Of Walks and Graphs

An Introduction to Walk Theory

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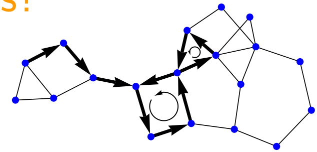
Outline

1. Introduction
   - Why walks?
   - Strange Observations
2. Walk Theory
   - Prime structure
   - Posets of walks, Ω-walks and ω-walks
   - Prime characterization of graphs
3. Algebraic Walk Theory
   - Path-sum representations
   - Algebraic structure and number theory
   - Prime walk theorem
4. Final Message

Why Walks?

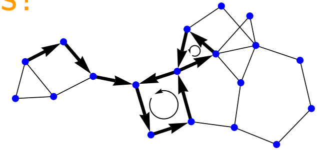
Walk: a *trajectory* on a graph



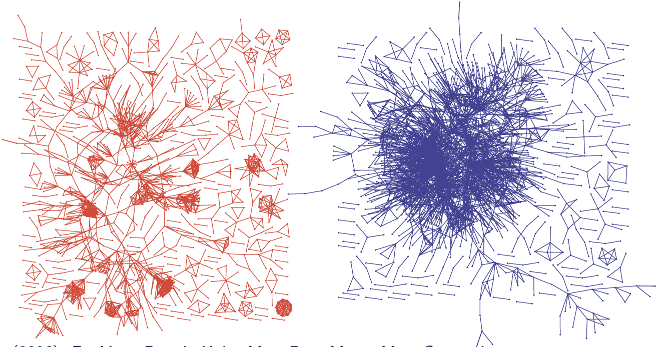
- Why walks?

Why Walks?

Walk: a *trajectory* on a graph



- Why walks?
  - ⟶ Random walks, quantum random walks
  - ⟶ Network analysis is often walk-based
  - ⟶ 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

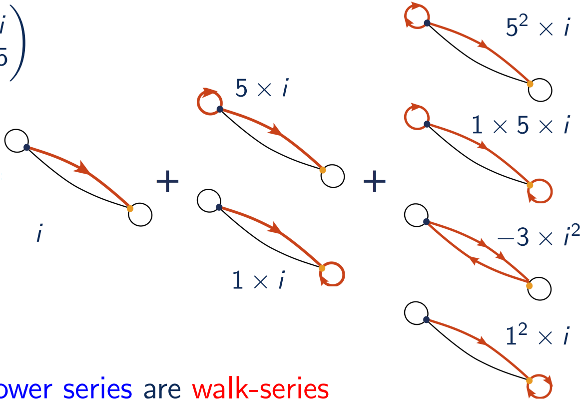
Why Walks?

Walks are pervasive objects!

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

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

$$\left(\sum_n \mathcal{M}^n\right)_{\blacksquare \to \blacksquare} =$$

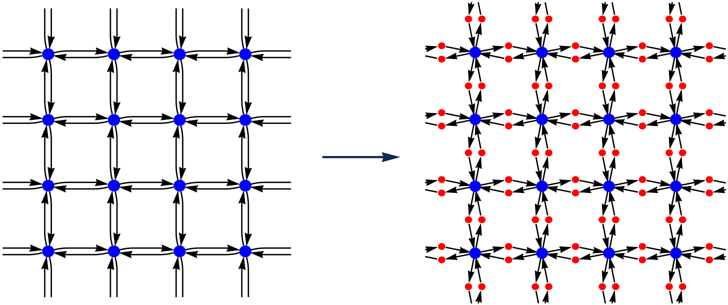


$\hookrightarrow$ Matrix power series are walk-series

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

Strange Observation 1

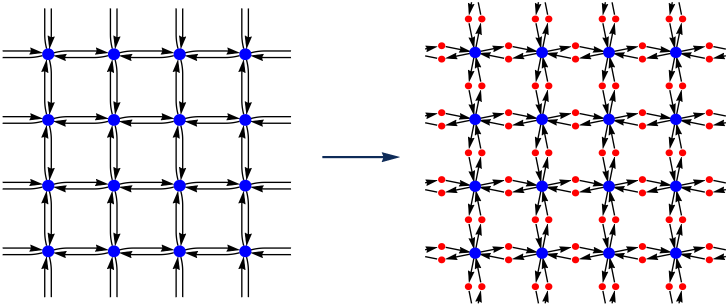
- Changing a square lattice



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

Strange Observation 1

- Changing a square lattice

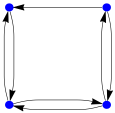


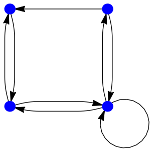
$$\#W_{\bullet \to \bullet'}(\ell) \;\longrightarrow\; \#W_{\bullet \to \bullet'}(2\ell)$$

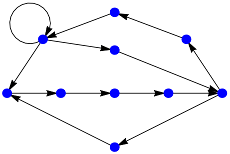
$\hookrightarrow$ Non-trivial for graphs: regularity is lost
$\hookrightarrow$ Trivial transformation for walks

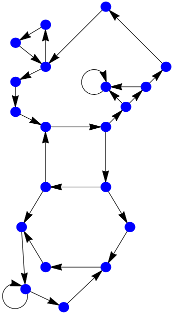
Strange Observation 2

Which graphs are "similar"?



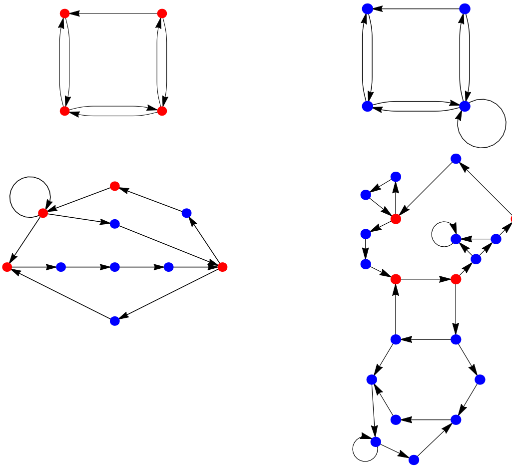






Strange Observation 2

Which graphs are "similar"?



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

Strange Observation 3

- Why is network analysis difficult?

  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

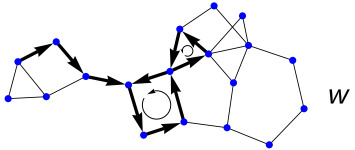
- Completely *dissimilar* graphs can have the *same* walk sets
- Even *fundamental* graph properties, *regularity*, may have little effect on walks
- Existence of *non-trivial* properties of walks *valid on all* multi-digraphs
- More strange objects to come (*walks without graphs!*)

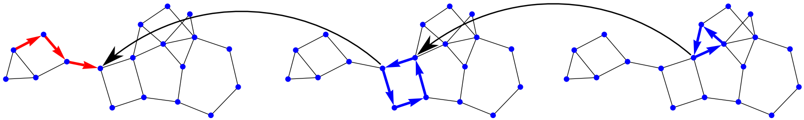
$\hookrightarrow$ Can we represent and manipulate walks without their graphs?

Elements of Walk Theory

Prime Structure

Observation : walk = simple path & simple cycle





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

  $\hookrightarrow w = \gamma_0 \odot \gamma_1 \odot \gamma_2$

What can we say in general?

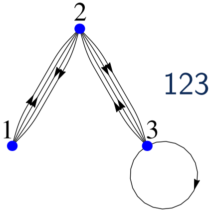
Prime Structure

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 $t \propto O(\ell_w)$



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

Primes provide walk sets with a *structure*

Posets of Walks

Construct a prime-based representation of walks

- Sets of walks ordered by divisibility

$$w \leq_{\odot} w' \iff w \,|\, w'$$

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

- 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: $P_\alpha^\Omega = (S_\Omega, \leq_\Omega)$

Poset of ω-walks

Sets of *distinct* prime factors...

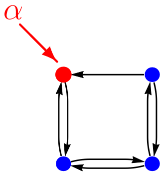
$$w = \gamma_0 \odot \gamma_1^3 \Rightarrow S_\omega(w) = \{\gamma_0, \gamma_1\}$$

...ordered by inclusion

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

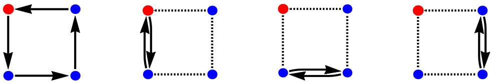
$\hookrightarrow$ Poset of ω-walks: $P_\alpha^\omega = (S_\omega, \leq_\omega)$

Example: P_α^ω on the Square



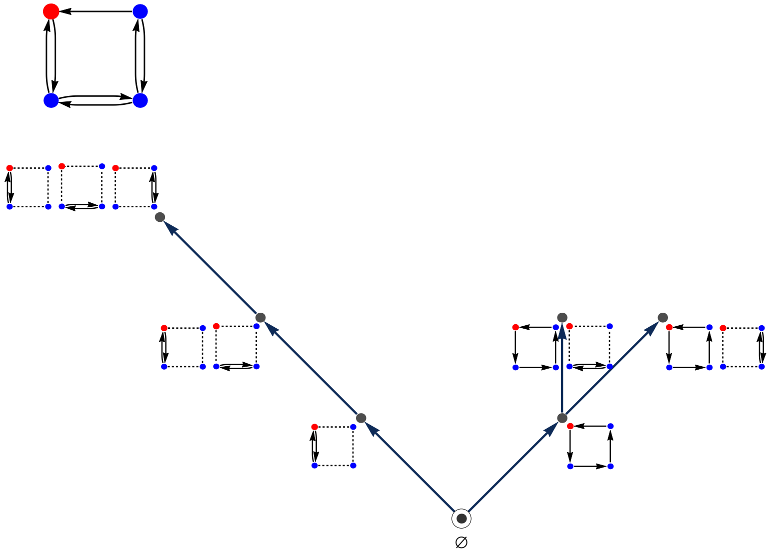
Walking from • to itself
Which primes can be reached?

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



Example: P^{ω}_{α} on the Square

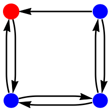
Relations between the primes

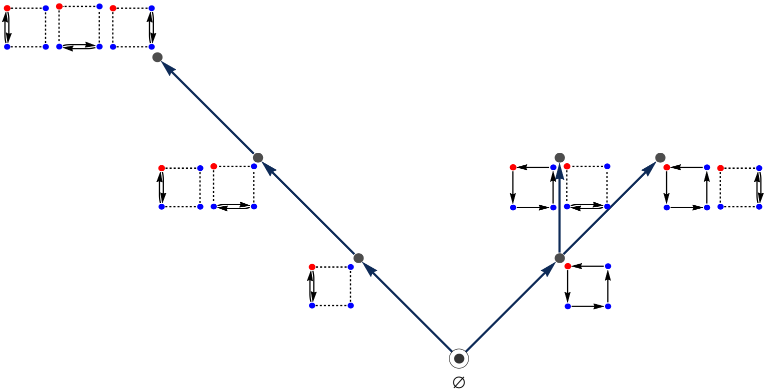


Example: P_α^ω on the Square

Relations between the primes

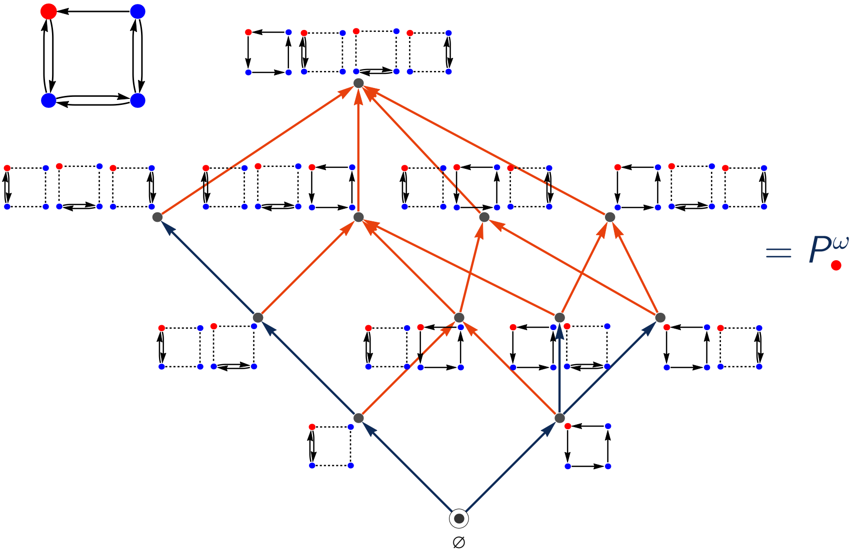
Prime Tree $T^\omega_{\bullet}$





Example: P_{α}^{ω} on the Square

Primes provide walk sets with a *structure*



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
  $\hookrightarrow$ Gradation is $\Omega(w) = \#\,$Prime factors of w
- P_α^ω is a *finite* lattice, has a smallest and largest element
- P_α^ω is the uniquely determined by the **prime tree** T_α^ω

Theorem

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

- Number of walk posets on n primes:

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

Strange Observation 4

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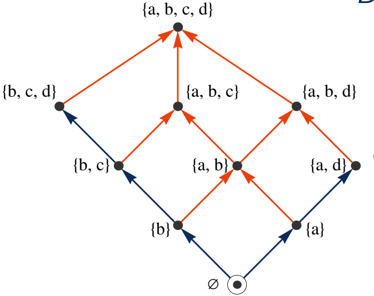
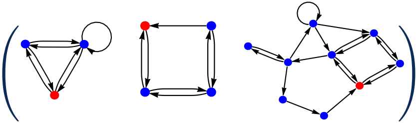


a, b, c, d primes

$\subseteq P^{\omega}_{\bullet}$



Strange Observation 4

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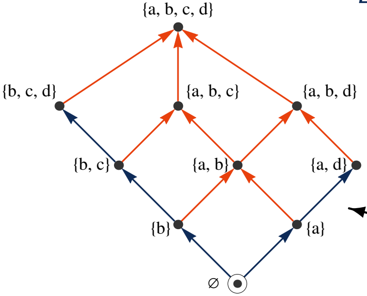
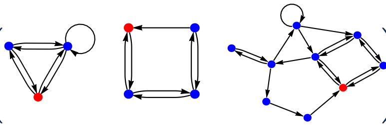


a, b, c, d primes

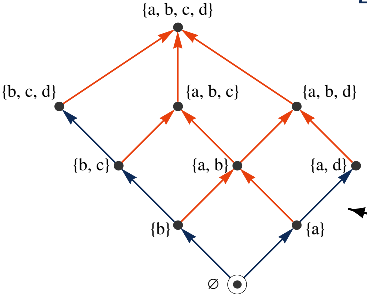
$\subseteq P^{\omega}_{\bullet}\left(\right.$  $\left.\right)$

No graph exists with exactly this walk poset

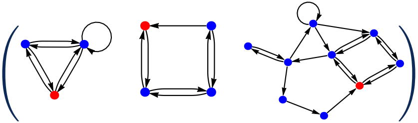
Strange Observation 4

- Number of walk posets on n primes:

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



a, b, c, d primes

$\subseteq P^{\omega}_{\bullet}\Big($  $\Big)$

No graph exists with exactly this walk poset

- Number of walk posets on n primes with exact graph realization

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

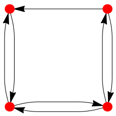
$\hookrightarrow$ *Most walk sets have no exact graph realization!*

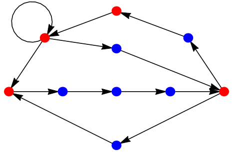
Isomorphic Walk Sets

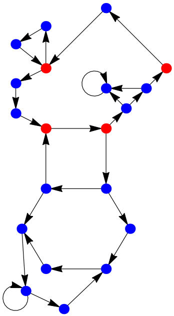
Isomorphic walk sets on dissimilar graphs

Theorem

Let $\mathcal{G}_1$ and $\mathcal{G}_2$ be two multi-digraphs and α and a two vertices on $\mathcal{G}_1$ and $\mathcal{G}_2$, respectively.
If $T^{\omega}_{\mathcal{G}_1;\alpha}$ is isomorphic to $T^{\omega}_{\mathcal{G}_2;a}$ then $(W_{\mathcal{G}_1;\alpha\alpha}, \odot)$ is isomorphic to $(W_{\mathcal{G}_2;aa}, \odot)$.







Length of prime ℓ_p is *unspecified*
$\hookrightarrow$ ∞-many graph realizations

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.

$\hookrightarrow$ Prime trees + length of primes + roots = unique graph

↑ location of the 1st vertex

Algebraic Walk Theory

Path-Sum Representations

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
$k(w) = \text{Weight}(w)$
$k(w) = z^{\Omega(w)}$

Path-Sum Representations

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
$k(w) = \text{Weight}(w)$
$k(w) = z^{\Omega(w)}$

Theorem

Let $w \odot w' = w_L \circ w' \circ w_R$. If $k(w \odot w') = k(w_L)k(w')k(w_R)$ then $\Sigma_{\mathcal{G};\,\alpha\beta}$ admits a finite, explicit form involving only prime walks.

$\hookrightarrow$ Extends to series of Ω- and ω-walks

Path-Sum Representations

Mathematics:

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

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

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

Physics:

Path-Sum Representations

Mathematics:

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

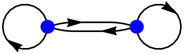
"Analytic matrix function $f(\mathcal{M})$ = series of walk weights"

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

Physics:

$\hookrightarrow$ Non-perturbative closed form for

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

$\hookrightarrow$ 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!*

$\hookrightarrow$ Path-sums too complicated for many quantum systems

Path-Sum Representations

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-Sum Representations

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)*

Algebraic Structure

Algebraic manipulation of walks

$Z_\alpha(w, w') = 1 \iff w|w'$

$\vec{d}(w) = \#$ divisors of w, $\vec{\omega}(w) = \#$ distinct prime factors of w

Why?

Algebraic Structure

Algebraic manipulation of walks

$Z_\alpha(w, w') = 1 \iff w|w'$

$\vec{d}(w) = \#$ divisors of w, $\vec{\omega}(w) = \#$ distinct prime factors of w

Why?

- $\#$ Divisors of the walks: $\vec{d} = \vec{\mathbf{1}} \, . \, Z_\alpha$

  $\hookrightarrow \sum_n \frac{d(n)}{n^s} = \sum_{\mathbf{n}} \frac{\mathbf{1}}{\mathbf{n^s}} \times \zeta(s)$

Algebraic Structure

Algebraic manipulation of walks

$Z_\alpha(w, w') = 1 \iff w|w'$

$\vec{d}(w) = \#$ divisors of w, $\vec{\omega}(w) = \#$ distinct prime factors of w

Why?

- # Divisors of the walks: $\vec{d} = \vec{\mathbf{1}} \,.\, Z_\alpha$

  $\hookrightarrow \sum_n \frac{d(n)}{n^s} = \sum_{\mathbf{n}} \frac{\mathbf{1}}{\mathbf{n^s}} \times \zeta(s)$

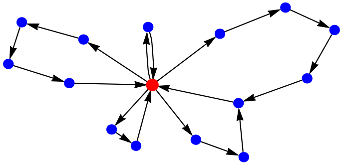
- # Distinct primes factors of w: $\vec{\omega} = \vec{\chi_p} \,.\, Z_\alpha$

  $\hookrightarrow \sum_n \frac{\omega(n)}{n^s} = \zeta_p(s) \times \zeta(s)$

- Probability prime p among factors of random walk $\vec{1}_p . Z_\alpha . \vec{P}[w]$ etc...

Relations in parallel to number theory?

Realization of Number Theory



A bouquet graph

On ∞-bouquet graphs $(\mathcal{S}_{\Omega;\bullet}, \odot) \sim (\mathbb{N}, \times)$

$\hookrightarrow$ Ω-walks $\equiv$ integers $\quad Z_\alpha^\Omega \equiv \zeta(s)$

$\hookrightarrow$ Path-sum representation $\quad Z_\alpha^\Omega \equiv \prod_p \frac{1}{1-p^{-s}}$

$$Z_\alpha^\omega \equiv \frac{\zeta(s)}{\zeta(2s)}$$

ω-walks $\equiv$ square-free integers

$$Z_\alpha \equiv \frac{1}{1-\zeta_p(s)}$$

walks $\equiv$ ordered prime factorisations

Esoteric results? all graphs are made of bouquets

The Prime Walk Theorem

Prime Walk Theorem (open problem):

- How many primes of length ℓ are there?

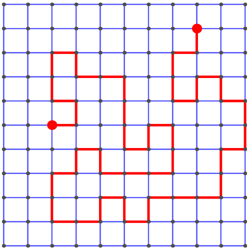
The Prime Walk Theorem

Prime Walk Theorem (open problem):

- 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?

$\hookrightarrow$ 70 years old problem in combinatorics & polymer physics



Walk Theory

Final Message

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
- Algebraic aspects in parallel with and producing number theory

Open problems

- Prime walk theorem
- Better exploit path-sums for quantum systems

Thank You!

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I am looking for a postdoctoral position!