# Euler Graphs as Basis for Higher-Order Derivatives of Spectral Functions

**Sebastian Krämer**

### Definition

A *spectral function* maps a matrix to some *symmetric* function of its eigenvalues,

$$F = f \circ \mathrm{eig} : M \subseteq \mathbb{C}^{n\times n} \to \mathbb{C}, \quad f : \mathrm{eig}(M) \subseteq \mathbb{C}^n \to \mathbb{C} \;\; (\mathrm{sym}),$$

where $\mathrm{eig}$ maps to the roots with multiplicity of the characteristic polynomial of $X$.

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$$F_g(X) = \mathrm{trace}\ g(X) = \sum_{i\in[n]} g(\lambda_i), \quad f_g(x) = \sum_{i\in[n]} g(x_i), \quad g : D \subseteq \mathbb{C} \to \mathbb{C}.$$

# Spectral Functions — Introduction

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Generally,

$$f(x) = f_\sim(\underbrace{[x]}_{\text{multiset of roots in } \mathbb{C}^n/S_n}) = F(\mathrm{diag}(x)).$$

## Spectral Functions — About Symmetry

For each $X$ with distinct $\lambda := \mathrm{eig}(X)$, there is an analytic $\mathrm{eig}^\circ : U_X \to U_\lambda \subset \mathbb{C}^n$,

$$f = f^\circ \circ \mathrm{sort}_{U_\lambda}, \quad \mathrm{eig}^\circ = \mathrm{sort}_{U_\lambda} \circ \mathrm{eig}, \quad \mathrm{sort}_{U_\lambda} : \Big( \bigcup_{i \in [n]} U_{\lambda_i} \Big)^n \to U_\lambda$$

such that

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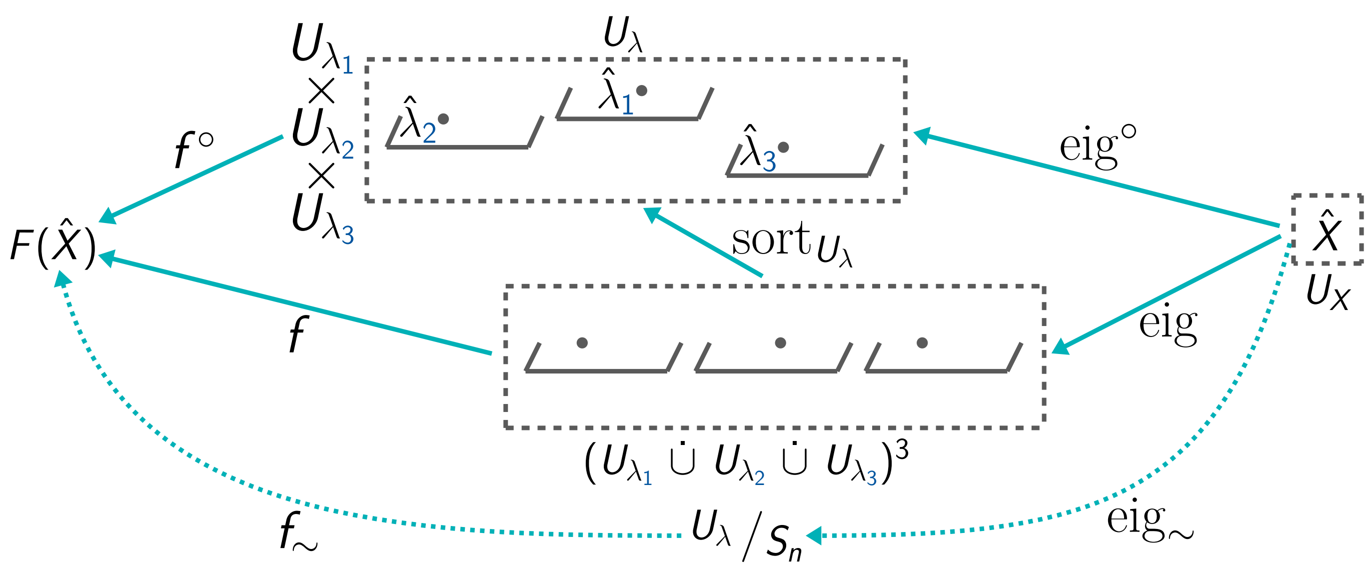

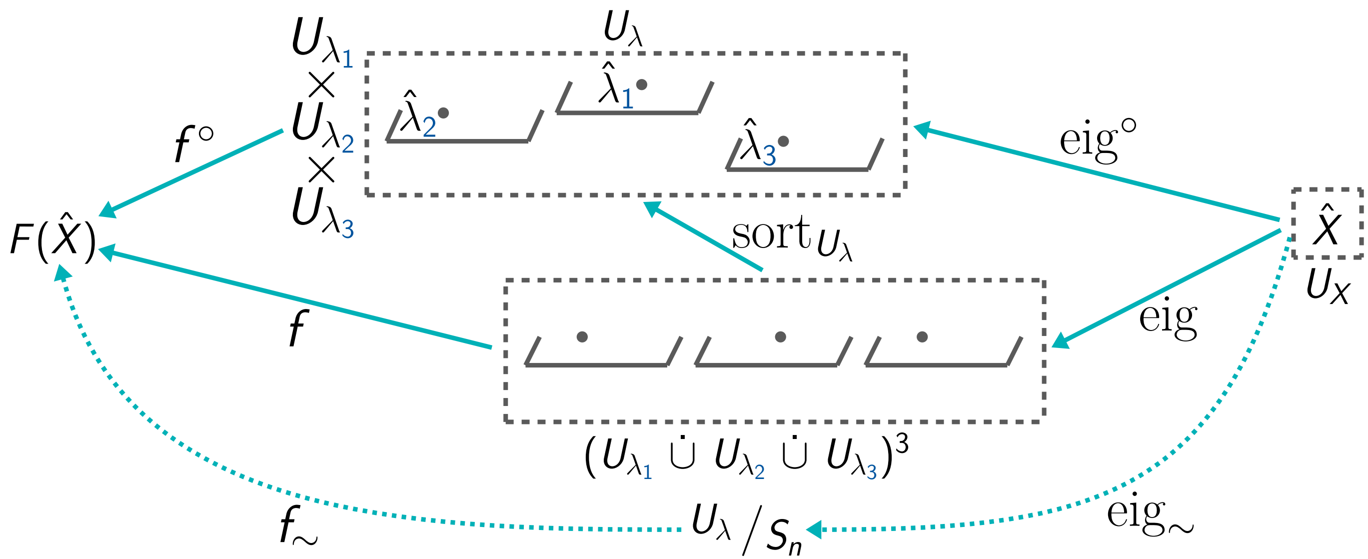


More general, for

$$\mathcal{D} = D_1 \times \ldots \times D_n \subseteq \mathbb{C}^n, \quad D_i \cap D_j := \emptyset \ \vee \ D_i = D_j$$

define

$$\mathcal{M}_\mathcal{D} := \{ T \mathrm{diag}(\lambda) T^{-1} \mid T \in \mathrm{GL}(n), \ \lambda \in \mathcal{D} \}$$

and let

$$f^\circ : \mathcal{D} \to \mathbb{C} \ (\textbf{d}\text{omain } \textbf{d}\text{ependent } \textbf{sym}), \quad F : \mathcal{M}_\mathcal{D} \to \mathbb{C}.$$

**Theorem (basically Riemann's Removable Singularity Theorem)**

*$f^\circ : \mathcal{D} \to \mathbb{C}$ analytic and d.d.sym $\Rightarrow F = f^\circ \circ \mathrm{eig}^\circ : \mathcal{M}_\mathcal{D} \to \mathbb{C}$ analytic*

**Proof**:

- $F$ is continuous on all of $\mathcal{M}_\mathcal{D}$ as $f^\circ$ and $\mathrm{eig}^\circ$ are continuous.
- Locally, around distinct eigenvalues, $\mathrm{eig}^\circ$ and $f^\circ$ are analytic.
- All other points are the root set of a polynomial in entries of $X$.
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### Example

For $\lambda_1 \in D_1$ with $D_1 \cap D_{\neq 1} = \emptyset$,

$$f^\circ : \mathcal{D} = D_1 \times D_{\neq 1} \times \ldots \times D_{\neq 1} \to \mathbb{C}, \quad f^\circ(\lambda) := \lambda_1$$

is an analytic (and d.d.sym) trace function with

$$f^\circ(\lambda) = g(\lambda_1) + \ldots + g(\lambda_n), \quad g : D_1 \cup D_{\neq 1} \to \mathbb{C},\ g(x) = \chi_{D_1}(x)x$$

Spectral functions on symmetric matrices:

**Theorem** ([J.Sylvester '85, M.Šilhavý '00])

*$f^\circ : \mathcal{D} \subset \mathbb{R}^n \to \mathbb{R}$ in $C^k$ and d.d.sym $\Rightarrow F = f^\circ \circ \mathrm{eig}^\circ : \mathcal{M}_{\mathcal{D},\,\mathrm{sym}} \to \mathbb{R}$ in $C^k$.*

**Proofs** (for $\mathcal{M}_{\mathcal{D},\,\mathrm{sym}} = \mathbb{R}^{n\times n}_{\mathrm{sym}}$, should generalize to $\mathcal{M}_{\mathcal{D}} \subseteq \mathbb{R}^{n\times n}_{\mathrm{sym}}$):

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# Spectral Functions — Inherited Differentiability

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[K. (ta)] algebraic argument based on graph recursions and removable singularities

$\downarrow$ Subsequent arguments are around matrices with distinct eigenvalues, where differentiability is given by analycity of $\mathrm{eig}^\circ$.

# Invariance based Euler Graph Relation — Diagonalization and Degree Condition

## Definition

$$\nabla^d F(X)[\Delta^{(1)}, \ldots, \Delta^{(d)}] := \frac{\partial^d}{\partial t_1 \ldots t_d} F(X + t_1 \Delta^{(1)} + \ldots + t_d \Delta^{(d)})\big|_{t_1,\ldots,t_d=0}$$

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For invariances $\mathcal{I} \in \mathrm{Lin}(\mathbb{K}^{n\times n}, \mathbb{K}^{n\times n})$ of $F$:

$$\nabla^d F(X)[\Delta^{(1)}, \ldots, \Delta^{(d)}] = \nabla^d F(\mathcal{I}(X))[\mathcal{I}(\Delta^{(1)}), \ldots, \mathcal{I}(\Delta^{(d)})]$$

In particular:

$$\nabla^d F(T\Lambda T^{-1})[\Delta^{(1)}, \ldots, \Delta^{(d)}] = \nabla^d F(\Lambda)[T^{-1}\Delta^{(1)}T, \ldots, T^{-1}\Delta^{(d)}T]$$

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## Lemma ([K. (ta)])

$$\nabla^d F(\Lambda)[e_{i_1 j_1}, \ldots, e_{i_d j_d}] = 0$$

*if there is $\ell \in [n]$ for which*

$$\deg_\ell^{(\mathrm{out})} := |\{\mu \mid i_\mu = \ell\}| \neq |\{\mu \mid j_\mu = \ell\}| =: \deg_\ell^{(\mathrm{in})}.$$

**Proof:** test $\mathcal{I}(X) := H_\ell X H_\ell^{-1}$, for $H_\ell = I + (\xi - 1)e_{\ell\ell}$ for certain root of unity $\xi$

# Invariance based Euler Graph Relation — Derivative Map $\Theta_f(\mathcal{G})$

## Definition

For a directed pseudograph (multigraph with loops allowed),

$$\mathcal{G} = \{i_1 \to j_1, \dots, i_d \to j_d\}_\#, \quad i, j \in [n]^d$$

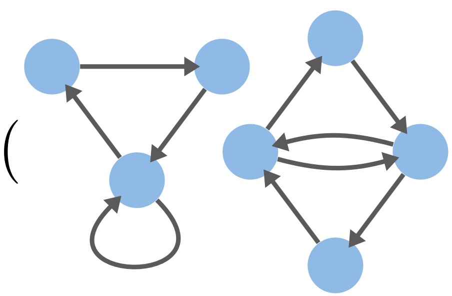
let

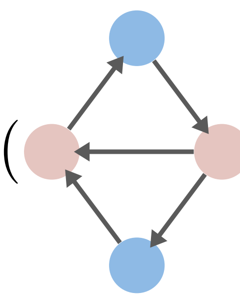
$$\Theta_f(\mathcal{G}) := \nabla^d F(\Lambda)[e_{i_1 j_1}, \dots, e_{i_d j_d}]$$

## Corollary ([K. (ta)])

*If $\mathcal{G}$ is not a union of Euler graphs, then $\Theta_f(\mathcal{G}) = 0$.*

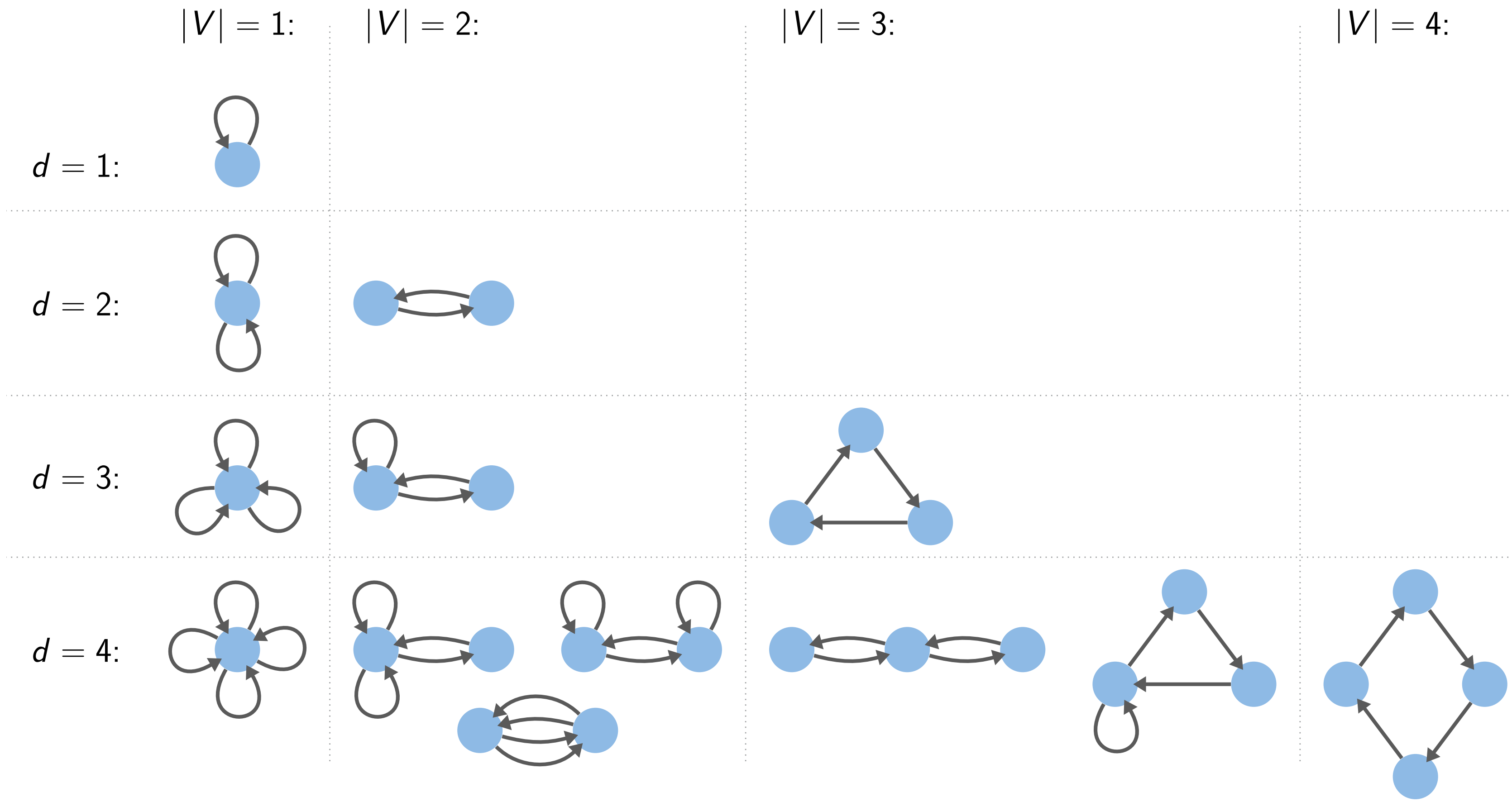
union of Euler graphs:
(in-deg $=$ out-deg)

$\Theta_f\Big($  $\Big) \in \mathbb{C}$,

$\Theta_f\Big($  $\Big) = 0$

# Invariance based Euler Graph Relation — Classes of Euler Graphs

All equivalence classes of connected Euler (pseudo-)graphs up to 4 edges:



## Invariance based Euler Graph Relation — Differentiation of Conjugation

For map of invariances $\mathcal{I} : (-\delta, \delta) \to \mathrm{Lin}(\mathbb{K}^{n\times n}, \mathbb{K}^{n\times n})$ with $\mathcal{I}_0 = \mathrm{id}$:

$$
\begin{aligned}
&- \nabla^d F(X)[\Delta^{(1)}, \dots, \Delta^{(d-1)}, \mathcal{I}_0'(X)] \\
&= \nabla^{d-1} F(X)[\mathcal{I}_0'(\Delta^{(1)}), \Delta^{(2)}, \dots] + \dots + \nabla^{d-1} F(X)[\dots, \Delta^{(d-2)}, \mathcal{I}_0'(\Delta^{(d-1)})].
\end{aligned}
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Use a basic idea of Lie group theory (turns out: generalizing [M.Šilhavý '00]),

$$
\mathcal{I}_\alpha(X) := T_\alpha X T_\alpha^{-1}, \;\; T_0 = I \quad \Rightarrow \quad \mathcal{I}_0'(E) = [T_0', E] = T_0' E - E T_0'
$$

Inside an identity matrix, set

$$
T_\alpha|_{(i,j)\times(i,j)} = \begin{pmatrix} \cos(\alpha) & \sin(\alpha) \\ -s\sin(\alpha) & \cos(\alpha) \end{pmatrix}, \quad s \in \{0, 1\}, \quad T_0' = e_{ij} - s e_{ji}.
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For $k$ and $i \neq j$:

$$[e_{ij} - s e_{ji}, \Lambda] = (\lambda_i - \lambda_j)(\boxed{e_{ij} + s e_{ji}})$$

$$[e_{ij} - s e_{ji}, \boxed{e_{jk} + s e_{kj}}\,] = \boxed{e_{ik} + s e_{ki}}, \quad [e_{ij} - s e_{ji}, e_{ji} + s e_{ij}] = (1 + s)(e_{ii} - e_{jj})$$

# Invariance based Euler Graph Relation — Recursion

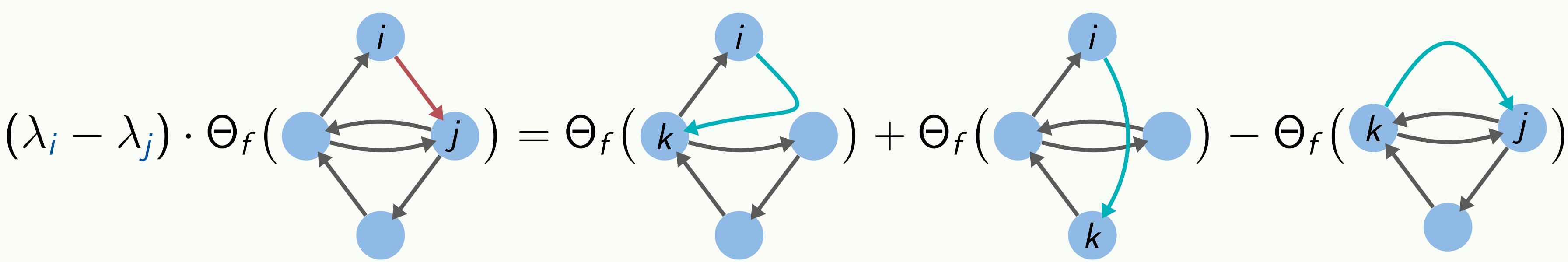
**Theorem ([K. (ta)])**

*Let* $r = i \to j \in \mathcal{G}$, $i \neq j$. *Then*

$$(\lambda_i - \lambda_j) \cdot \Theta_f(\mathcal{G}) = \sum_{e \in \mathcal{G} \,:\, e = j \to k} \Theta_f(\mathcal{G} \setminus \{r, e\} \cup \{i \to k\}) - \sum_{e \in \mathcal{G} \,:\, e = k \to i} \Theta_f(\mathcal{G} \setminus \{r, e\} \cup \{k \to j\})$$

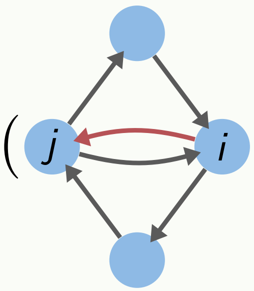
**Example**

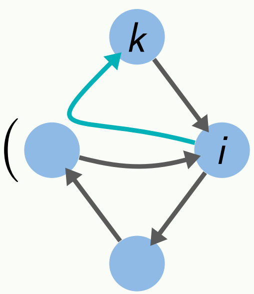
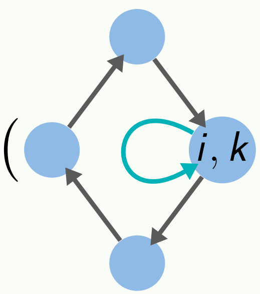
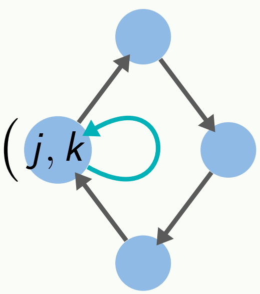
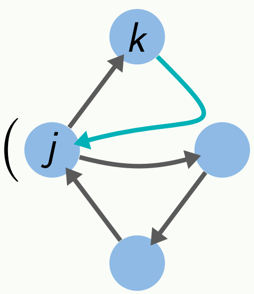
One choice of $r$:



### Example

With another choice:

$(\lambda_i - \lambda_j) \cdot \Theta_f\Big($  $\Big)$


$= \Theta_f\Big($  $\Big) + \Theta_f\Big($  $\Big) - \Theta_f\Big($  $\Big) - \Theta_f\Big($  $\Big)$


derivatives of $F$ (edges and loops) reduce to those of $f$ (loops only)
*(as in chain rule evaluation for $f^\circ \circ \mathrm{eig}^\circ$)*

# Euler Graph Relation — Differential Polynomial $\theta_1(\mathcal{G})$

## Definition

Capture derivatives in

$$\theta(\mathcal{G}) \in \mathbb{C}[\{\frac{1}{\lambda_i - \lambda_j}\}_{i\neq j}][\delta_1, \ldots, \delta_n] \quad s.t. \quad \theta(\mathcal{G})(\frac{\partial}{\partial\lambda_1}, \ldots, \frac{\partial}{\partial\lambda_n})f = \Theta_f(\mathcal{G})$$

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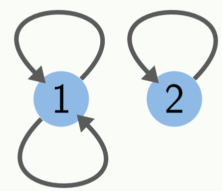
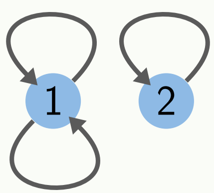
## Example

The differential polynomial of the loop-only graph

$$\theta\Big($$


$$\Big) = \delta_1^2 \delta_2$$

corresponds to

$$\Theta_f\Big($$


$$\Big) = \nabla^3 F(\Lambda)[e_{11}, e_{11}, e_{22}] = \frac{\partial^2}{\partial X_{11}^2} \frac{\partial}{\partial X_{22}} F(\Lambda) \overset{f = F \circ \mathrm{diag}}{=} \frac{\partial^2}{\partial \lambda_1^2} \frac{\partial}{\partial \lambda_2} f(\lambda)$$


Euler Graphs as Basis for Higher-Order Derivatives of Spectral Functions — Sebastian Krämer, kraemer@igpm.rwth-aachen.de — RWTH Aachen University — 08.01.26

# Euler Graph Relation — The Simple Cycle

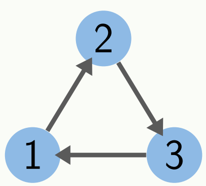
## Lemma

*For a canonical, simple cycle:*

$$\mathcal{G} = \{1 \to 2, \dots, d \to 1\}, \quad \theta(\mathcal{G}) = \sum_{i=1}^{d} \Big( \prod_{j=1,\ j \neq i}^{d} \frac{1}{\lambda_i - \lambda_j} \Big) \cdot \delta_i .$$

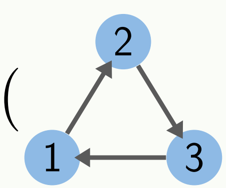
*For trace functions* $f_g(x) = g(x_1) + \ldots + g(x_n)$ *follows* $\Theta_{f_g}(\mathcal{G}) = [\lambda_1, \dots, \lambda_d] g'$.

## Example

$\theta\Big($


$\Big) = \frac{1}{\lambda_2 - \lambda_1} \frac{1}{\lambda_3 - \lambda_1} \delta_1 + \frac{1}{\lambda_1 - \lambda_2} \frac{1}{\lambda_3 - \lambda_2} \delta_2 + \frac{1}{\lambda_1 - \lambda_3} \frac{1}{\lambda_2 - \lambda_3} \delta_3$

and for trace functions,

$\Theta_{f_g}\Big($


$\Big) = [\lambda_1, \lambda_2, \lambda_3] g'$

## Lemma

*The linear part* $\theta_1(\mathcal{G}) := \theta(\mathcal{G})|_{degree\ 1\ terms}$ *is locally given via*

$$\theta_1(\mathcal{G}) = \Theta_{f_{g^{(1)}}}(\mathcal{G}) \cdot \delta_1 + \ldots + \Theta_{f_{g^{(n)}}}(\mathcal{G}) \cdot \delta_n$$

*where*

$$f_{g^{(i)}}(\lambda) = \lambda_i, \qquad g^{(i)}(x) = \chi_{U_{\lambda_i}}(x) \cdot x, \qquad F_{g^{(i)}}(X) = \mathrm{eig}_i^\circ(X)$$

*where* $\chi_{U_{\lambda_i}}$ *are the indicator functions on sufficiently small neighborhoods of* $\lambda_i$

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The graph recursion holds true for

- derivatives $\Theta_f(\mathcal{G})$,
- differential polynomial $\theta(\mathcal{G})$,
- its linear part $\theta_1(\mathcal{G})$,

for distinct eigenvalues $\lambda$ (though generalizes in certain ways to all)

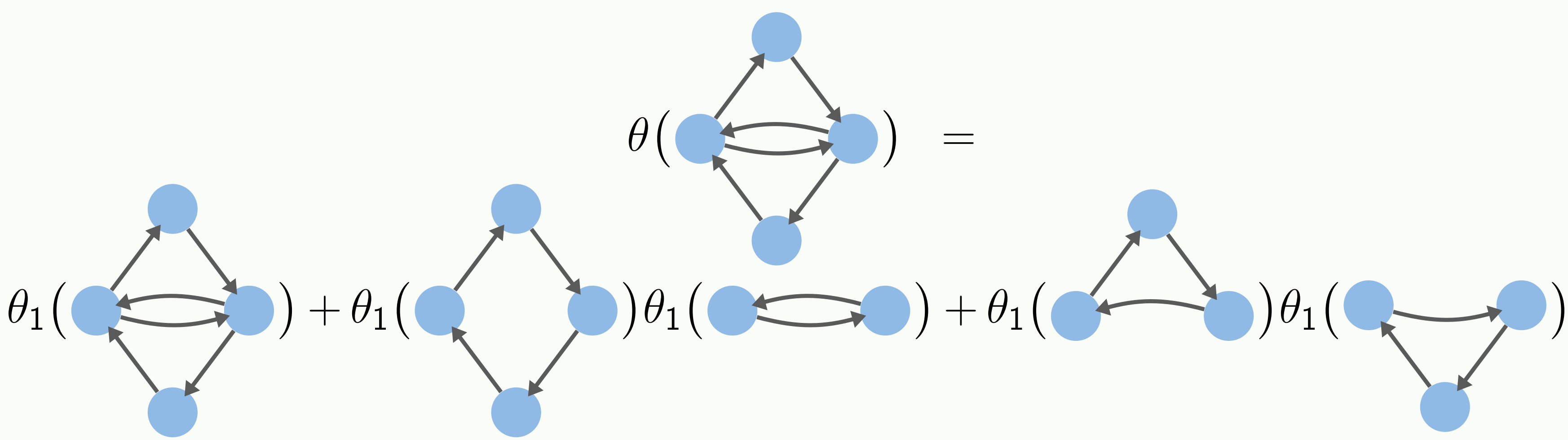
# Euler Graph Relation — Factorization of Differential Polynomial

## Theorem ([K. (ta)])

*Factorization via,*

$$\theta(\mathcal{G}) = \sum_{\bigcup_\nu \mathrm{Euler}_\nu = \mathcal{G}} \prod_\nu \theta_1(\mathrm{Euler}_\nu)$$

## Example



### Theorem ([K. (ta)])

*Factorization via,*

$$\theta(\mathcal{G}) = \sum_{\bigcup_\nu \mathrm{Euler}_\nu = \mathcal{G}} \prod_\nu \theta_1(\mathrm{Euler}_\nu)$$

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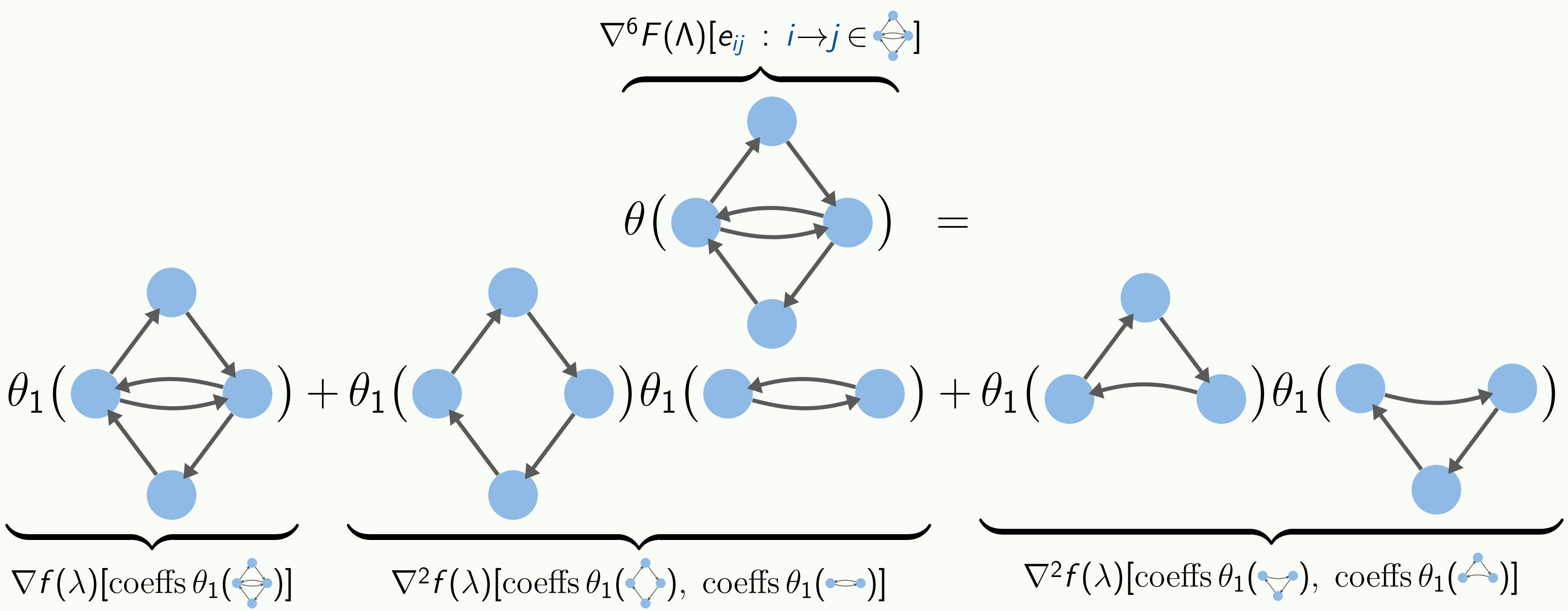

## Corollary ([K. (ta)])

*Let $i \neq j$. If $\lambda_i = \lambda_j$, then*

$$\sum_{e \in \mathcal{G}\,:\, e = j \to k} \Theta_f(\mathcal{G} \setminus \{j \to k\} \cup \{i \to k\}) = \sum_{e \in \mathcal{G}\,:\, e = k \to i} \Theta_f(\mathcal{G} \setminus \{k \to i\} \cup \{k \to j\}).$$

(At least) for trace functions, we can augment $i := n + 1 \notin \mathcal{G}$:

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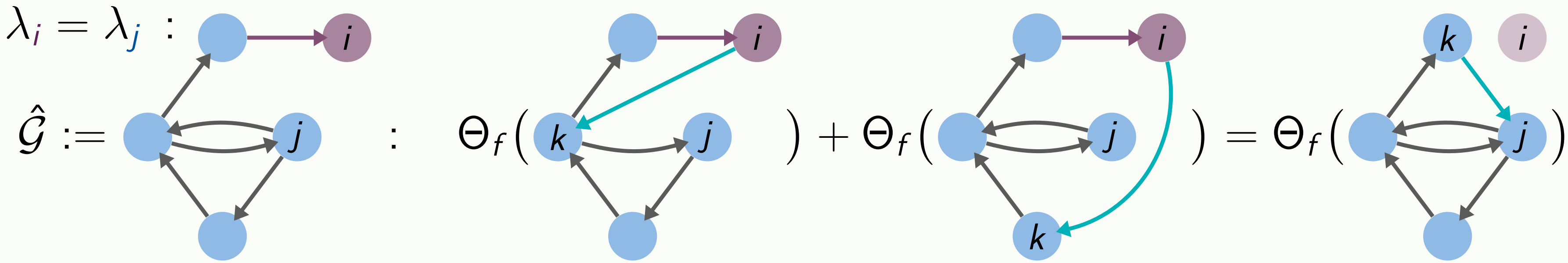

## Inflation to Euler Circuits — Vertex Exchange

### Corollary ([K. (ta)])

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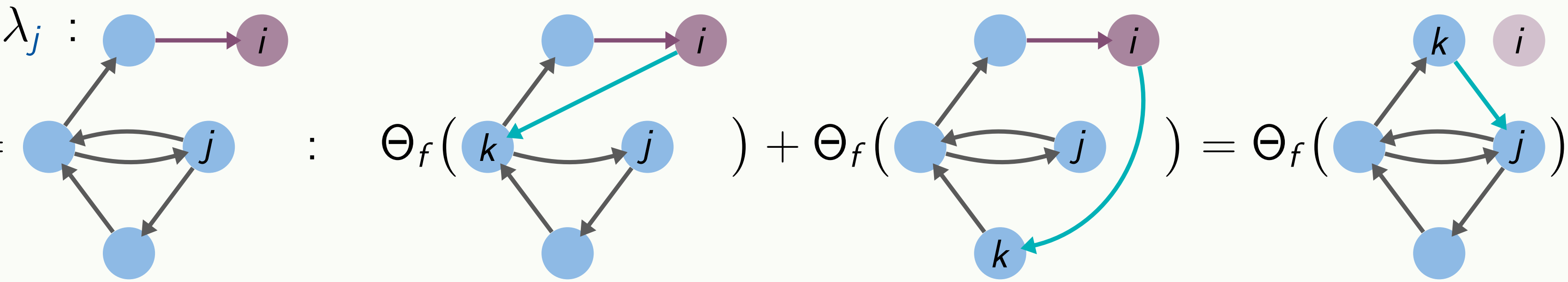
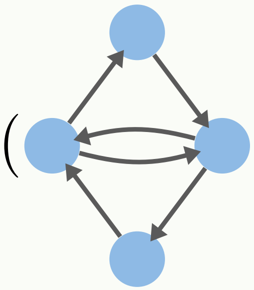
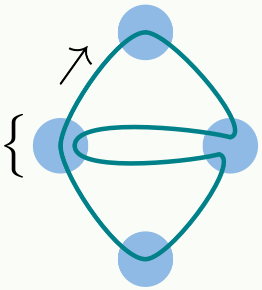
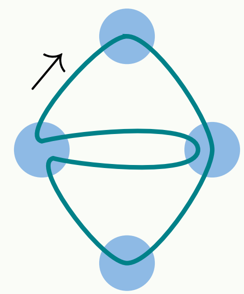
$\lambda_i = \lambda_j$ :

$\hat{\mathcal{G}} :=$

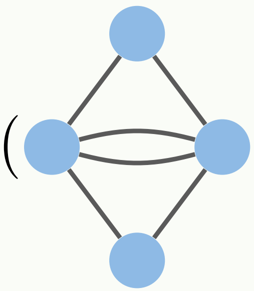


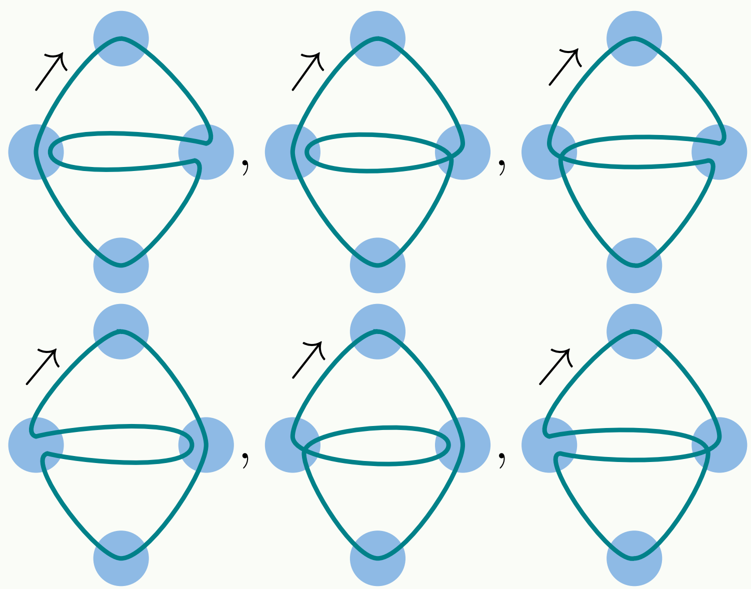

Iterating this encounts Euler circuits! $=: \mathfrak{C}_1(\mathcal{G})$

## Example

$\mathfrak{C}_1\Big($  $\Big) = \Big\{$   $\Big\}$

## Example

$\mathfrak{E}_1\big($  $\big) = \{ \swarrow \} \,\dot\cup\, \{ \nearrow \}$

$\{ \nearrow \} = \{$  $\}$

**Theorem** ([K. (ta)])

*Let*

$$\mathcal{G} = \{i_1 \to j_1, \ldots, i_d \to j_d\} \quad s.t. \quad \Theta_f(\mathcal{G}) = \nabla^d F(\Lambda)[e_{i_1 j_1}, \ldots, e_{i_d j_d}]$$

*For trace functions,*

$$\Theta_{f_g}(\mathcal{G}) = |\mathfrak{C}_1(\mathcal{G})| \cdot [\lambda_{i_1}, \ldots, \lambda_{i_d}]g'$$

*For the linear part of the differential polynomial,*

$$\theta_1(\mathcal{G}) = |\mathfrak{C}_1(\mathcal{G})| \cdot \sum_{k=1}^{n} [\lambda_{i_1}, \ldots, \lambda_{i_d}]\chi_{U_{\lambda_k}} \cdot \delta_k$$

**Proof:** inflate graph to sums of simple cycles / use $\theta_1(\mathcal{G})$ relation

- $\Theta_{f_g}(\mathcal{G})$ identity valid for all $\lambda$ (under Hermite scheme)
- $\theta_1(\mathcal{G})$ identity **not** compatible with coinciding eigenvalues (but uses $\chi'_{U_{\lambda_k}}(\lambda_k) = 0$)

## Theorem

*For trace functions $F_g$ (as for instance also by [F.Hansen '06, N.Highem '08])*

$$\nabla^d F_g(\Lambda)[\Delta^{(1)}, \ldots, \Delta^{(d)}] = \frac{1}{d} \sum_{m \in [n]^d} [\lambda_m] g' \cdot \sum_{\pi \in S_d} \Delta^{(\pi(1))}_{m_1 m_2} \cdot \Delta^{(\pi(2))}_{m_2 m_3} \cdots \Delta^{(\pi(d))}_{m_d m_1}$$

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*as well as (generalizing [H.S.Sendov '07] to non-symmetric matrices)*

$$\nabla^d F_g(\Lambda)[\Delta^{(1)}, \dots, \Delta^{(d)}] = \sum_{m \in [n]^d} [\lambda_m] g' \cdot \sum_{\tau \in S_d : \tau \text{ cyclic}} \prod_{\mu \in [d]} \Delta^{(\mu)}_{m_\mu, m_{\tau(\mu)}}.$$

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## Corollary

*For an isolated eigenvalue* $E_1^{(0)} := \lambda_1$,

$$F(X) := \mathrm{eig}_1^\circ(\Lambda + t\Delta) = E_1^{(0)} + \sum_{d\in\mathbb{N}} t^d E_1^{(d)}$$

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*Then* $E_1^{(1)} = \Delta_{11}$ *and (as also by* [T.Kato '95]*)*

$$E_1^{(d)} = \frac{1}{d!}\nabla^d \mathrm{eig}_1^\circ(\Lambda)[\Delta, \ldots, \Delta] = \frac{1}{d}\sum_{m\in[n]^d} \Delta_{m_1 m_2}\ldots\Delta_{m_d m_1}\cdot[\lambda_m]\chi_{U_{\lambda_1}}$$

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$$= \sum_{\substack{p\in\{0,\dots,d-1\}^{d-1}\\ s.t.\ p_1+\dots+p_{d-1}=d-1}} (-1)^{1+|\{\mu\,|\,p_\mu=0\}|}\cdot e_1^T\Delta\Big(\prod_{\mu\in[d-1]} S^{p_\mu}\cdot\Delta\Big)e_1$$

*with* $S^0 := e_{11}$ *and* $S^q := \mathrm{diag}(0, \frac{1}{\lambda_1-\lambda_2},\dots,\frac{1}{\lambda_1-\lambda_n})^q$, $q\in\mathbb{N}$.

**Proof:** combinatorics and symmetric polynomial expression for $[\lambda_m]\chi_{U_{\lambda_1}}$
[T.Kato '95] contour-integral around expanded trace-resolvant

Use

$$\Theta_{f_{\log}}(\mathcal{G}_{\mathrm{undir}})(\mathbf{1}) = \pm|\mathfrak{C}_1(\mathcal{G}_{\mathrm{undir}})|, \quad \mathrm{trace}\,\log = \log\det, \quad \mathcal{X} := \begin{pmatrix} 1 & X_{12} & \dots & X_{1n} \\ X_{12} & 1 & \dots & X_{2n} \\ \vdots & \vdots & & \vdots \\ X_{1n} & X_{2n} & \dots & 1 \end{pmatrix}$$

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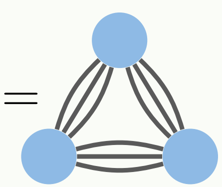
### Example

$\mathcal{G} =$  : $\log\det(\mathcal{X}) \xrightarrow{\left(\frac{\partial^3}{\partial X_{12}^3} u\right)|_{X_{12}=0}} \dfrac{-4X_{13}X_{23}(4X_{13}^2X_{23}^2 - 3X_{13}^2 - 3X_{23}^2 + 3)}{(X_{13}^2 + X_{23}^2 - 1)^3}$

$$\xrightarrow{\left(\frac{\partial^3}{\partial X_{23}^3} u\right)|_{X_{23}=0}} \frac{-48X_{23}(2X_{23}^2 + 3)}{(X_{23} - 1)^3(X_{23} + 1)^3} \xrightarrow{\left(\frac{\partial^3}{\partial X_{13}^3} u\right)|_{X_{13}=0}} 3168 = |\mathfrak{C}_1(\mathcal{G})|.$$

# Reverse Applications — Counting Euler Circuits in Undirected Graphs

Use

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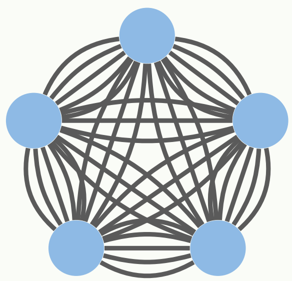
$\mathfrak{C}_1\Bigg($  $\Bigg) = 15414462840434593737631334400000$

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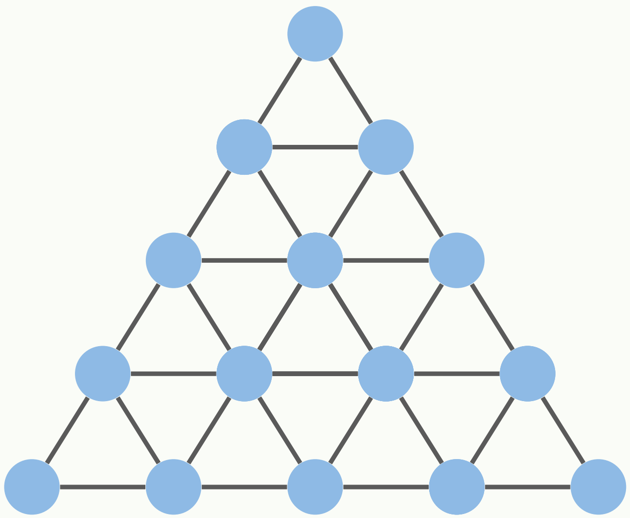
$\mathfrak{C}_1($  $) = 30480384$

## Singular Value Functions —

### Definition

An *sv function* maps a matrix to a symmetric **and even** function of its singular values,

$$F = f \circ \mathrm{sv} : M \subseteq \mathbb{R}^{n\times n} \to \mathbb{R}, \quad f : \mathrm{sv}(M) \subseteq \mathbb{R}^n \to \mathbb{R} \text{ (sym \& even)}$$

- orthogonally invariant: $F(U\Sigma V^T) = F(\Sigma)$ for $U, V \in \mathrm{O}(n)$

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- here, not every Euler circuit yields same summand
- for graph-independent expressions for even trace functions, may also use

$$\nabla^d F_g^{(\mathrm{sv})}(\Sigma)[\Delta^{(1)}, \ldots, \Delta^{(d)}] = \frac{1}{2} \nabla^d F_g^{(\mathrm{eig})}(\mathrm{diag}(-\Sigma, \Sigma))[\Omega^{(1)}, \ldots, \Omega^{(d)}]$$

$$\Omega^{(\mu)} := \frac{1}{2} \begin{pmatrix} -\Delta^{(\mu)} - \Delta^{(\mu)T} & -\Delta^{(\mu)} + \Delta^{(\mu)T} \\ \Delta^{(\mu)} - \Delta^{(\mu)T} & \Delta^{(\mu)} + \Delta^{(\mu)T} \end{pmatrix}$$

## Open ends of this approach:

- simplify derivatives at low-rank and non-symmetric matrices
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## Thank you for your attention!

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## Slide overview: