Evaluating Matrix Functions by Resummations on Graphs

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Goal : compute $f(\mathcal{M})$

1. From Matrices to Graphs

2. Factoring Walks on Graphs

3. Back to Matrices

4. Summary & Outlook

Goal : compute $f(\mathcal{M})$

From Matrices to Graphs

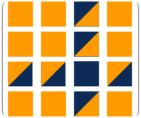
- Adjacency matrix $\mathcal{A}^n =$ number of walks on graph

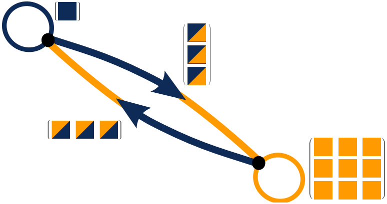
What about arbitrary matrices ?

From Matrices to Graphs

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

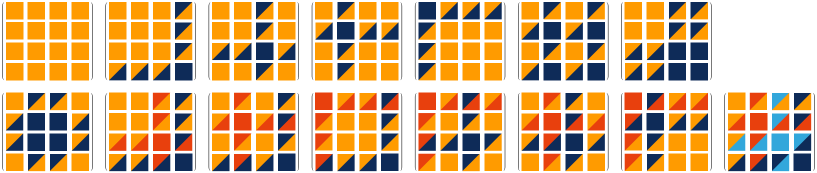
What about arbitrary matrices ?





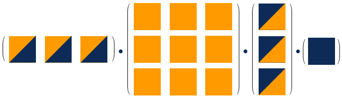
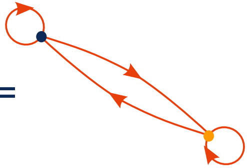
Matrix partition

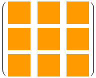
Division of a matrix into blocks & mapping on graph



From Matrices to Graphs

Product of blocks $\Longleftrightarrow$ walk

 $=$ 

 $= \mathcal{M}_{\color{navy}\blacksquare\leftarrow\color{navy}\blacksquare}$  $= \mathcal{M}_{\color{orange}\blacksquare\leftarrow\color{navy}\blacksquare}$  $= \mathcal{M}_{\color{navy}\blacksquare\leftarrow\color{orange}\blacksquare}$  $= \mathcal{M}_{\color{orange}\blacksquare\leftarrow\color{orange}\blacksquare}$

Edge weights

$$(\mathcal{M}^4)_{\color{navy}\blacksquare\leftarrow\color{navy}\blacksquare} = \mathcal{M}_{\color{navy}\blacksquare\leftarrow\color{orange}\blacksquare}\cdot\mathcal{M}_{\color{orange}\blacksquare\leftarrow\color{orange}\blacksquare}\cdot\mathcal{M}_{\color{orange}\blacksquare\leftarrow\color{navy}\blacksquare}\cdot\mathcal{M}_{\color{navy}\blacksquare\leftarrow\color{navy}\blacksquare} + \ldots$$

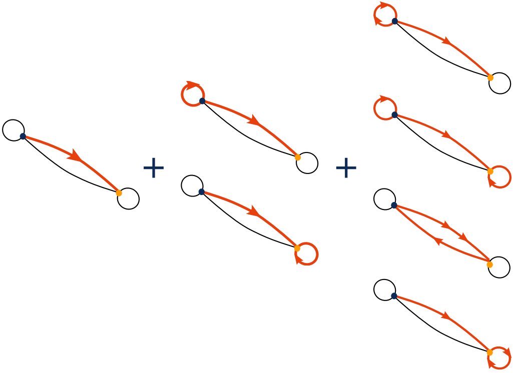
Walk weight

Arbitrary matrix $\mathcal{M}^n =$ sum of walk weights

From Matrices to Graphs

Taylor series are recast into walk-sums

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

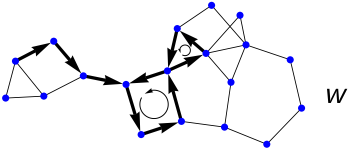


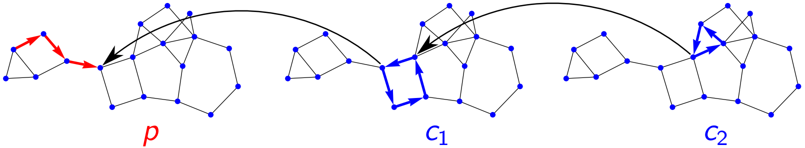
Accelerate convergence via graph theory

Goal : compute $f(\mathcal{M})$

Factoring Walks on Graphs

Observation : walk = simple path & simple cycle





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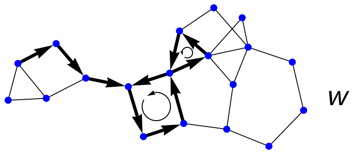
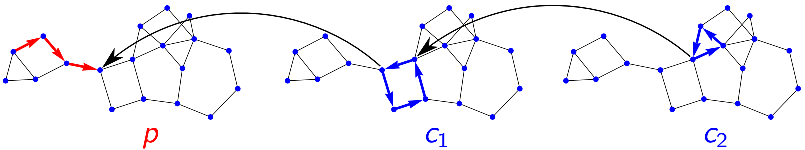




- Walks factor into simple paths, simple cycles

  $\hookrightarrow w = p \odot c_1 \odot c_2$

Prime factorization on graphs arXiv:1202.5523

Factoring Walks on Graphs

Why ?

- Factorized forms ...

$$p \odot c_1 \odot c_2 + p \odot c_1 \odot (c_2)^2 + p \odot c_1 \odot (c_2)^3 + p \odot c_1 \odot (c_2)^4 + \cdots$$

... are easy to sum !

$$p \odot c_1 \odot (\mathcal{I} - c_2)^{-1}$$

- We can sum all walks this way

Prime factorization on graphs arXiv:1202.5523

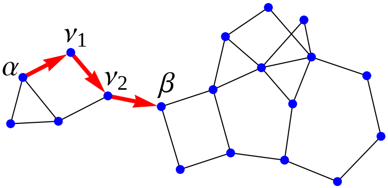
Factoring Walks on Graphs

How does it works ?

- Factor sums of walks

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

Ensemble of simple paths



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

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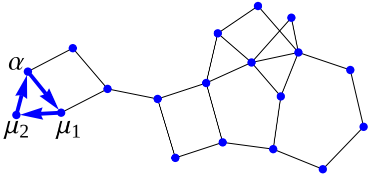
$$(\alpha)\to\Big[\mathcal{I}-\sum_{c:\,\alpha\to\alpha}(\alpha\mu_1)(\mu_1)\cdots(\mu_\ell)(\mu_\ell\alpha)\Big]^{-1}$$



Factoring Walks on Graphs

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

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

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 ?

- Sums of walks

  $\hookrightarrow$ Sum of simple paths

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

  $\hookrightarrow$ Continued fraction of simple cycles

$$[\alpha]_{\mathcal{G}} = \Big[\mathcal{I} - \sum_{c:\,\alpha\to\alpha}(\alpha\mu_1)[\mu_1]_{\mathcal{G}\backslash\{\alpha\}}\cdots[\mu_\ell]_{\mathcal{G}\backslash\{\alpha,\mu_1,\cdots,\mu_{\ell-1}\}}(\mu_\ell\alpha)\Big]^{-1}$$

- 'Few' simple paths & cycles + vertex removal

  $\hookrightarrow$ **Finite** number of operations

And for matrices ?

Goal : compute $f(\mathcal{M})$

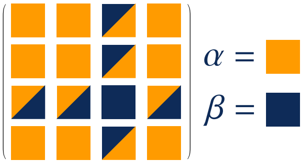
Back to Matrices

Same, with weights

- Replace edges $\Rightarrow$ weights
  $\hookrightarrow$ factorizes $\sum_n \mathcal{M}^n$

$$\Big(\sum_n \mathcal{M}^n\Big)_{\beta\alpha} = \sum_{P_{\mathcal{G}}} [\beta]_{\mathcal{G}\backslash\{\alpha,\nu_2,\dots,\nu_p\}}\, \mathcal{M}_{\beta\nu_p} \cdots [\nu_2]_{\mathcal{G}\backslash\{\alpha\}}\, \mathcal{M}_{\nu_2\alpha}\, [\alpha]_{\mathcal{G}}$$

Indices of the partition



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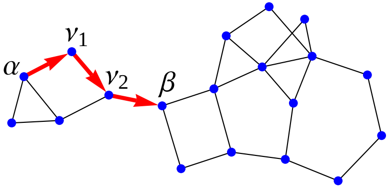
Sum over the simple paths



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Edge weights

Back to Matrices

Same, with weights

- Replace edges ⇒ weights
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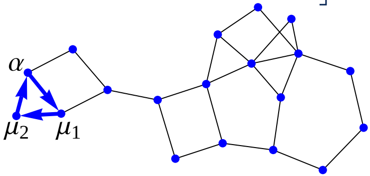
$$\Big(\sum_n \mathcal{M}^n\Big)_{\beta\alpha} = \sum_{P_{\mathcal{G}}} [\beta]_{\mathcal{G}\backslash\{\alpha,\nu_2,\dots,\nu_p\}}\, \mathcal{M}_{\beta\nu_p} \cdots [\nu_2]_{\mathcal{G}\backslash\{\alpha\}}\, \mathcal{M}_{\nu_2\alpha}\, [\alpha]_{\mathcal{G}}$$

Effective vertex weights

$$[\alpha]_{\mathcal{G}} = \Big[\mathcal{I} - \sum_{C_{\mathcal{G};\alpha}} \mathcal{M}_{\alpha\mu_\ell}\, [\mu_\ell]_{\mathcal{G}\backslash\{\alpha,\mu_2,\dots,\mu_{\ell-1}\}} \cdots [\mu_2]_{\mathcal{G}\backslash\{\alpha\}}\, \mathcal{M}_{\mu_2\alpha}\Big]^{-1}$$

Sum over simple cycles



Back to Matrices

Same, with weights

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Effective vertex weights

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$\Rightarrow$ Builds a continued fraction

Back to Matrices

What did we obtain ?

- A factorized form for $\sum_n \mathcal{M}^n$
- Valid for any partition
- Valid for any $\|\mathcal{M}\|$ by analytic continuation

Back to Matrices

What did we obtain ?

- A factorized form for $\sum_n \mathcal{M}^n$
- Valid for any partition
- Valid for any $\|\mathcal{M}\|$ by analytic continuation

Did we accelerate the Taylor series ?

- Only a finite number of terms left
- Continued fraction

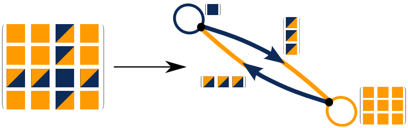
Other $f(\mathcal{M})$?

- Compute resolvent matrix $\mathcal{R}_{\mathcal{M}}$

Back to Matrices

Step by step procedure :

- Partition $\mathcal{M} \Rightarrow \mathcal{G}$



- Calculate $\mathcal{R}_{\mathcal{M}}$ with path-sums
- Compute the inverse transform $f(\mathcal{M})$
- Already done for $\mathcal{M}^q$, $\exp(\mathcal{M})$, $\mathcal{M}^{-1}$, $\log(\mathcal{M})$

The method of path-sums arXiv:1112.1588

Back to Matrices

Remarks :

- $\mathcal{M}^q$, $q = -1$, $\mathcal{M}$ singular $\Rightarrow$ Drazin inverse
- Matrices with non-commuting elements
- $K_2 \Rightarrow$ 4 blocks inversion formula

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{C} & \mathcal{D} \end{pmatrix}^{-1} =$$
$$\begin{pmatrix} (\mathcal{A} - \mathcal{B}\mathcal{D}^{-1}\mathcal{C})^{-1} & -\mathcal{A}^{-1}\mathcal{B}\,(\mathcal{D} - \mathcal{C}\mathcal{A}^{-1}\mathcal{B})^{-1} \\ -\mathcal{D}^{-1}\mathcal{C}\,(\mathcal{A} - \mathcal{B}\mathcal{D}^{-1}\mathcal{C})^{-1} & (\mathcal{D} - \mathcal{C}\mathcal{A}^{-1}\mathcal{B})^{-1} \end{pmatrix}$$

- Block tridiagonal $\Rightarrow$ continued fraction

Conjecture:

Exponential convergence, weight of simple path $\propto e^{-\ell(p)}$

Goal : compute $f(\mathcal{M})$

Summary & Outlook

Main Results

- Matrix function $\Rightarrow$ sum of simple paths & simple cycles

Prime factorization on graphs arXiv:1202.5523
The method of path-sums arXiv:1112.1588

- Successfully implemented in quantum mechanics

Physical approach arXiv:1204.5087
Quantum dynamics arXiv:1108.1177

Open questions

- Numerics: stability
- Convergence behavior
- Continuous matrices, functions of operators $(\partial_x + m)^q$

Thank you!

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