Of Walks and Graphs
An Introduction to Walk Theory I

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Seminar
September 2014
Outline

1 Introduction
   - Why walks?
   - Strange Observations

2 Walk Theory
   - Prime factorisation of walks
   - Posets of walks, \( \Omega \)-walks and \( \omega \)-walks
   - Prime characterization of graphs

3 Algebraic Walk Theory
   - Path-sum representations
   - Applications
   - Prime walk theorem

4 Conclusion
Why Walks?

Walk: a *trajectory* on a graph

➤ Why walks?

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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 = $ number of walks on graph
- Arbitrary matrix $M^n = $ sum of walk weights

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

$$\sum_n M^n = \begin{pmatrix} 1 & i \\ -3 & 5 \end{pmatrix} = \begin{pmatrix} 5 \times i \\ 1 \times i \end{pmatrix} + \begin{pmatrix} 5 \times i \\ 1 \times i \end{pmatrix} + \begin{pmatrix} 1 \times 5 \times i \\ -3 \times i^2 \end{pmatrix} + \begin{pmatrix} 1 \times 5 \times i \\ -3 \times i^2 \end{pmatrix}$$

Matrix power series are walk-series

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

- Changing a square lattice

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

- Changing a square lattice

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

\[\rightarrow \text{Non-trivial for graphs: regularity is lost}\]
\[\rightarrow \text{Trivial transformation for walks}\]
Strange Observation 2

Which graphs are “similar”? 

[Diagrams of graphs]
Strange Observation 2

Which graphs are “similar”? 

Yet the walk sets $W_{\rightarrow}$ are \textit{isomorphic} (I will come back on this)
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>Backtrackless walk kernel</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>Feature vector from backtrackless random walk</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>
<td>89.4%</td>
</tr>
<tr>
<td>Feature vector from backtrackless random walk</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 factorisation of walks
   - Posets of walks, Ω-walks and ω-walks
   - Prime characterization of graphs

3. Algebraic Walk Theory
   - Path-sum representations
   - Applications
   - Prime walk theorem

4. Conclusion
Prime factorisation of walks

Observation: walk = simple path & simple cycle

$w \xleftarrow{\gamma_0} \rightarrow (\gamma_1 \xleftarrow{\gamma_2})$

What can we say in general?
Nesting product

- Nesting product \( \circ \) nests a walk into another iff

\[
\begin{align*}
\alpha & \quad \circ \quad w_1 \quad \circ \quad w_2 \\
\alpha & \quad \circ \quad w_1 \quad = \quad w_1 \quad \circ \quad w_2 \\
\alpha & \quad \circ \quad w_1 \quad = \quad \alpha \quad w_1 \quad \circ \quad w_2
\end{align*}
\]

or

\[
\begin{align*}
\alpha & \quad \alpha \alpha \quad w_1 \\
\alpha & \quad \alpha \alpha \quad w_2 \\
\alpha & \quad \alpha \alpha \quad w_2
\end{align*}
\]

\[w = \gamma_0 \circ (\gamma_1 \circ \gamma_2)\]
Nesting product

- Nesting product \( \circ \) nests a walk into another iff

\[
\alpha \quad \circ \quad \alpha \quad \circ \quad \alpha \quad = \quad \alpha \quad \circ \quad w_1 \quad = \quad \alpha \quad \circ \quad w_2 \quad \alpha
\]

or

\[
\alpha \quad \circ \quad \alpha \alpha \quad = \quad \alpha \quad \circ \quad \alpha \quad \circ \quad w_1 \quad = \quad \alpha \quad \circ \quad \alpha \alpha \quad \circ \quad w_2 \quad \alpha
\]

\[\text{Does not visit any of these vertices except } \alpha\]

\[\rightarrow w = \gamma_0 \circ (\gamma_1 \circ \gamma_2)\]

- Ad-hoc? consider loop-erasing
The Fundamental Theorem

**Theorem**

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

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

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

$$1232332121 = \left(121 \odot (232 \odot (232 \odot 33))\right) \odot 121$$
Posets of Walks

Construct a prime-based representation of walks

- Sets of walks ordered by divisibility

\[ w \preceq \odot w' \iff w | w' \]

Example: \( 121 | 1221 = 121 \odot 22 \implies 121 \preceq \odot 1221 \)

- Poset of walks \( P_\alpha = (W_G;\alpha\alpha, \preceq_{\odot}) \)

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

Construct a prime-based representation of walks

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

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

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

\[ \mapsto P_\alpha \text{ is a complicated object: } \infty-\text{many walks} \]

\[ \mapsto \text{Nesting } \circ \text{ is non-commutative, non-associative} \]

\[ \mapsto \text{Difficult to find all divisors} \]

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

**Poset of $\Omega$-walks**

Sets of prime factors...

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

...ordered by inclusion

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

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

- $\Omega$-walk = loop-erased walk + set of loops

$\bigcirc$ (almost) commutative!
Posets of $\Omega$-walks and $\omega$-walks

**Poset of $\omega$-walks**

Sets of *distinct* prime factors...

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

...ordered by inclusion

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

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

$\blacktriangleright \quad P_\alpha^\omega$ finite graded lattice

$\blacktriangleright$ Let’s see what $P_\alpha^\omega$ looks like
Example: $P^\omega_\alpha$ on the Square

Walking from $\bullet$ to itself
Which primes can be reached?

$\alpha$

$\rightarrow$ Set of accessible primes, walking from $\bullet$ to itself
Example: $P^\omega_\alpha$ on the Square

Relations between the primes

Prime Tree $T^\omega$
Example: $P^\omega_\alpha$ on the Square

The complete poset

$= P^\omega$
Example: $P_\alpha^\omega$ on the Square

Primes provide walk sets with a *structure*

$= P_\cdot^\omega$
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 lattices
- $P^\omega_\alpha$ finite

... and lossless

Theorem

Knowledge of $P^\Omega_\alpha$, $P^\omega_\alpha$ or $T^\omega_\alpha$ is equivalent to that of $P_\alpha$

Proof

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

$$T^\omega(w) \subseteq T^\omega_\alpha \Rightarrow w \in P_\alpha$$
Corollary

Let $G_1$ and $G_2$ be two graphs and $\alpha \in V(G_1)$, $a \in V(G_2)$

$$T_{G_1;\alpha}^\omega \cong T_{G_2;a}^\omega \iff (W_{G_1;\alpha\alpha; \bigcirc}) \cong (W_{G_2;aa; \bigcirc})$$
Isomorphic Walk Sets

Invariance of $P_\alpha$ 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

$$(W_{\mathcal{G}}; \alpha \beta, \circ) \simeq (W_{\mathcal{G}'}; \alpha \beta, \circ)$$
Isomorphic Walk Sets

Invariance of $P_\alpha$ 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

$$(W_\mathcal{G}; \alpha\beta, \circlearrowleft) \cong (W_{\mathcal{G}}'; \alpha\beta, \circlearrowleft)$$

More $P_\alpha$-invariant graph transformations

`Broad’ classification possible
$P_\alpha$-invariant graph transformations as *generators*

$T^\omega_\alpha$ a *graph-free* representation of walk sets?

$\rightarrow$ Depends weakly on any specific $G$

$\rightarrow$ Walks without graphs?
Strange Observation 4

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

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

No graph exists with exactly this walk poset
Strange Observation 4

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

- Conjectured # walk posets on $n$ primes with exact graph realization:
  \[ C_n \sim 4^n n^{-3/2} / \sqrt{\pi} \ll B_n \]

\[ \iff \text{Most walk sets have no exact graph realization!} \]
Prime Characterization of Graphs

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

\[ \bigcup_{\alpha, \beta} T \omega_{\alpha \beta} = G \]

Walk set structure Specific realization of the structure
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:

$$
\bigcup_{\alpha,\beta} T_{\alpha\beta}^\omega + \text{length of primes} + \text{roots} = \mathcal{G}
$$

Walk set structure

Specific realization of the structure
Prime Characterization of Graphs

Let $\alpha, \beta \in V(G)$

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

Proof

Graphs determined by their primes
- Walks $W_{G;\alpha\beta} = \text{words of language } L_{\alpha\beta}$
- Automaton with skeleton $G^{\alpha, \beta}$ is minimal for $L_{\alpha\beta}$
- Minimal automaton unique

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

- Unique factorization
  $W_{G;\alpha\beta} \iff \text{Prime set}$

Unique graph realization
- $T^\omega_{\alpha\beta}$ determines inter-prime relations
- $T^\omega_{\alpha\beta} + \text{length of primes} + \text{roots} = \text{Prime set}$
Algebraic Walk Theory

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4. Conclusion
Path-Sums

Prime representations of walk-series

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

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

A function of walks

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

\[ k(w) = z^{\Omega(w)} \]

Theorem

Let \( w, w' \) be two walks with \( w \circ w' = w_1 \circ w' \circ w_2 \). If

\[ k(w \circ w') = k(w_1) k(w') k(w_2) \]

then \( \sum_{G; \alpha \beta} \) admits a unique, explicit and universal form involving only prime walks.

\[ \leftarrow \text{Extends to series of } \Omega- \text{ and } \omega-\text{walks (next talk)} \]
Path-Sums

How does it works?

- Factorized forms ...

\[ \gamma_0 \otimes \gamma_1 + \gamma_0 \otimes \gamma_1 \otimes (\gamma_2)^1 + \gamma_0 \otimes \gamma_1 \otimes (\gamma_2)^2 + \gamma_0 \otimes \gamma_1 \otimes (\gamma_2)^3 + \cdots \]

... are easy to sum!

\[ \gamma_0 \otimes \gamma_1 \otimes (\mathbb{I} - \gamma_2)^{-1} \]

- We can sum all walks this way
Factoring Walks on Graphs

How does it work?

- Factor formal series of walks

\[ \sum w = \sum (\alpha)(\alpha \nu_1)(\nu_1)(\nu_1 \nu_2) \cdots (\nu_p \beta)(\beta) \]

Ensemble of simple paths
Factoring Walks on Graphs

*How does it works?*

- Factor formal series of walks

\[
\sum_{w: \alpha \to \beta} w = \sum_{p: \alpha \to \beta} (\alpha)(\alpha \nu_1)(\nu_1)(\nu_1 \nu_2) \cdots (\nu_p \beta)(\beta)
\]

Insert simple cycles: \( G \), \( G \setminus \{\alpha\} \), \( G \setminus \{\alpha, \nu_1, \cdots, \nu_p\} \)
Factoring Walks on Graphs

How does it work?

- Factor formal series of walks

\[ \sum_{w: \alpha \rightarrow \beta} w = \sum_{p: \alpha \rightarrow \beta} (\alpha)(\alpha \nu_1)(\nu_1)(\nu_1 \nu_2) \cdots (\nu_p \beta)(\beta) \]

Insert simple cycles:

\[ (\alpha) \rightarrow [I - \sum_{c: \alpha \rightarrow \alpha} (\alpha \mu_1)(\mu_1) \cdots (\mu_\ell)(\mu_\ell \alpha)]^{-1} \]
Factoring Walks on Graphs

*How does it work?*

- Factor formal series of walks

\[
\sum_{w: \alpha \to \beta} w = \sum_{p: \alpha \to \beta} (\alpha)(\alpha \nu_1)(\nu_1)(\nu_1 \nu_2) \cdots (\nu_p \beta)(\beta)
\]

Insert simple cycles:

\[
(\alpha) \to [I - \sum_{c: \alpha \to \alpha} (\alpha \mu_1)(\mu_1) \cdots (\mu_\ell)(\mu_\ell \alpha)]^{-1}
\]

*Insert simple cycles again…*
Factoring Walks on Graphs

What does it bring?

- Series of walks
  - Sum of simple paths
    \[
    \sum_{p: \alpha \to \beta} [\alpha]_g (\alpha \nu_1)[\nu_1]_g \{\alpha\} (\nu_1 \nu_2) \cdots (\nu_p \beta)[\beta]_g \{\alpha, \nu_1, \ldots, \nu_p\}
    \]
  - Continued fraction of simple cycles
    \[
    [\alpha]_g = \left[ I - \sum_{c: \alpha \to \alpha} (\alpha \mu_1)[\mu_1]_g \{\alpha\} \cdots [\mu_{\ell}]_g \{\alpha, \mu_1, \ldots, \mu_{\ell-1}\} (\mu_{\ell} \alpha) \right]^{-1}
    \]
- Evaluate \( k \left( \sum_{w: \alpha \to \beta} w \right) \) by distributing \( k(.) \)
Factoring Walks on Graphs

The path-sum

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

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

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

Mathematics:

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

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

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

Structure? the prime tree!

Physics:

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

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

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

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

Wow? not quite!

\[ \text{Too complicated for naive use in many quantum systems} \]
Path-Sums

Prime representations of *dynamical* walk-series

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

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

**Physics:**
Path-Sums
Prime representations of *dynamical* walk-series

Extends to \(\{\) dynamical graphs
\(\}\) time-dependent Hamiltonians

**Mathematics:**
\(-\rightarrow\) Solves systems of diff. equations with variable coefficients

**Physics:**
\(-\rightarrow\) Treat time on equal footing with all degrees of freedom
\(-\rightarrow\) ‘Timeless’ quantum mechanics (*weird*)
The Prime Walk Theorem

Prime Walk Theorem:

- How many primes of length $\ell$ are there?

- Square-lattice: a new take on an old problem

**How many self avoiding walks of length $\ell$?**

Next talk: walk zeta functions and number theory on graphs
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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 $T^\omega_\alpha$ and $G$

Come back for next talk!
Thank You!

Work supported by: EPSRC Grant EP/K038311/1


I am looking for a postdoctoral position!