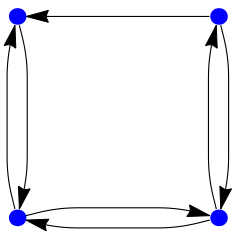
$$\#W_{\bullet\to\bullet'}(\ell) \longrightarrow \#W_{\bullet\to\bullet'}(2\ell)$$

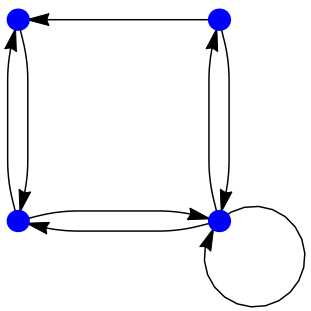
$\hookrightarrow$ Non-trivial for graphs: regularity is lost

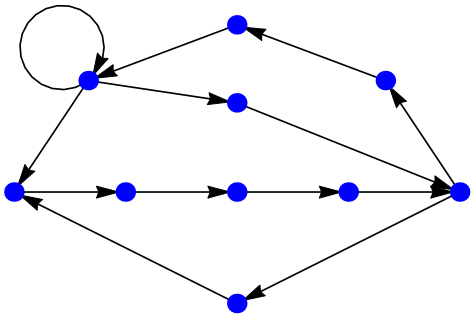
$\hookrightarrow$ Trivial transformation for walks

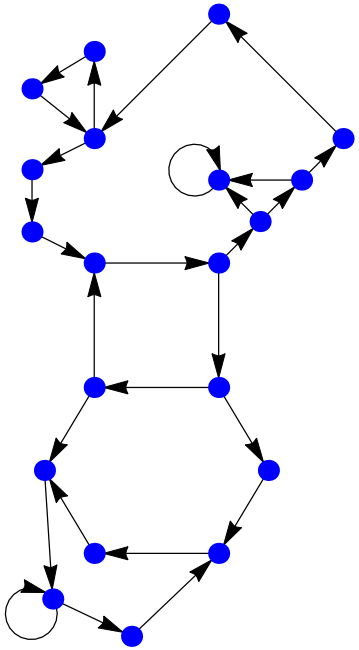
Strange Observation 2

Which graphs are "similar"?









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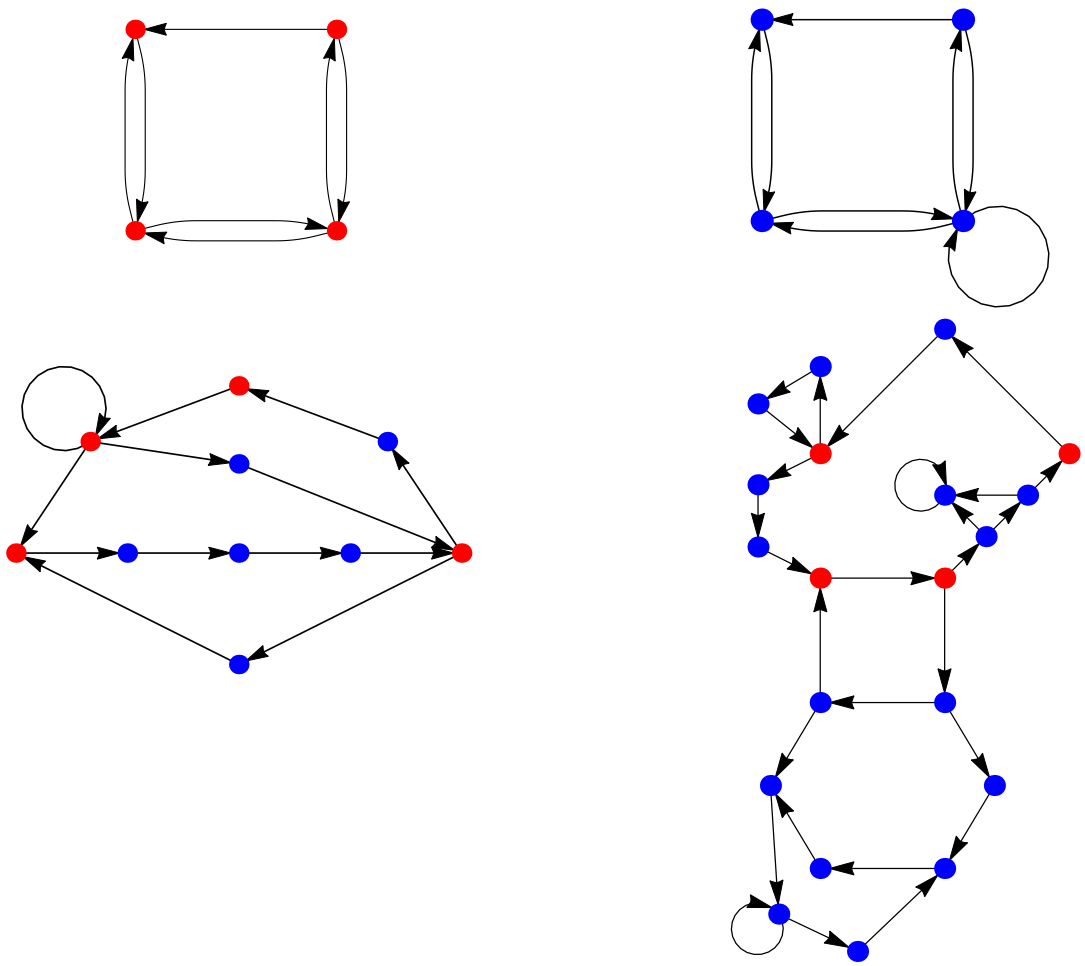


Yet the walk sets $W_{\bullet \to \bullet'}$ are *isomorphic* (I will come back on this)

Strange Observation 3

- Why is network analysis not perfect?

  Example: characterizing molecules

Method	Dataset	Accuracy
Random walk kernel	Mutag(labelled)	90. 0%
Backtrackless walk kernel	Mutag(labelled)	**91.1**%
Feature vector from Random walk	COIL(unlabeled)	94.4%
Feature vector from backtrackless random walk	COIL(unlabeled)	**95.5**%
Feature vector from Ihara coefficients	COIL(unlabeled)	94.4%
Shortest Path Kernel	COIL(unlabeled)	86.7%
Feature vector from Random walk	Mutag(unlabeled)	89.4%
Feature vector from backtrackless random walk	Mutag(unlabeled)	**90.5**%
Feature vector from Ihara coefficients	Mutag(unlabeled)	80.5%

R. Wilson (2013), *Characterisation of Networks and their Applications*.
http://www.cs.york.ac.uk/cvpr/talks/Char.pdf

F. Aziz, R. Wilson, E. Hancock, *Backtrackless Walks on a Graph*,
IEEE Trans. Neural Netw. Learning Syst. 24(6): 977-989 (2013)

Walk-based methods

Strange Observations

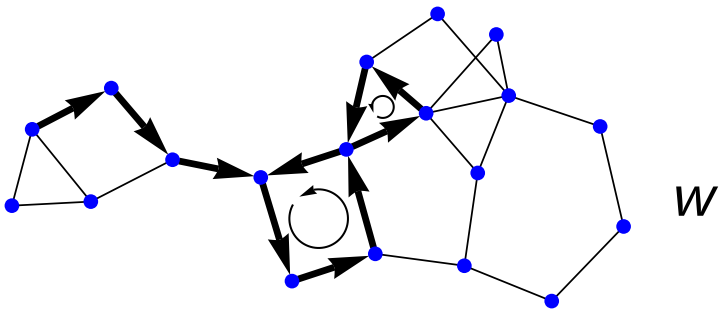
- Completely *dissimilar* graphs can have the *same* walk sets
- Even *fundamental* graph properties, *regularity*, may have little effect on walks
- Existence of *non-trivial* properties of walks *valid on all* multi-digraphs
- More strange objects to come (*walks without graphs!*)

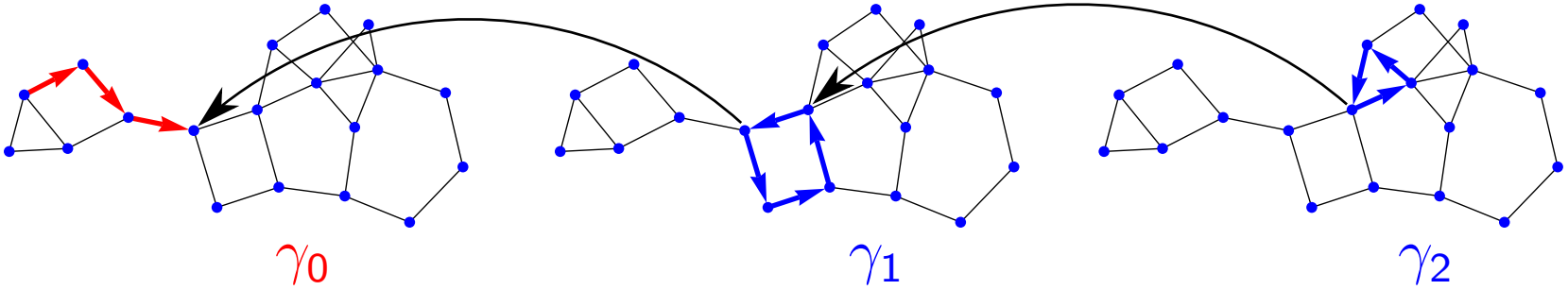
$\hookrightarrow$ Can we represent and manipulate walks without their graphs?

Elements of Walk Theory

Prime factorisation of walks

Observation : walk = simple path & simple cycle





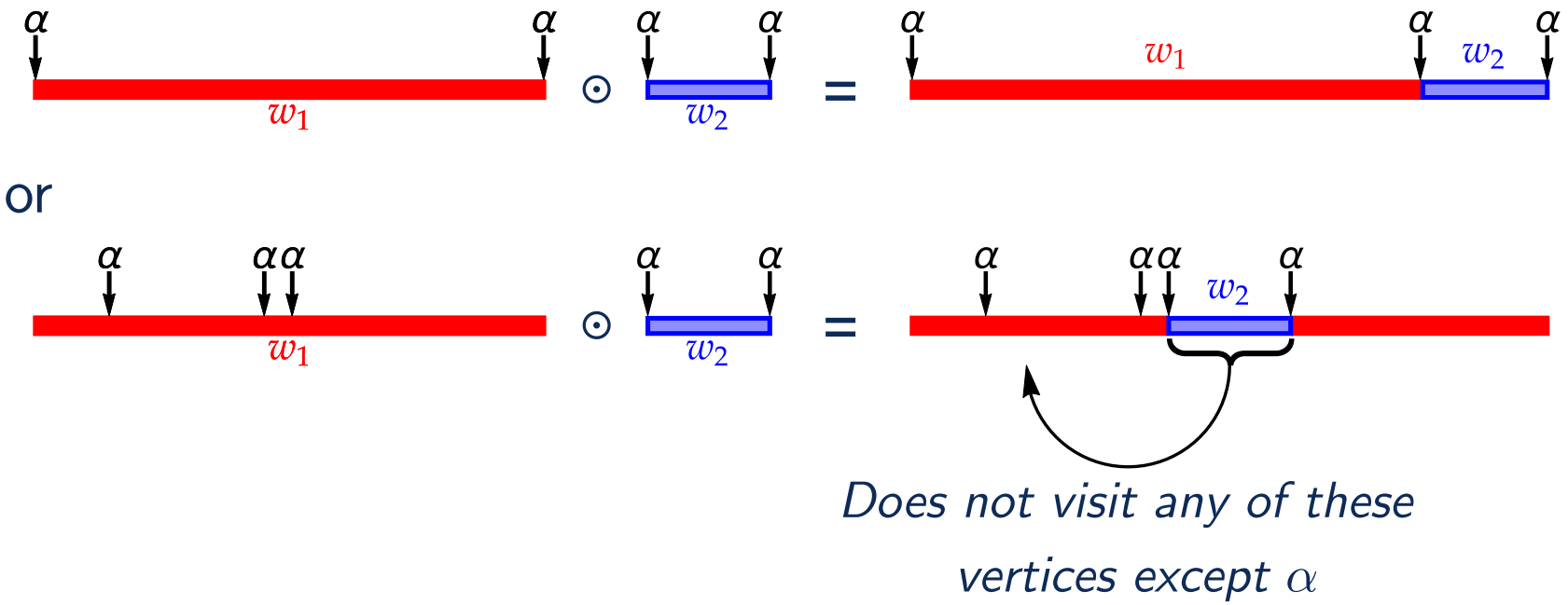
- Walk w 'factors' into 1 simple path and 2 simple cycles

$$\hookrightarrow w = \gamma_0 \leftarrow (\gamma_1 \leftarrow \gamma_2)$$

What can we say in general?

Nesting product

- Nesting product $\odot$ nests a walk into another iff



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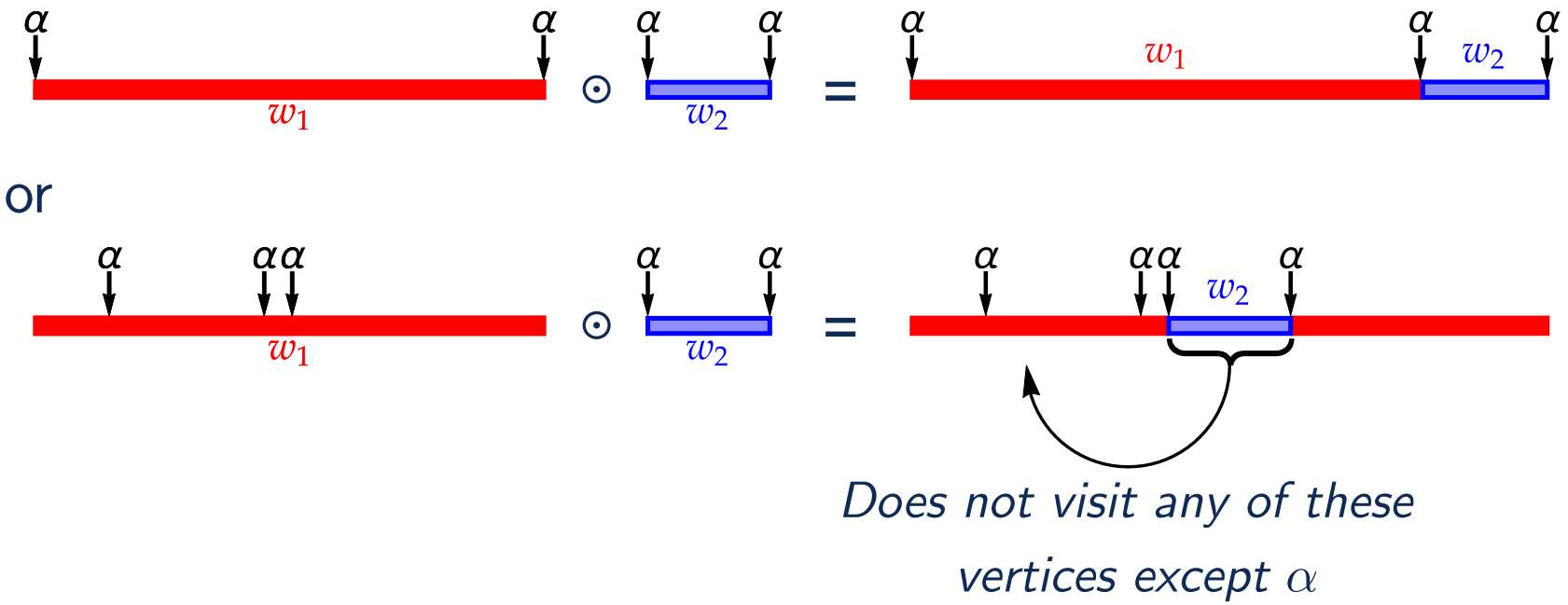


$$\longrightarrow \; w = \gamma_0 \odot \left(\gamma_1 \odot \gamma_2\right)$$

- Ad-hoc? consider loop-erasing

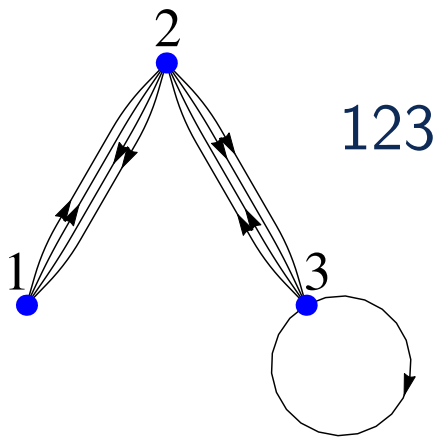
The Fundamental Theorem

Theorem

Let $\mathcal{G}$ be a graph and w a walk on $\mathcal{G}$.
Then there exists a unique factorisation of w into $\odot$-products of prime walks, the simple paths and simple cycles on $\mathcal{G}$.

Prime walks: $\gamma \,|\, w \odot w' \Rightarrow \gamma \,|\, w$ or $\gamma \,|\, w'$

$\hookrightarrow$ This holds on *all* multi-digraphs!
$\hookrightarrow$ Walk factorization is efficient $t \propto O(\ell_w)$



$$1232332121 = \Big(121 \odot \big(232 \odot (232 \odot 33)\big)\Big) \odot 121$$

Posets of Walks

Construct a prime-based representation of walks

- Sets of walks ordered by divisibility

$$w \leq_{\odot} w' \iff w \mid w'$$

Example: $121 \mid 1221 = 121 \odot 22 \Longrightarrow 121 \leq_{\odot} 1221$

- Poset of walks $P_\alpha = (W_{\mathcal{G};\alpha\alpha}, \leq_{\odot})$

Set of walks from α to α on $\mathcal{G}$

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Set of walks from α to α on $\mathcal{G}$

$\hookrightarrow$ P_α is a complicated object: ∞-many walks
$\hookrightarrow$ Nesting $\odot$ is non-commutative, non-associative
$\hookrightarrow$ Difficult to find all divisors

Can we make things simpler?

Posets of Ω-walks and ω-walks

Poset of Ω-walks

Sets of prime factors...

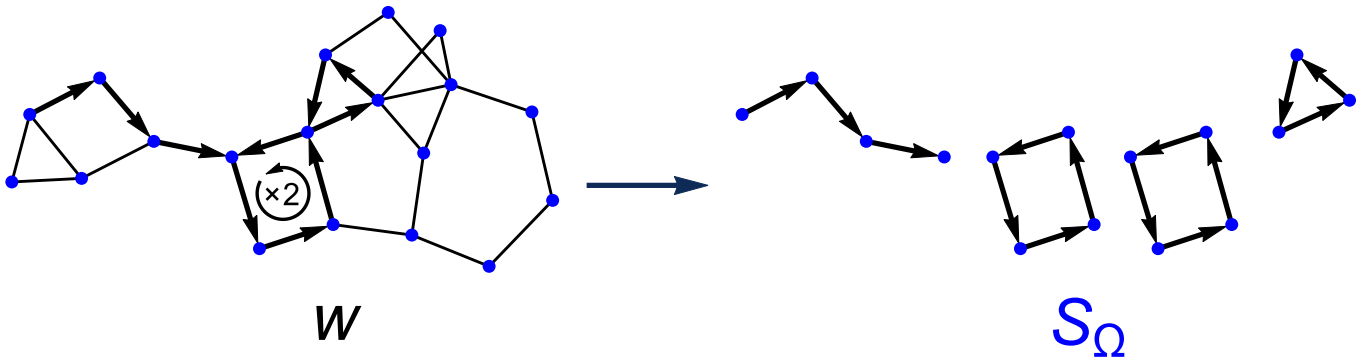
$$w = \gamma_0 \odot \gamma_1^3 \Rightarrow S_\Omega(w) = \{\gamma_0, \gamma_1, \gamma_1, \gamma_1\}$$

...ordered by inclusion

$$S_\Omega(w) \leq_\Omega S_\Omega(w') \iff S_\Omega(w) \subseteq S_\Omega(w')$$

$\hookrightarrow$ Poset of Ω-walks: $P_\alpha^\Omega = (S_\Omega, \leq_\Omega)$

- Ω-walk = loop-erased walk + set of loops



- $\odot$ (almost) commutative!

Posets of Ω-walks and ω-walks

Poset of ω-walks

Sets of *distinct* prime factors...

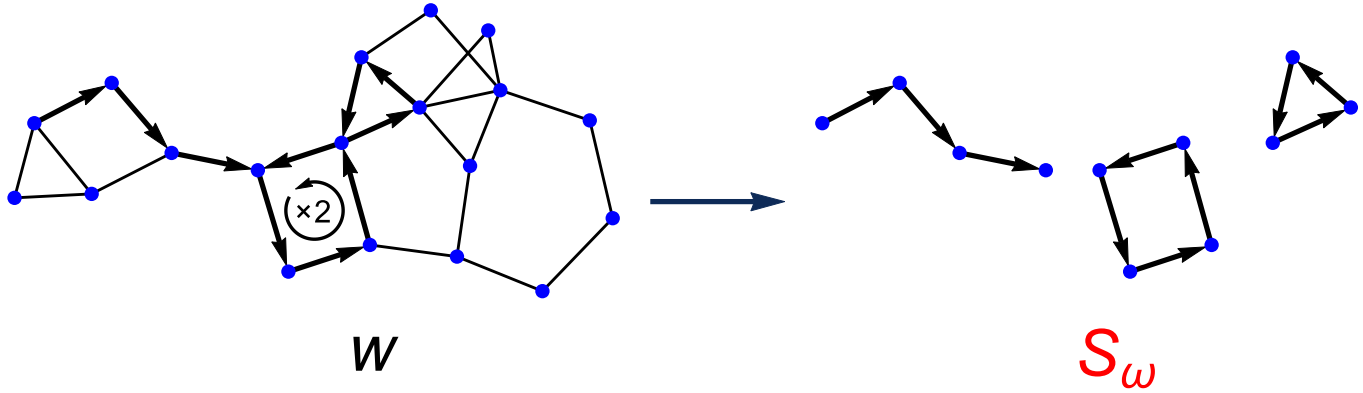
$$w = \gamma_0 \odot \gamma_1^3 \Rightarrow S_\omega(w) = \{\gamma_0, \gamma_1\}$$

...ordered by inclusion

$$S_\omega(w) \leq_\omega S_\omega(w') \iff S_\omega(w) \subseteq S_\omega(w')$$

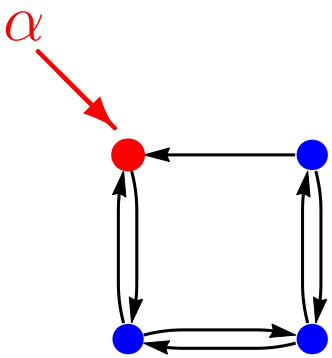
$\hookrightarrow$ Poset of ω-walks: $P_\alpha^\omega = (S_\omega, \leq_\omega)$

- P_α^ω *finite* graded lattice



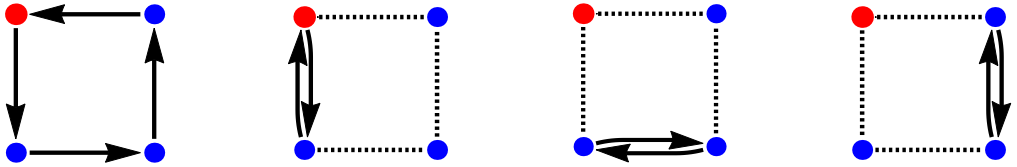
- Let's see what P_α^ω looks like

Example: P_α^ω on the Square



Walking from • to itself
Which primes can be reached?

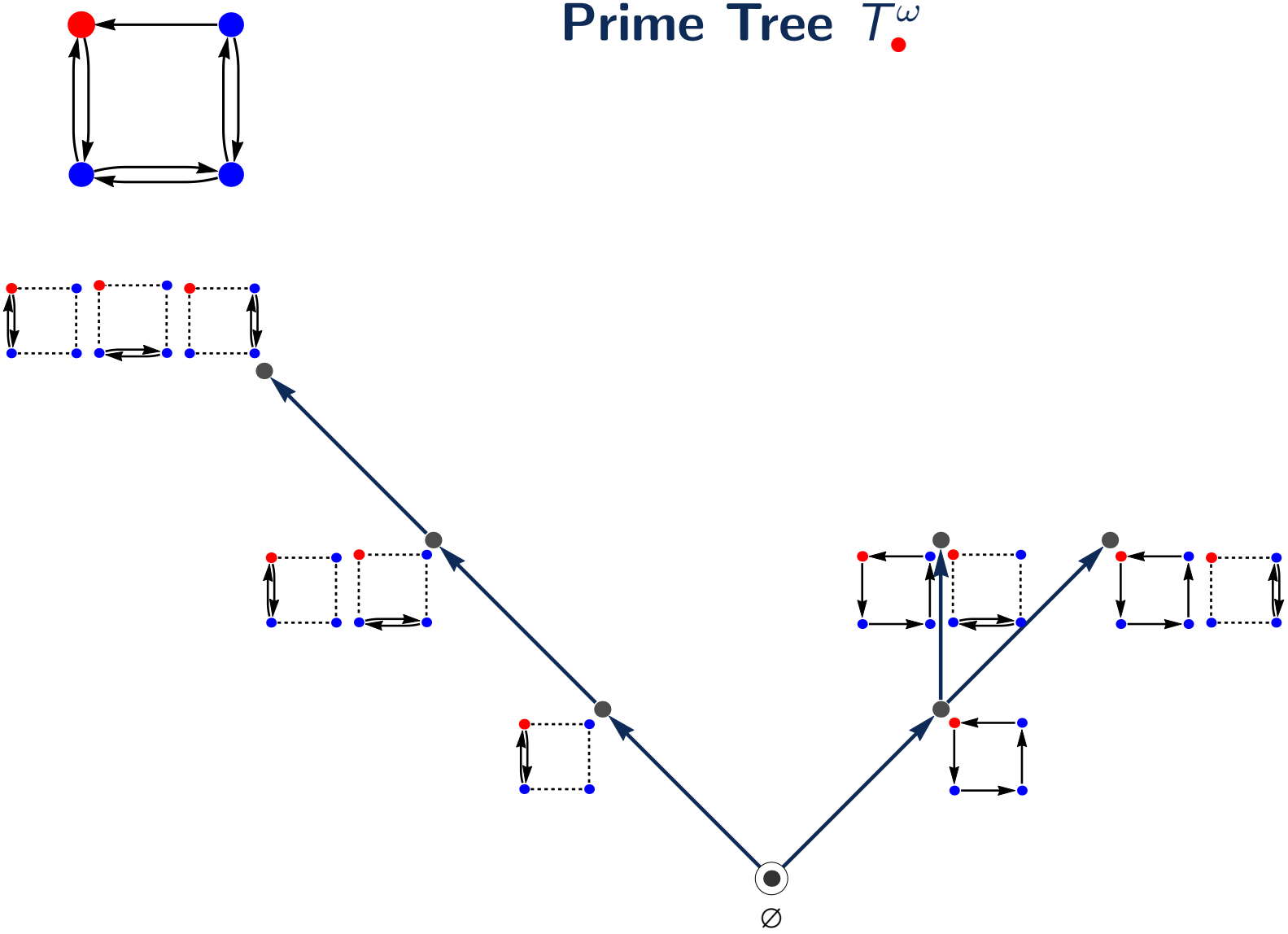
$\hookrightarrow$ *Set of accessible primes*, walking from • to itself



Example: P_α^ω on the Square

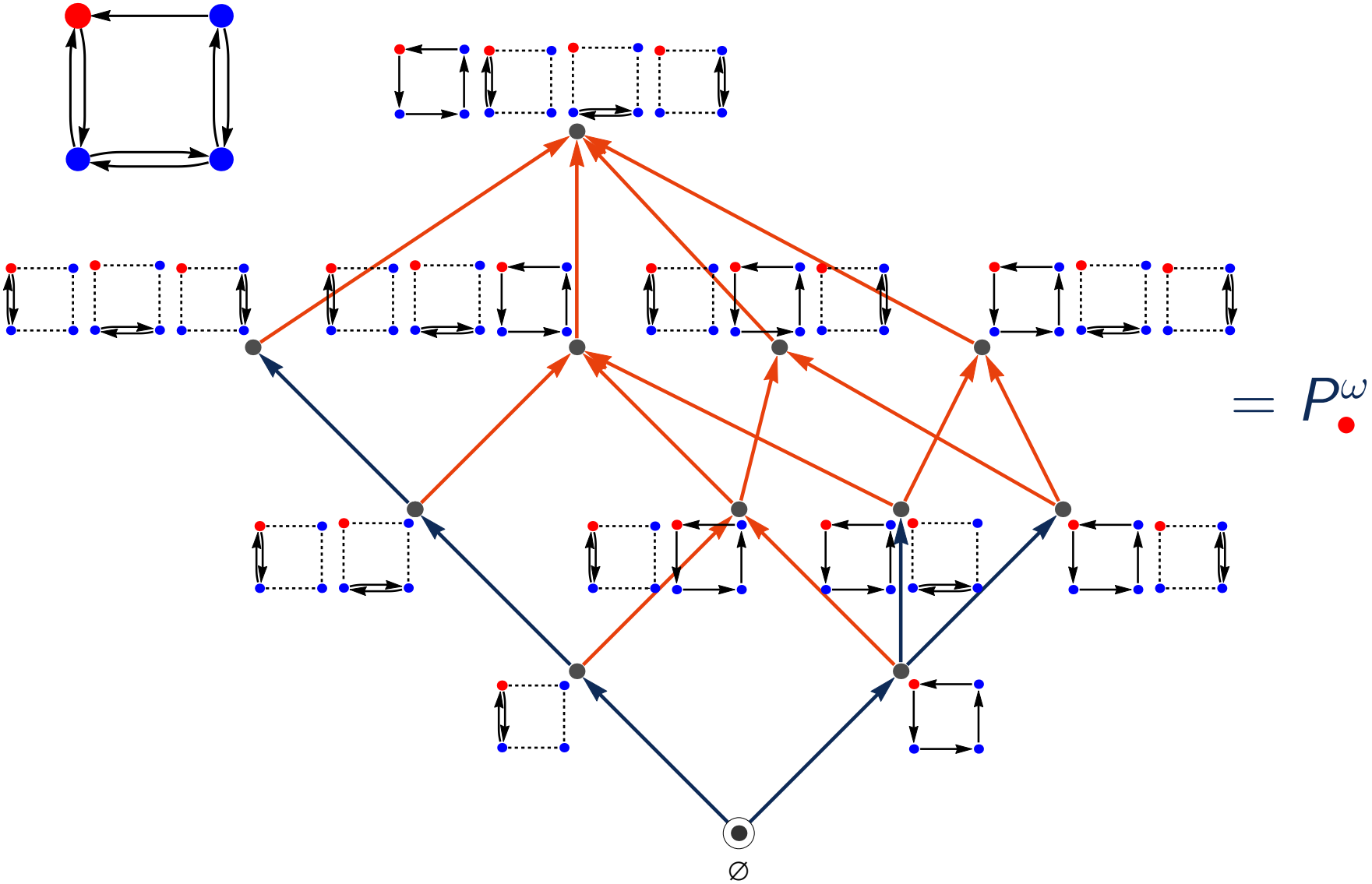
Relations between the primes

Prime Tree $T_{\bullet}^{\omega}$



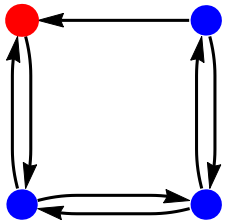
Example: P_α^ω on the Square

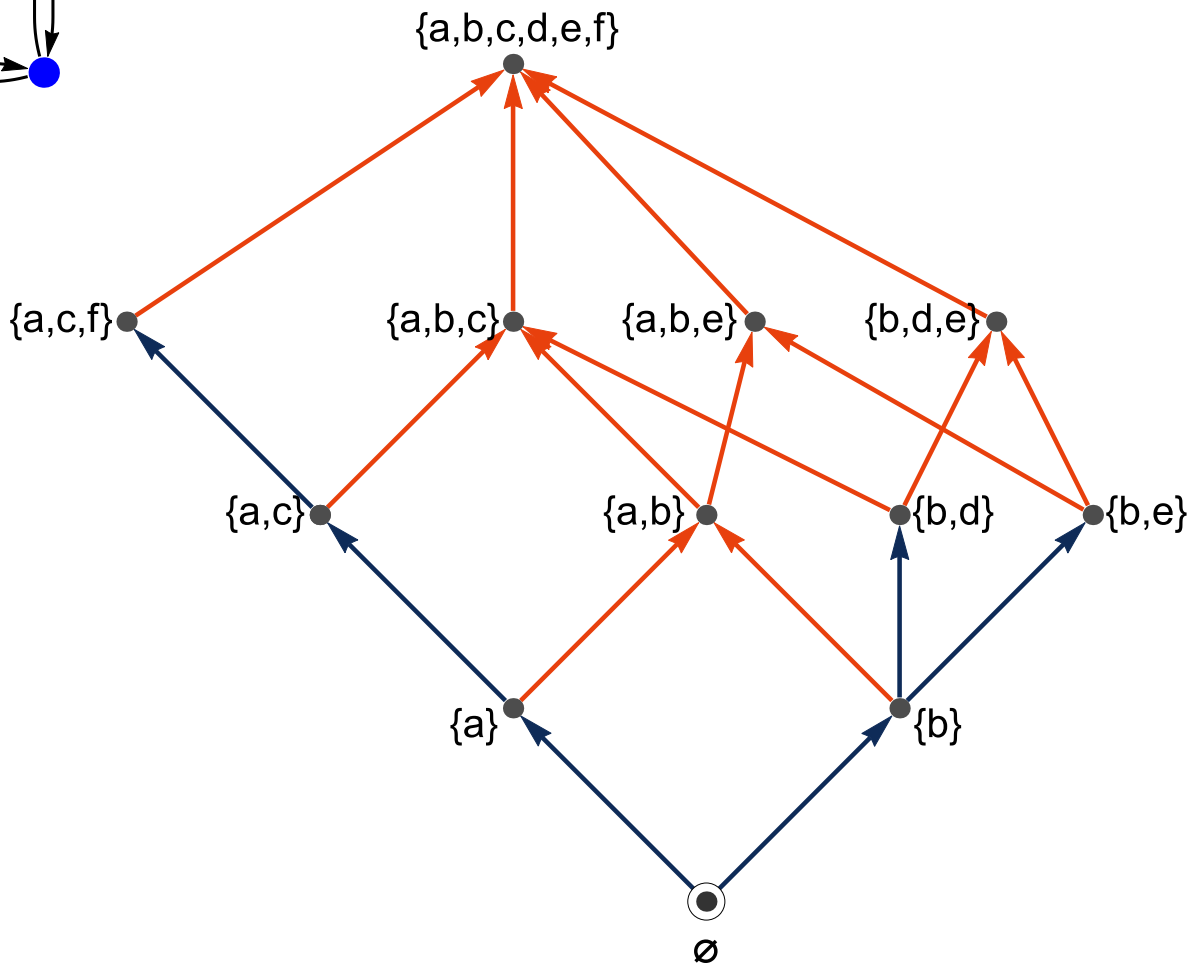
The complete poset



Example: P_α^ω on the Square

Primes provide walk sets with a *structure*





$= P_\bullet^\omega$

Posets of Ω-walks and ω-walks

P_α^Ω and P_α^ω are simpler than P_α ...

- P_α^Ω and P_α^ω are graded lattices
- P_α^ω finite

... and lossless

Theorem

Knowledge of P_α^Ω, P_α^ω or T_α^ω is equivalent to that of P_α

Proof

- T_α^ω = set of join-irreducibles in P_α^ω
- P_α^ω is the join-closure of T_α^ω
- For w a walk, construct $(S_\omega(w), \leq_\omega)$ and its prime tree $T^\omega(w)$

$$T^\omega(w) \subseteq T_\alpha^\omega \Rightarrow w \in P_\alpha \qquad \square$$

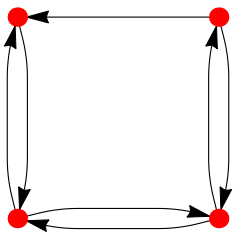
Isomorphic Walk Sets

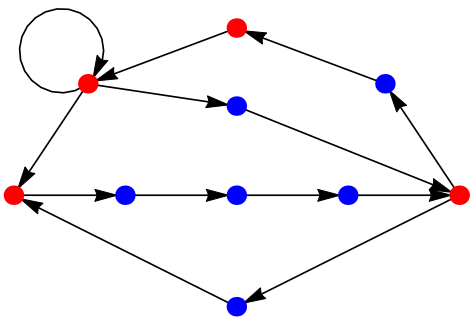
Isomorphic walk sets on dissimilar graphs

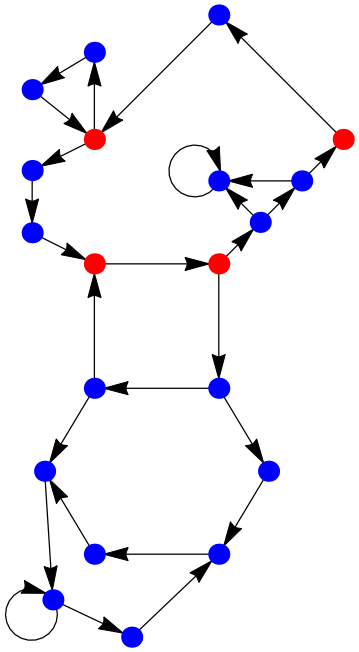
Corollary

Let $\mathcal{G}_1$ and $\mathcal{G}_2$ be two graphs and $\alpha \in \mathcal{V}(\mathcal{G}_1)$, $a \in \mathcal{V}(\mathcal{G}_2)$

$$T^{\omega}_{\mathcal{G}_1;\alpha} \simeq T^{\omega}_{\mathcal{G}_2;a} \iff (W_{\mathcal{G}_1;\,\alpha\alpha}, \odot) \simeq (W_{\mathcal{G}_2;\,aa}, \odot)$$







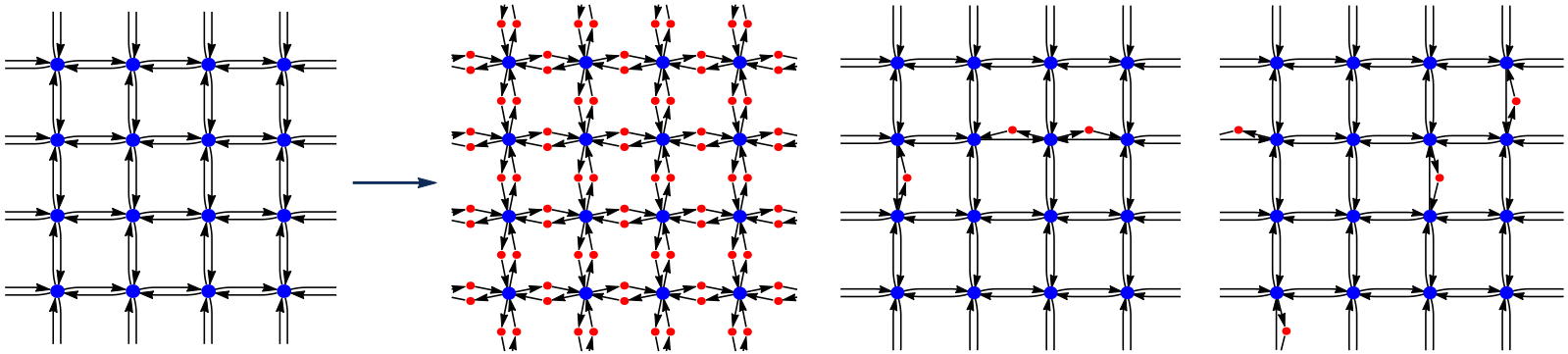
Isomorphic Walk Sets

Invariance of P_α under graph transformations

Corollary

Let $\mathcal{G}$ be a graph $\alpha, \beta \in \mathcal{V}(\mathcal{G})$ and $\mathcal{G}$' the graph $\mathcal{G}$ with some added vertices on edges. Then

$$(W_{\mathcal{G};\,\alpha\beta}, \odot) \simeq (W_{\mathcal{G}';\,\alpha\beta}, \odot)$$



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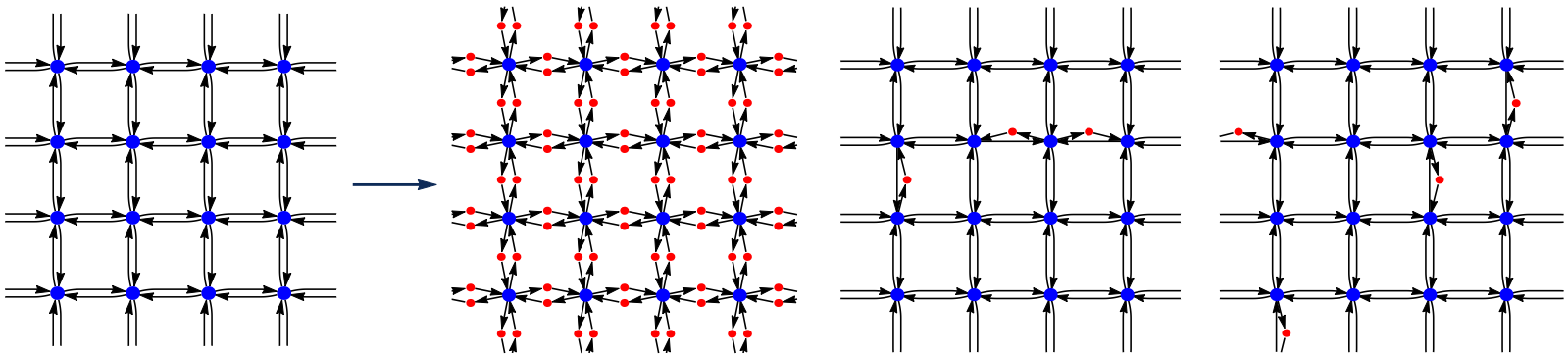
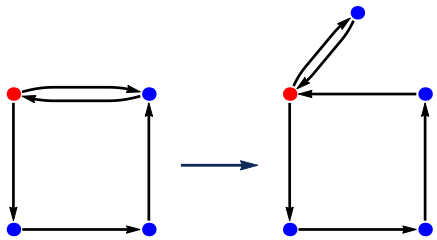


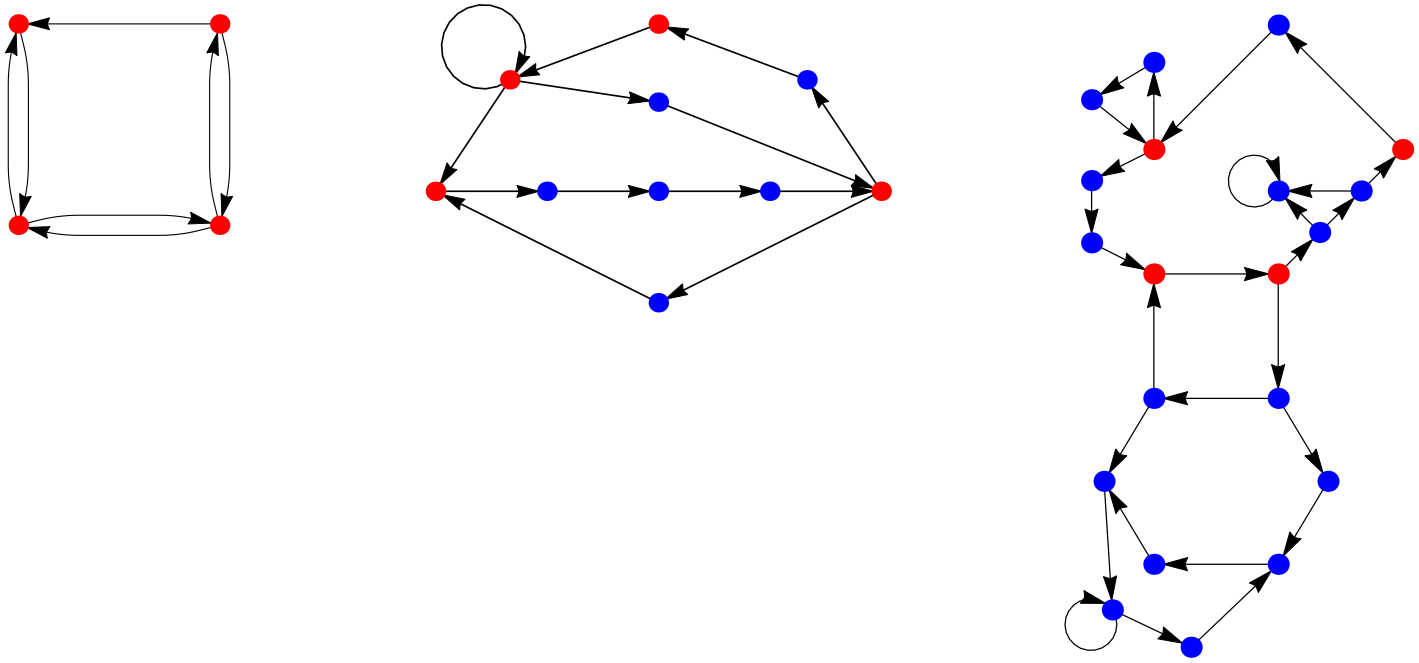
More P_α-invariant graph transformations

$\hookrightarrow$ 'Broad' classification possible



Isomorphic Walk Sets

P_α-invariant graph transformations as *generators*



T_α^ω a *graph-free* representation of walk sets?

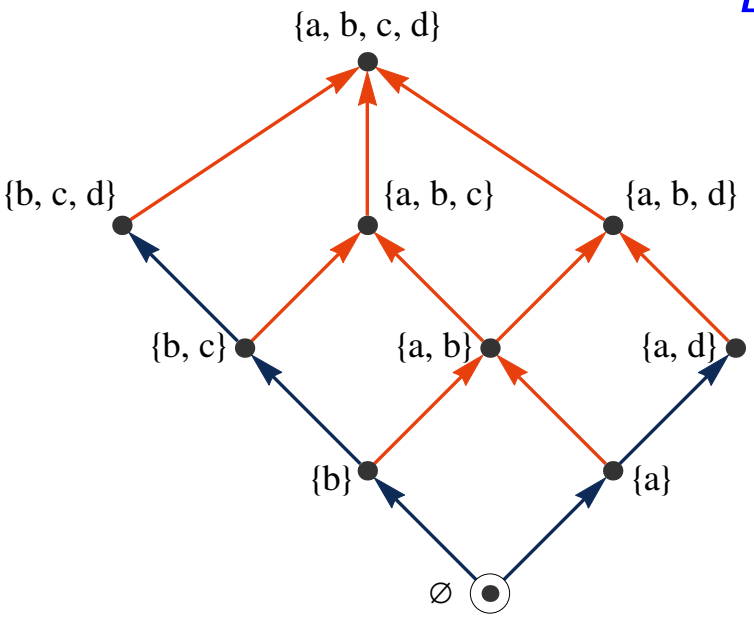
$\hookrightarrow$ Depends weakly on any specific $\mathcal{G}$

$\hookrightarrow$ Walks without graphs?

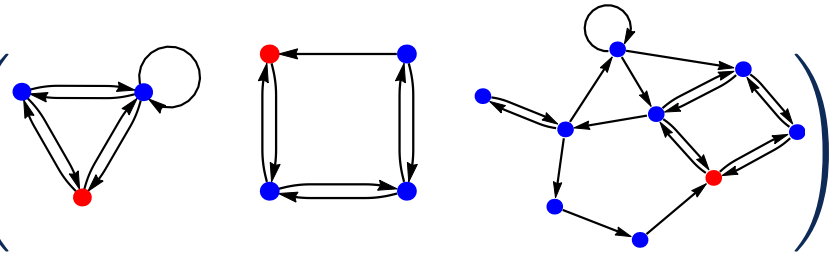
Strange Observation 4

- Number of walk posets on n primes:

$$B_n \sim \left(.792\, n/\log n\right)^n$$



$a,\ b,\ c,\ d$ primes

$\subseteq P_{\bullet}^{\omega}\Bigg($  $\Bigg)$

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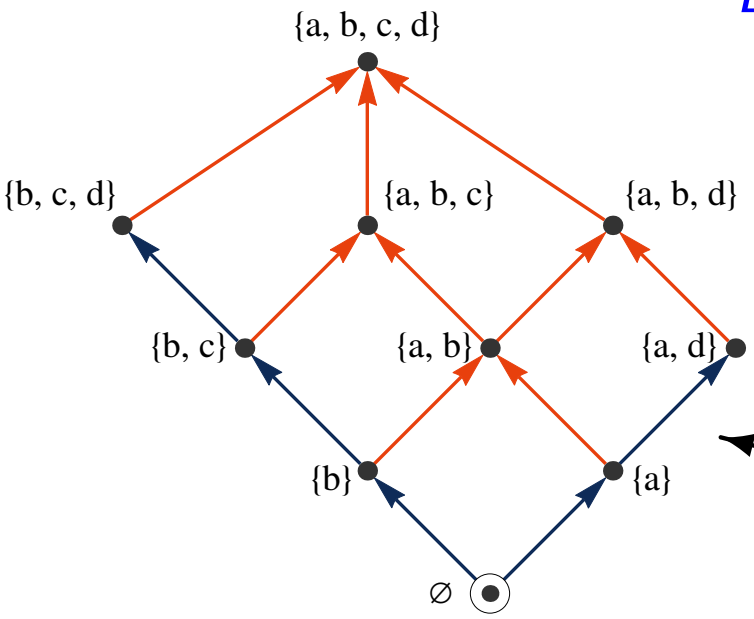
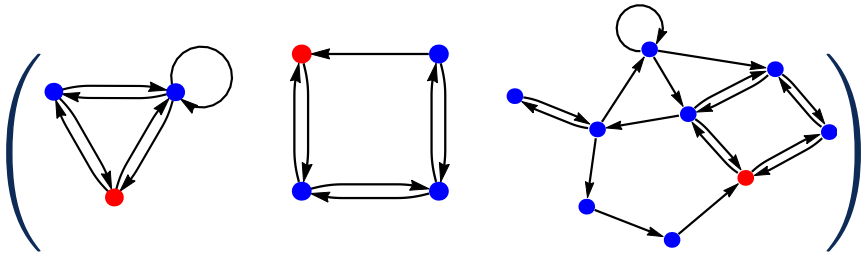


a, b, c, d primes

$\subseteq P_{\bullet}^{\omega}$ 

No graph exists with exactly this walk poset

Strange Observation 4

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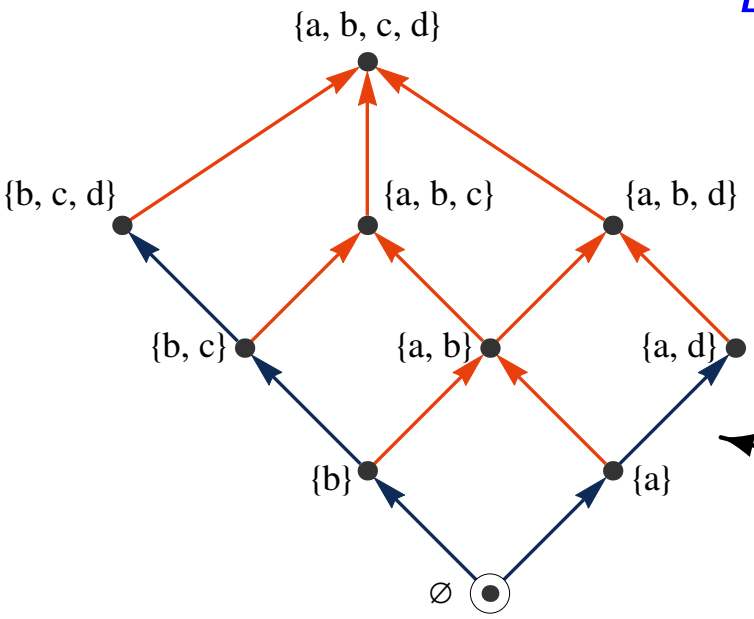

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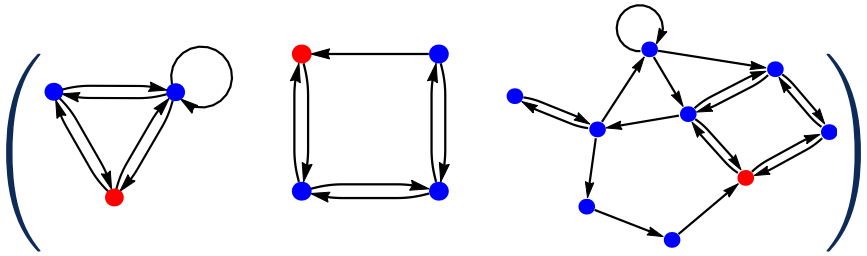
$\subseteq P_{\bullet}^{\omega}$ 

No graph exists with exactly this walk poset

- Conjectured # walk posets on n primes with exact graph realization

$$C_n \sim 4^n n^{-3/2}/\sqrt{\pi} \ll B_n$$

$\longrightarrow$ *Most walk sets have no exact graph realization!*

Prime Characterization of Graphs

Graphs determine walks... *do walks determine graphs?*

Prime Characterization of Graphs

Graphs determine walks... *do walks determine graphs?*

YES

Theorem

Let $\mathcal{G}$ be a connected multi-digraph.
Then $\mathcal{G}$ is uniquely determined, up to an isomorphism, by the primes it sustains. In particular:

$$\bigcup_{\alpha,\beta} \underbrace{T^{\omega}_{\alpha\beta}}_{\text{Walk set structure}} + \underbrace{\textit{length of primes} + \textit{roots}}_{\text{Specific realization of the structure}} = \mathcal{G}$$

Prime Characterization of Graphs

Let $\alpha, \beta \in \mathcal{V}(\mathcal{G})$

$\mathcal{G}^{\alpha,\beta}$ largest strongly connected component with α, β

Proof

Graphs determined by their primes

- Walks $W_{\mathcal{G};\alpha\beta}$ = words of language $L_{\alpha\beta}$
- Automaton with skeleton $\mathcal{G}^{\alpha,\beta}$ is minimal for $L_{\alpha\beta}$
- Minimal automaton unique

$$W_{\mathcal{G};\alpha\beta} \text{ determines } \mathcal{G}^{\alpha,\beta} \text{ uniquely}$$

- Unique factorization

$$W_{\mathcal{G};\alpha\beta} \iff \text{Prime set}$$

Unique graph realization

- $T^{\omega}_{\alpha\beta}$ determines inter-prime relations
- $T^{\omega}_{\alpha\beta}$ + length of primes + roots = Prime set $\square$

Algebraic Walk Theory

Path-Sums

Prime representations of walk-series

$$\Sigma_{\mathcal{G};\,\alpha\beta} := \sum_{w \in W_{\mathcal{G};\alpha\beta}} k(w)$$

Sum of all walks from α to β

A function of walks
$k(w) = \mathrm{Weight}(w)$
$k(w) = z^{\Omega(w)}$

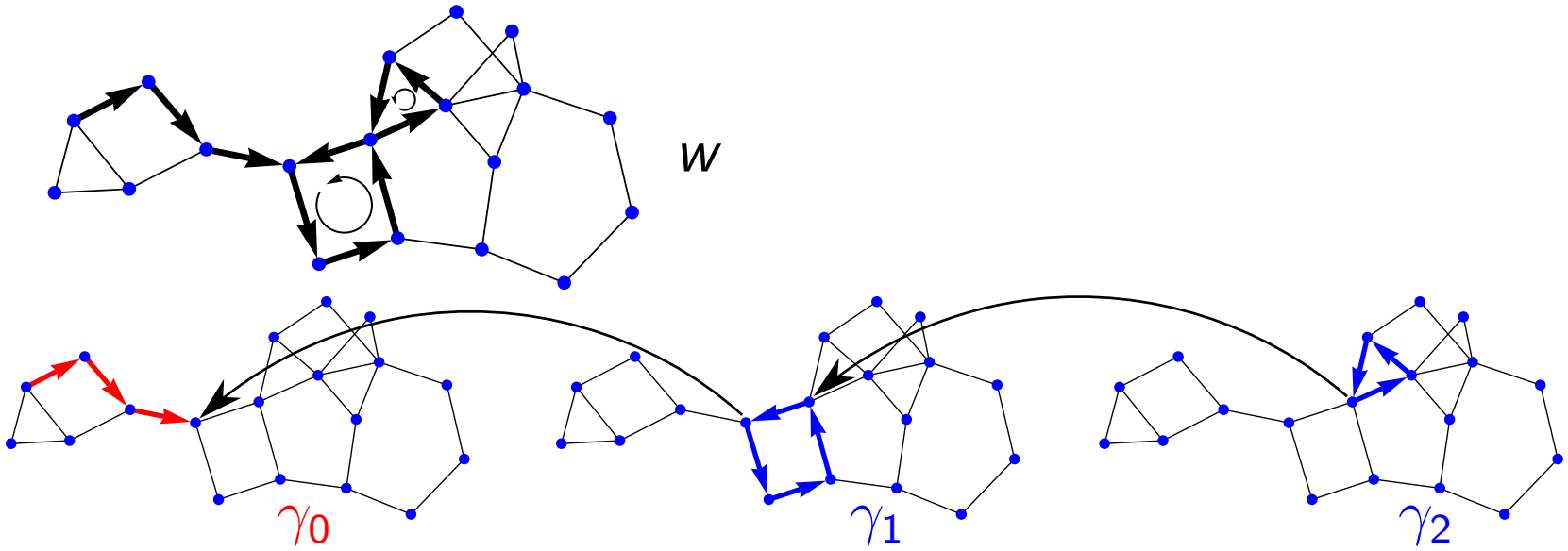
Theorem

Let w, w' be two walks with $w \odot w' = w_1 \circ w' \circ w_2$. If $k(w \odot w') = k(w_1)k(w')k(w_2)$ then $\Sigma_{\mathcal{G};\,\alpha\beta}$ admits a unique, explicit and universal form involving only prime walks.

$\hookrightarrow$ Extends to series of Ω- and ω-walks (next talk)

Path-Sums

How does it works?



- Factorized forms ...

$$\gamma_0 \odot \gamma_1 + \gamma_0 \odot \gamma_1 \odot (\gamma_2)^1 + \gamma_0 \odot \gamma_1 \odot (\gamma_2)^2 + \gamma_0 \odot \gamma_1 \odot (\gamma_2)^3 + \cdots$$

... are easy to sum !

$$\gamma_0 \odot \gamma_1 \odot (\mathcal{I} - \gamma_2)^{-1}$$

- We can sum all walks this way

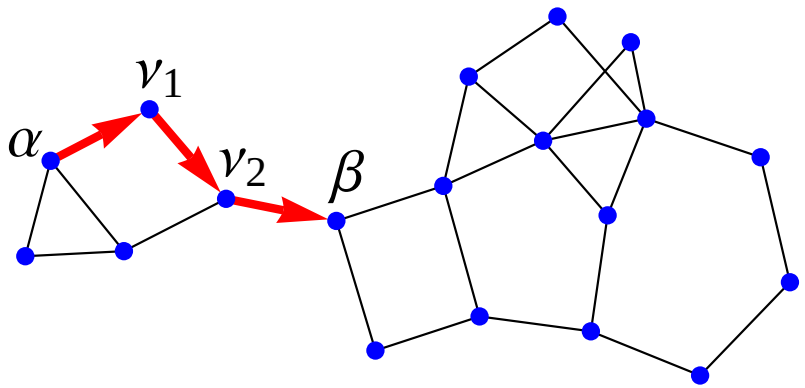
Factoring Walks on Graphs

How does it works?

- Factor formal series of walks

$$\sum_{w\colon \alpha\to\beta} w = \sum_{p\colon \alpha\to\beta} (\alpha)(\alpha\nu_1)(\nu_1)(\nu_1\nu_2)\cdots(\nu_p\beta)(\beta)$$

Ensemble of simple paths



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Insert simple cycles: $\mathcal{G}$ $\mathcal{G}\backslash\{\alpha\}$ $\mathcal{G}\backslash\{\alpha,\nu_1,\cdots\nu_p\}$

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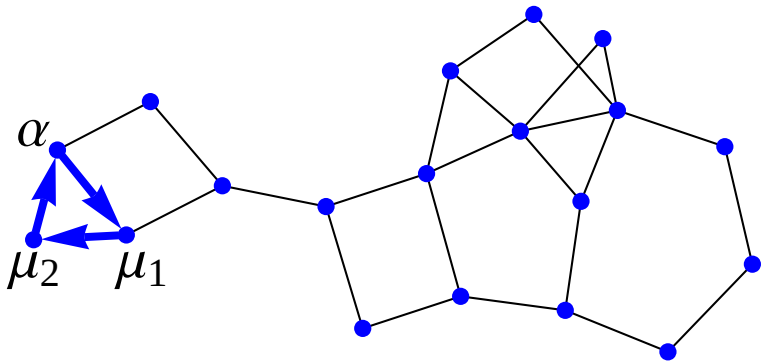
$$(\alpha) \to \Big[\mathcal{I} - \sum_{c\colon \alpha\to\alpha} (\alpha\mu_1)(\mu_1)\cdots(\mu_\ell)(\mu_\ell\alpha)\Big]^{-1}$$



Factoring Walks on Graphs

How does it works?

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$$\sum_{w\colon \alpha\to\beta} w = \sum_{p\colon \alpha\to\beta} (\alpha)(\alpha\nu_1)(\nu_1)(\nu_1\nu_2)\cdots(\nu_p\beta)(\beta)$$

Insert simple cycles: $\mathcal{G}\backslash\{\alpha\}$ $\mathcal{G}\backslash\{\alpha,\nu_1,\cdots\nu_p\}$

$$(\alpha) \to \Big[\mathcal{I} - \sum_{c\colon \alpha\to\alpha} (\alpha\mu_1)(\mu_1)\cdots(\mu_\ell)(\mu_\ell\alpha)\Big]^{-1}$$

Insert simple cycles again...

$\mathcal{G}\backslash\{\alpha\}$ $\mathcal{G}\backslash\{\alpha,\mu_1,\cdots\mu_{\ell-1}\}$

Factoring Walks on Graphs

What does it bring ?

- Series of walks

  $\hookrightarrow$ Sum of simple paths

$$\sum_{p\colon \alpha\to\beta} [\alpha]_{\mathcal{G}}(\alpha\nu_1)[\nu_1]_{\mathcal{G}\setminus\{\alpha\}}(\nu_1\nu_2)\cdots(\nu_p\beta)[\beta]_{\mathcal{G}\setminus\{\alpha,\nu_1,\cdots,\nu_p\}}$$

  $\hookrightarrow$ Continued fraction of simple cycles

$$[\alpha]_{\mathcal{G}} = \left[\mathcal{I} - \sum_{c\colon \alpha\to\alpha} (\alpha\mu_1)[\mu_1]_{\mathcal{G}\setminus\{\alpha\}}\cdots[\mu_\ell]_{\mathcal{G}\setminus\{\alpha,\mu_1,\cdots,\mu_{\ell-1}\}}(\mu_\ell\alpha)\right]^{-1}$$

- Evaluate $k\left(\sum_{w\colon \alpha\to\beta} w\right)$ by distributing $k(.)$

Factoring Walks on Graphs

The path-sum

$$\Sigma_{\mathcal{G};\,\alpha\beta} = \sum_{p\in\Pi_{\mathcal{G};\,\alpha\beta}} \prod_{j=1}^{\ell_p} \left\{ \Sigma_{\mathcal{G}\setminus\{\alpha,\nu_1,\cdots,\nu_{j-1}\};\,\nu_j\nu_j} k(e_{\nu_{j+1}\nu_j}) \right\} \Sigma_{\mathcal{G};\,\alpha\alpha}$$

$$\Sigma_{\mathcal{G};\,\alpha\alpha} = \left[1 - \sum_{\gamma\in\Gamma_{\mathcal{G};\,\alpha\alpha}} \prod_{j=1}^{\ell_\gamma} \left\{ \Sigma_{\mathcal{G}\setminus\{\alpha,\mu_1,\mu_{j-1}\};\,\mu_j\mu_j} k(e_{\mu_j\mu_{j-1}}) \right\} \right]^{-1}$$

- Explicit universal formula for series of walks
- Terminates on any finite graph
- Gives rise to branched continued fractions

Path-Sums

Mathematics:

$$k(w) = \mathrm{Weight}(w)$$

"Analytic matrix function $f(\mathcal{M})$ = series of walk weights"

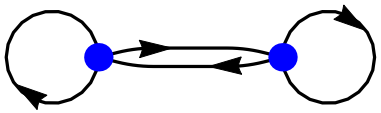
$\hookrightarrow$ Path-sum: *universal* formula for functions of matrices

Structure? the prime tree!

Physics:

$\hookrightarrow$ Non-perturbative closed form for

$$\mathrm{U} = e^{-i\mathrm{H}t}, \;\; \mathrm{Z} = e^{-\beta\mathrm{H}}, \;\; \mathrm{R} = (z\mathrm{I} - \mathrm{H})^{-1}$$

$\hookrightarrow$ Dyson equation? $\Rightarrow$ path-sum on 

$\hookrightarrow$ Exact finite formula for the *self-energy*

$\hookrightarrow$ Anderson localisation in many-body interacting systems

Wow? *not quite!*

$\hookrightarrow$ Too complicated for naive use in many quantum systems

Path-Sums

Prime representations of *dynamical* walk-series

Extends to $\begin{cases} \text{dynamical graphs} \\ \text{time-dependent Hamiltonians} \end{cases}$

Mathematics:

$\hookrightarrow$ Solves systems of diff. equations with variable coefficients

Physics:

Path-Sums

Prime representations of *dynamical* walk-series

Extends to $\begin{cases} \text{dynamical graphs} \\ \text{time-dependent Hamiltonians} \end{cases}$

Mathematics:

$\hookrightarrow$ Solves systems of diff. equations with variable coefficients

Physics:

$\hookrightarrow$ Treat time on equal footing with all degrees of freedom

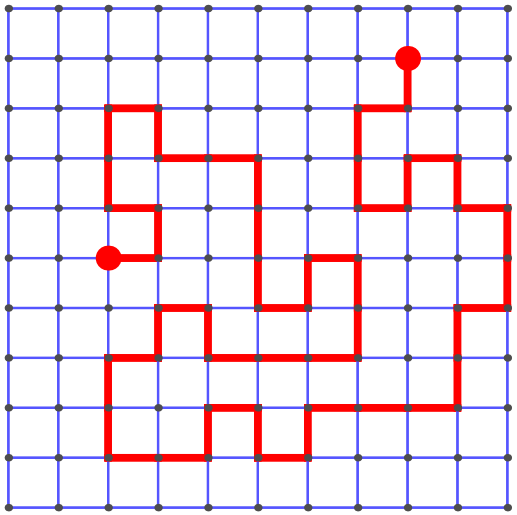
$\hookrightarrow$ 'Timeless' quantum mechanics *(weird)*

The Prime Walk Theorem

Prime Walk Theorem:

- How many primes of length ℓ are there?
- Square-lattice: a new take on an old problem

How many self avoiding walks of length ℓ?



Next talk: walk zeta functions and number theory on graphs

Walk Theory

An Introduction to Walk Theory I

Main Message

Walks are not slaves to graphs and need to be treated by a separate approach from graph theory; a theory of walks.

Results

- Prime factorization of walks
- Graph-free approach to walks using prime orderings
- Path-sum representation of walk-series

Open problems

- Count walk sets with exact graph realizations
- Better understanding of the relation between T_α^ω and $\mathcal{G}$

Come back for next talk!

Thank You!

Work supported by: EPSRC Grant EP/K038311/1

- G.-C. Rota, *On the Foundations of Combinatorial Theory, I. Theory of Möbius Functions*, Z. Wahrscheinlichkeitstheorie, 2:340–368, (1964).
- P. Doubilet, G.-C. Rota, and R. Stanley, *On the Foundations of Combinatorial Theory (VI): the Idea of Generating Function*, Proc. Sixth Berkeley Symp. on Math. Statist. and Prob., 2:267–318, (1972).
- P.-L. Giscard, S. J. Thwaite, and D. Jaksch, *Continued fractions and unique factorization on digraphs*, arXiv 1202.5523, under review.
- P.-L. Giscard, S. J. Thwaite, and D. Jaksch, *Evaluating matrix functions by resummations on graphs: the method of path-sums*, SIAM. J. Matrix Anal. & Appl., 34:445–469, (2013).
- P.-L. Giscard, Z. Choo, M. Mitchison, J.-J. Mendoza-Arenas, and D. Jaksch, *An explicit bound for dynamical localisation in an interacting many-body System*, arXiv:1402.1421, under review.
- P.-L. Giscard, *A graph theoretic approach to matrix functions and quantum dynamics*, DPhil thesis (2014).
- P.-L. Giscard, *The Theory of Walks*, unpublished notes (2014).

I am looking for a postdoctoral position!