

# Evaluating Matrix Functions by Resummations on Graphs

P.-L. Giscard, S. Thwaite, D. Jaksch



*Numerical Analysis Seminar*  
13th November 2012

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

- 1 From Matrices to Graphs
- 2 Factoring Walks on Graphs
- 3 Back to Matrices
  - Live examples
- 4 Summary & Outlook

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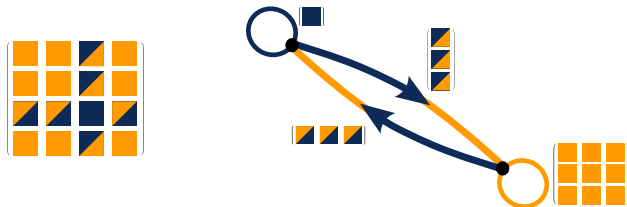
# From Matrices to Graphs

- Adjacency matrix  $\mathcal{A}^n =$  number of walks on graph  
*What about arbitrary matrices ?*

# From Matrices to Graphs

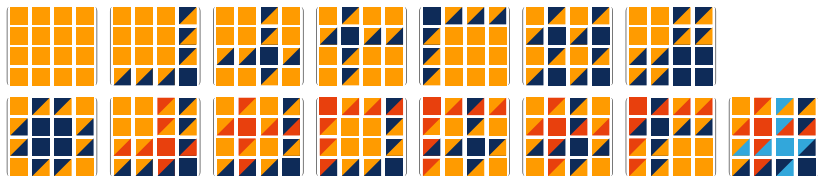
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*What about arbitrary matrices ?*



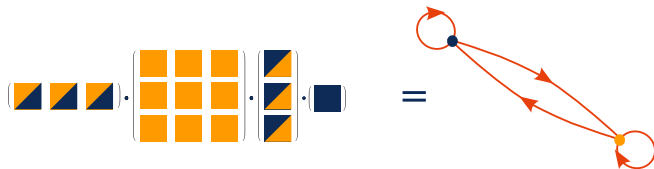
## Matrix partition

Division of a matrix into blocks & mapping on graph



# From Matrices to Graphs

Product of blocks  $\iff$  walk



$$\begin{array}{cccc}
 \blacksquare = \mathcal{M}_{\blacksquare \leftarrow \blacksquare} & \begin{array}{|c|} \hline \blacksquare \\ \hline \blacksquare \\ \hline \blacksquare \\ \hline \end{array} = \mathcal{M}_{\blacksquare \leftarrow \blacksquare} & \begin{array}{|c|} \hline \blacksquare \blacksquare \blacksquare \\ \hline \end{array} = \mathcal{M}_{\blacksquare \leftarrow \blacksquare} & \begin{array}{|c|} \hline \blacksquare \blacksquare \blacksquare \\ \hline \blacksquare \blacksquare \blacksquare \\ \hline \blacksquare \blacksquare \blacksquare \\ \hline \end{array} = \mathcal{M}_{\blacksquare \leftarrow \blacksquare} \\
 & \text{Edge weights} & & 
 \end{array}$$

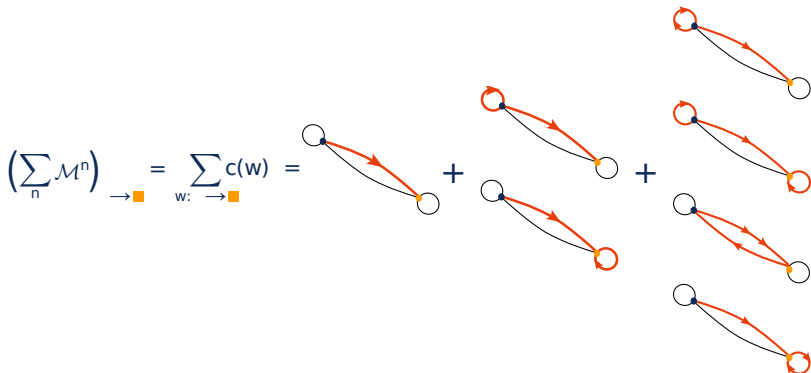
$$(\mathcal{M}^4)_{\blacksquare \leftarrow \blacksquare} = \mathcal{M}_{\blacksquare \leftarrow \blacksquare} \cdot \mathcal{M}_{\blacksquare \leftarrow \blacksquare} \cdot \mathcal{M}_{\blacksquare \leftarrow \blacksquare} \cdot \mathcal{M}_{\blacksquare \leftarrow \blacksquare} + \dots$$

*Walk weight*

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

# From Matrices to Graphs

Taylor series are recast into walk-sums



Accelerate convergence via **graph theory**

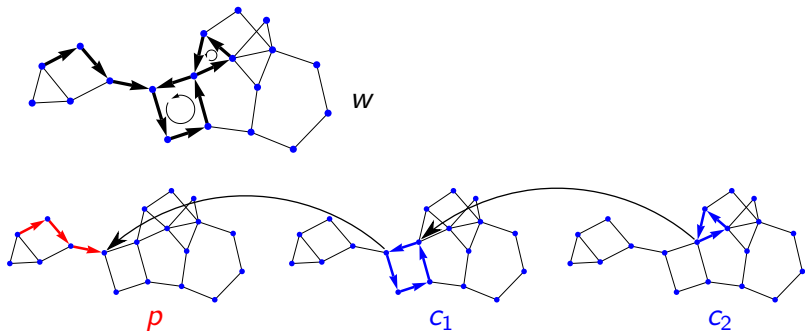
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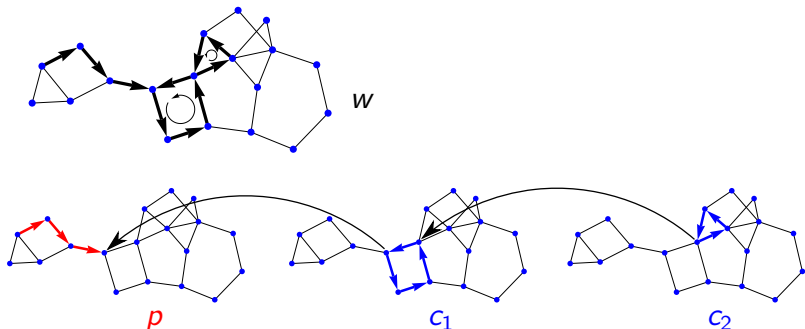
# Factoring Walks on Graphs

Observation : walk = simple path & simple cycle



# Factoring Walks on Graphs

Observation : walk = simple path & simple cycle



- Walks factor into simple paths, simple cycles

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

Prime factorization on graphs [arXiv:1202.5523](https://arxiv.org/abs/1202.5523)

# Factoring Walks on Graphs

*Why ?*

- Factorized forms ...

$$p \odot c_1 \odot (c_2)^0 + p \odot c_1 \odot (c_2)^1 + p \odot c_1 \odot (c_2)^2 + p \odot c_1 \odot (c_2)^3 + \dots$$

... 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](https://arxiv.org/abs/1202.5523)

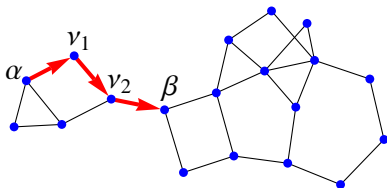
# Factoring Walks on Graphs

*How does it work ?*

- Factor sums of walks

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

Ensemble of simple paths



# Factoring Walks on Graphs

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Insert simple cycles:

$\mathcal{G}$

$\mathcal{G} \setminus \{\alpha\}$

$\mathcal{G} \setminus \{\alpha, \nu_1, \dots, \nu_p\}$

# Factoring Walks on Graphs

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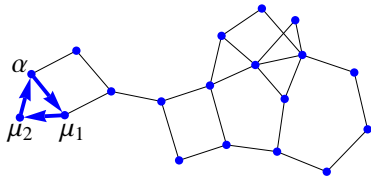
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$\mathcal{G} \setminus \{\alpha\}$

$\mathcal{G} \setminus \{\alpha, \nu_1, \dots, \nu_p\}$

$$(\alpha) \rightarrow \left[ \mathcal{I} - \sum_{c: \alpha \rightarrow \alpha} (\alpha \mu_1) (\mu_1) \cdots (\mu_\ell) (\mu_\ell \alpha) \right]^{-1}$$



# Factoring Walks on Graphs

*How does it work?*

- Factor sums 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:

$\mathcal{G} \setminus \{\alpha\}$

$\mathcal{G} \setminus \{\alpha, \nu_1, \dots, \nu_p\}$

$$(\alpha) \rightarrow \left[ \mathcal{I} - \sum_{c: \alpha \rightarrow \alpha} (\alpha\mu_1)(\mu_1) \cdots (\mu_\ell)(\mu_\ell\alpha) \right]^{-1}$$

*Insert simple cycles again...*

$\mathcal{G} \setminus \{\alpha\}$

$\mathcal{G} \setminus \{\alpha, \mu_1, \dots, \mu_{\ell-1}\}$

# Factoring Walks on Graphs

*What does it bring ?*

- Sums of walks  
     $\longleftrightarrow$  Sum of **simple paths**

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

- $\longleftrightarrow$  Continued fraction of **simple cycles**

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

- 'Few' simple paths & cycles + vertex removal  
     $\longleftrightarrow$  **Finite** number of operations

*And for matrices ?*



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# Back to Matrices

*Same, with weights*

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

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

Indices of the partition

$$\left( \begin{array}{cccc} \alpha & \alpha & \beta & \alpha \\ \alpha & \alpha & \beta & \alpha \\ \beta & \beta & \beta & \beta \\ \alpha & \alpha & \beta & \alpha \end{array} \right) \quad \begin{array}{l} \alpha = \text{orange square} \\ \beta = \text{dark blue square} \end{array}$$

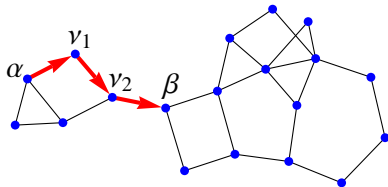
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Sum over the simple paths



# Back to Matrices

*Same, with weights*

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$$\left(\sum_n \mathcal{M}^n\right)_{\beta\alpha} = \sum_{P_G} [\beta]_{G \setminus \{\alpha, \nu_2, \dots, \nu_p\}} \mathcal{M}_{\beta\nu_p} \cdots [\nu_2]_{G \setminus \{\alpha\}} \mathcal{M}_{\nu_2\alpha} [\alpha]_G$$

Edge weights

# Back to Matrices

Same, with weights

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 $\hookrightarrow$  factorizes  $\sum_n \mathcal{M}^n$

$$\left(\sum_n \mathcal{M}^n\right)_{\beta\alpha} = \sum_{P_G} [\beta]_{G \setminus \{\alpha, \nu_2, \dots, \nu_p\}} \mathcal{M}_{\beta\nu_p} \cdots [\nu_2]_{G \setminus \{\alpha\}} \mathcal{M}_{\nu_2\alpha} [\alpha]_G$$

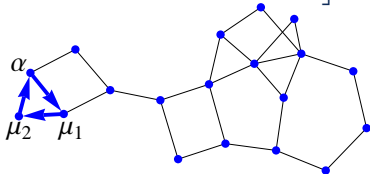
Effective vertex weights

$$[\alpha]_G =$$

$$\left[ \mathcal{I} - \sum_{\mu_1, \dots, \mu_\ell} \mathcal{M}_{\alpha\mu_\ell} [\mu_\ell]_{G \setminus \{\alpha, \mu_2, \dots, \mu_{\ell-1}\}} \cdots [\mu_2]_{G \setminus \{\alpha\}} \mathcal{M}_{\mu_2\alpha} \right]^{-1}$$

$C_{G;\alpha}$

Sum over simple cycles



# Back to Matrices

*Same, with weights*

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

$$\left(\sum_n \mathcal{M}^n\right)_{\beta\alpha} = \sum_{P_G} [\beta]_{G \setminus \{\alpha, \nu_2, \dots, \nu_p\}} \mathcal{M}_{\beta\nu_p} \cdots [\nu_2]_{G \setminus \{\alpha\}} \mathcal{M}_{\nu_2\alpha} [\alpha]_G$$

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

Effective vertex weights

$\Rightarrow$  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  $f(\mathcal{M})$  ?*

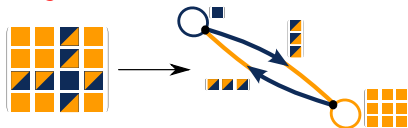
- Compute resolvent matrix  $\mathcal{R}_{\mathcal{M}}$



# 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](https://arxiv.org/abs/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

# Live Examples !

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# 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

- *MATLAB implementation*
- Works for functions of operators ! (*Chebfun style*)
- Extension to tensors, TNT algorithm

# Thank you!



Simon Thwaite



Dieter Jaksch

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