Outline

1 Introduction
   - Why walks?
   - Strange Observations

2 Walk Theory
   - Prime structure
   - Posets of walks, $\Omega$-walks and $\omega$-walks
   - Prime characterization of graphs

3 Algebraic Walk Theory
   - Path-sum representations
   - Algebraic structure
   - 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

Why Walks?

*Walks are pervasive objects!*

- Adjacency matrix $A^n = \text{number of walks on graph}$
Why Walks?

Walks are pervasive objects!

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

\[
M = \begin{pmatrix} 1 & i \\ -3 & 5 \end{pmatrix}
\]

\[
\left( \sum_n M^n \right) = \begin{pmatrix} i \\ 5 \end{pmatrix} = 5^2 \times i + 5 \times i + 1 \times 5 \times i + 1 \times i + 1^2 \times i + 3 \times i^2 + 1 \times i
\]

\rightarrow \text{Matrix power series are walk-series}

Analytic matrix function $f(M) = \text{series of walk weights}$
Strange Observation 1

• Changing a square lattice

\[
\# W_{\bullet \rightarrow \bullet'}(\ell) \quad \rightarrow \quad \# W_{\bullet \rightarrow \bullet'}(2\ell)
\]
Strange Observation 1

- Changing a square lattice

\[ \# W_{\bullet \rightarrow \bullet'}(\ell) \quad \rightarrow \quad \# W_{\bullet \rightarrow \bullet'}(2\ell) \]

\[ \text{←→ Non-trivial for graphs: } \text{regularity is lost} \]

\[ \text{←→ Trivial transformation for walks} \]
Strange Observation 2

Which graphs are “similar”? 

[Diagrams of graphs]
Strange Observation 2

Which graphs are “similar”?  

Yet the walk sets $W_{\bullet \rightarrow \bullet}$ are \textit{isomorphic}.
Strange Observation 3

- Why is network analysis not perfect?

Example: characterizing molecules

<table>
<thead>
<tr>
<th>Method</th>
<th>Dataset</th>
<th>Accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Random walk kernel</td>
<td>Mutag(labelled)</td>
<td>90.0%</td>
</tr>
<tr>
<td><em>Backtrackless walk kernel</em></td>
<td>Mutag(labelled)</td>
<td>91.1%</td>
</tr>
<tr>
<td>Feature vector from Random walk</td>
<td>COIL(unlabeled)</td>
<td>94.4%</td>
</tr>
<tr>
<td><em>Feature vector from backtrackless random walk</em></td>
<td>COIL(unlabeled)</td>
<td>95.5%</td>
</tr>
<tr>
<td>Feature vector from Ihara coefficients</td>
<td>COIL(unlabeled)</td>
<td>94.4%</td>
</tr>
<tr>
<td>Shortest Path Kernel</td>
<td>COIL(unlabeled)</td>
<td>86.7%</td>
</tr>
<tr>
<td>Feature vector from Random walk</td>
<td>Mutag(unlabeled)</td>
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<tr>
<td><em>Feature vector from backtrackless random walk</em></td>
<td>Mutag(unlabeled)</td>
<td>90.5%</td>
</tr>
<tr>
<td>Feature vector from Ihara coefficients</td>
<td>Mutag(unlabeled)</td>
<td>80.5%</td>
</tr>
</tbody>
</table>

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*,  
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!*)

→ Can we represent and manipulate walks without their graphs?
Elements of Walk Theory

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
   - Prime walk theorem

4. Final Message
Prime Structure

Observation: walk = simple path & simple cycle

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

$w = \gamma_0 \circ \gamma_1 \circ \gamma_2$

What can we say in general?
**Theorem**

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

**Prime walks:** $\gamma | w \circ w' \Rightarrow \gamma | w$ or $\gamma | w'$

This holds on all multi-digraphs!

Walk factorization is efficient $t \propto O(\ell_w)$

Primes provide walk sets with a structure
Posets of Walks

Construct a **prime-based** representation of walks

- Sets of walks ordered by divisibility

\[ w \leq \circ w' \iff w | w' \]

Example: \( 121 | 1221 = 121 \circ 22 \implies 121 \leq \circ 1221 \)

- Poset of walks \( P_\alpha = (W_G, \alpha, \leq \circ) \)

Set of walks from \( \alpha \) to \( \alpha \) on \( G \)
Posets of Walks

Construct a **prime-based** representation of walks

- Sets of walks **ordered by divisibility**

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- Poset of walks \( P_\alpha = (W_G;_\alpha \alpha, \leq_\circ) \)
  
  Set of walks from \( \alpha \) to \( \alpha \) on \( G \)

  \( P_\alpha \) is a complicated object: \( \infty \)-many walks
  
  Nesting \( \circ \) is non-commutative, non-associative
  
  Difficult to find all divisors

  **Can we make things simpler?**
Posets of $\Omega$-walks and $\omega$-walks

**Poset of $\Omega$-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 $\Omega$-walks: $P^\Omega_\alpha = (S_\Omega, \leq_\Omega)$

**Poset of $\omega$-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 $\omega$-walks: $P^\omega_\alpha = (S_\omega, \leq_\omega)$
Example: $P^\omega_\alpha$ on the Square

Walking from • to itself
Which primes can be reached?

→ Set of accessible primes, walking from • to itself
Example: $P_{\alpha}^\omega$ on the Square

Relations between the primes
Example: $P_\omega^\alpha$ on the Square

Relations between the primes

**Prime Tree** $T_\omega$

\[\Phi\]
Example: $P_{\omega}^\omega$ on the Square

Primes provide walk sets with a *structure*
Posets of $\Omega$-walks and $\omega$-walks

$P_\Omega^\alpha$ and $P_\omega^\alpha$ are simpler than $P_\alpha$

- $P_\Omega^\alpha$ and $P_\omega^\alpha$ are graded
  - Gradation is $\Omega(w) = \#$ Prime factors of $w$
- $P_\omega^\alpha$ is a finite lattice, has a smallest and largest element
- $P_\omega^\alpha$ is the uniquely determined by the prime tree $T_\omega^\alpha$

Theorem

Knowledge of $P_\Omega^\alpha$, $P_\omega^\alpha$ or $T_\omega^\alpha$ is equivalent to that of $P_\alpha$

- Number of walk posets on $n$ primes:
  $$B_n \sim \left(\frac{.792 n}{\log n}\right)^n$$
Strange Observation 4

- Number of walk posets on $n$ primes:
  \[ B_n \sim \left(\frac{.792 \, n}{\log n}\right)^n \]
Strange Observation 4

- Number of walk posets on $n$ primes:

$$B_n \sim (0.792 \frac{n}{\log n})^n$$

$a, b, c, d$ primes
Strange Observation 4

- Number of walk posets on $n$ primes:
  $$B_n \sim (0.792 n/ \log n)^n$$

No graph exists with exactly this walk poset

$\{a, b, c, d\}$
$\{b, c, d\}$
$\{b, c\}$
$\{b\}$
$\emptyset$

$a, b, c, d$ primes

$\subseteq P^\omega$

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

Most walk sets have no exact graph realization!
Strange Observation 4

- Number of walk posets on \( n \) primes:
  \[ B_n \sim \left( \frac{.792}{\log n} \right)^n \]

- Number of walk posets on \( n \) primes with exact graph realization:
  \[ C_n \sim 4^n n^{-3/2} / \sqrt{\pi} \ll B_n \]

\( \rightarrow \) Most walk sets have no exact graph realization!
Theorem

Let $G_1$ and $G_2$ be two multi-digraphs and $\alpha$ and $a$ two vertices on $G_1$ and $G_2$, respectively. If $T^\omega_{G_1;\alpha}$ is isomorphic to $T^\omega_{G_2;a}$ then $(W_{G_1;\alpha\alpha}, \odot)$ is isomorphic to $(W_{G_2;aa}, \odot)$.

Length of prime $\ell_p$ is unspecified

$\infty$-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 $G$ be a connected multi-digraph.*

*Then $G$ is uniquely determined, up to an isomorphism, by the primes it sustains.*

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

$\uparrow$ location of the 1\textsuperscript{st} vertex
Algebraic Walk Theory

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4 Final Message
Path-Sum Representations

Prime representations of walk-series

\[ \Sigma_{G, \alpha \beta} := \sum_{w \in W_{G, \alpha \beta}} k(w) \]

Sum of all walks from \( \alpha \) to \( \beta \)

A function of walks

\[ k(w) = \text{Weight}(w) \]
\[ k(w) = z^{\Omega(w)} \]
Path-Sum Representations

Prime representations of walk-series

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

Sum of all walks from $\alpha$ to $\beta$

A function of walks $k(w) = \text{Weight}(w)$

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

Theorem

If $k(w \odot w') = k(w)k(w')$ then $\Sigma_{G; \alpha \beta}$ admits a finite form involving only prime walks.

→ Extends to series of $\Omega$- and $\omega$-walks
Path-Sum Representations

Mathematics:

\[ k(w) = \text{Weight}(w) \]

“Analytic matrix function \( f(M) = \text{series of walk weights} \)”

\[ \rightarrow \text{Path-sum: universal formula for functions of matrices} \]

Physics:

\[ U = e^{-iHt}, \quad Z = e^{-\beta H}, \quad R = (zI - H)^{-1} \]

\[ \Rightarrow \text{Dyson equation?} \]

\[ \rightarrow \text{Exact finite formula for the self-energy} \]

\[ \rightarrow \text{Anderson localisation in many-body interacting systems} \]

Wow?

\[ \rightarrow \text{not quite!} \]

\[ \rightarrow \text{Path-sums too complicated for many quantum systems} \]
Path-Sum Representations

Mathematics:

\[ k(w) = \text{Weight}(w) \]

“Analytic matrix function \( f(M) = \) series of walk weights”

\[ \Rightarrow \text{Path-sum: universal formula for functions of matrices} \]

Physics:

\[ \Rightarrow \text{Non-perturbative closed form for} \]

\[ U = e^{-iHt}, \ Z = e^{-\beta H}, \ R = (zI - H)^{-1} \]

\[ \Rightarrow \text{Dyson equation? } \Rightarrow \text{path-sum on} \]

\[ \Rightarrow \text{Exact finite formula for the self-energy} \]

\[ \Rightarrow \text{Anderson localisation in many-body interacting systems} \]

Wow? not quite!

\[ \Rightarrow \text{Path-sums too complicated for many quantum systems} \]
Path-Sum Representations
Prime representations of *dynamical* walk-series

Extends to \{ dynamical graphs, time-dependent Hamiltonians \}

**Mathematics:**
\[ \text{Solves systems of diff. equations with variable coefficients} \]

**Physics:**
Path-Sum Representations

Prime representations of *dynamical* walk-series

Extends to \( \{ \text{dynamical graphs} \}
\begin{align*}
\text{time-dependent Hamiltonians}
\end{align*}

**Mathematics:**
\[ \rightarrow \text{Solves systems of diff. equations with variable coefficients} \]

**Physics:**
\[ \rightarrow \text{Treat time on equal footing with all degrees of freedom} \]
\[ \rightarrow \text{Timeless quantum mechanics *(weird)*} \]
Algebraic Structure

Algebraic manipulation of walks

\[ Z_\alpha(w, w') = 1 \iff w | w' \]
\[ Z_{\ell_\alpha}(w, w') = 1 \iff \ell_w < \ell_{w'} \text{ or } w = w' \]

Why?
Algebraic manipulation of walks

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

\[ Z_\ell^\ell(w, w') = 1 \iff \ell_w < \ell_{w'} \text{ or } w = w' \]

Why?

- # Divisors of the walks: \( \vec{d} = \vec{1} \cdot Z_\alpha \)

\[ \sum n \frac{d(n)}{n^s} = \sum n \frac{1}{n^s} \times \zeta(s) \]
Algebraic Structure

Algebraic manipulation of walks

\[ Z_\alpha(w, w') = 1 \iff w | w' \]
\[ Z_\ell(w, w') = 1 \iff \ell_w < \ell_{w'} \text{ or } w = w' \]

Why?

- **# Divisors of the walks:** \( \vec{d} = \vec{1} \cdot Z_\alpha \)

  \[ \sum_n \frac{d(n)}{n^s} = \sum_n \frac{1}{n^s} \times \zeta(s) \]

- **# Primes shorter than \( w \):** \( \pi(w) = \vec{\omega} \cdot (Z_\alpha)^{-1} \cdot Z_\ell \cdot \vec{1}_w \)

  \[ \pi(n) = \sum_m \frac{\omega(m)}{m^s} \times \zeta(s)^{-1} \times \sum_{m \leq n} m^s \]

- **Probability prime \( p \) among factors of random walk \( \vec{1}_p \cdot Z_\alpha \cdot \vec{P}[w] \)

  etc...

Relations in parallel to number theory?
Realization of Number Theory

A bouquet graph

On $\infty$-bouquet graphs $(S_\Omega;\bullet, \odot) \sim (\mathbb{N}, \times)$

$\Omega$-walks $\equiv$ integers

Path-sum representation

$Z_\alpha^\Omega \equiv \zeta(s)$

$Z_\alpha^\Omega \equiv \prod_p \frac{1}{1 - p^{-s}}$

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

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

$\omega$-walks $\equiv$ square-free integers

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 $\ell$ are there?
Prime Walk Theorem (open problem):

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

\[ \text{How many self avoiding walks of length } \ell? \]

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