Asymptotic Spectral Analysis of Markov Chains with Rare Transitions: A Graph-Algorithmic Approach

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Outline

- The problem
- Backgrounds and motivations
- The essence of the main results
- Optimal W-graphs and asymptotic eigenvalues
- The construction of optimal W-graphs
- Typical transitions graphs and the rediscovery of Freidlin's cycles
- Asymptotic estimates of eigenvectors
- What if optimal W-graphs are not unique?
- An application to LJ75 network
- Conclusion

Continuous-time Markov chains with exponentially small transition rates

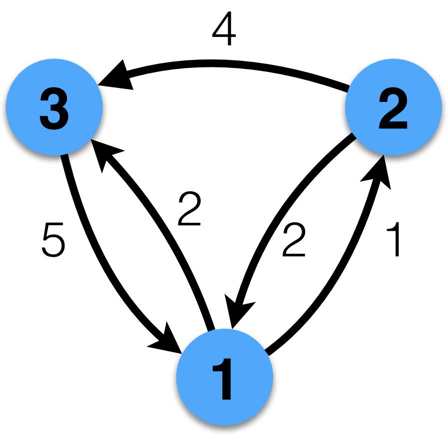
- Consider jump processes with dynamics described by generator matrices L.
    - The transition rate from state i to state j (for $i \neq j$):

$$L_{ij} \asymp \exp\left(-U_{ij}/\varepsilon\right), \text{ or } \lim_{\varepsilon \to 0} \varepsilon \ln L_{ij} = -U_{ij}$$

    - The escape rates from state i: $-L_{ii} = \sum_{j \neq i} L_{ij}$
- Such a Markov chain can be represented, up to exponential order, by a weighted directed graph $G(S, A, U)$.
- Assume all Markov chains under consideration have finite states and are irreducible.
- **Do not assume reversibility**, i.e. the process is not required to satisfy the *detailed balance* equation $\pi_i L_{ij} = \pi_j L_{ji}$, where π is the invariant distribution.

A simple example

$$L \asymp \begin{bmatrix} -(e^{-1/\varepsilon} + e^{-2/\varepsilon}) & e^{-1/\varepsilon} & e^{-2/\varepsilon} \\ e^{-2/\varepsilon} & -(e^{-2/\varepsilon} + e^{-4/\varepsilon}) & e^{-4/\varepsilon} \\ e^{-5/\varepsilon} & 0 & -e^{-5/\varepsilon} \end{bmatrix}$$

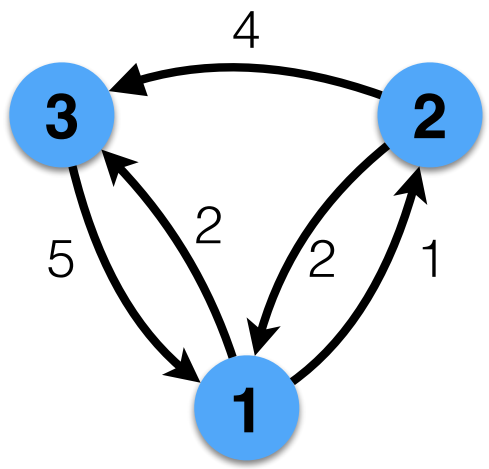


The problem: spectral decomposition of the generator L

- **Goal**: Estimate the eigenvalues and eigenvectors of the generator L.
- **Main story**: How such a problem can be translated into optimization problems over graphs, how we solve it efficiently, and what are the associated physical interpretations.

A simple example

$$L \asymp \begin{bmatrix} -(e^{-1/\varepsilon}+e^{-2/\varepsilon}) & e^{-1/\varepsilon} & e^{-2/\varepsilon} \\ e^{-2/\varepsilon} & -(e^{-2/\varepsilon}+e^{-4/\varepsilon}) & e^{-4/\varepsilon} \\ e^{-5/\varepsilon} & 0 & -e^{-5/\varepsilon} \end{bmatrix}$$



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Theoretical backgrounds

Markov chain approximation in the Freidlin-Wentzell regime

Freidlin and Wentzell developed the Large Deviation Theory in their study of random perturbations of dynamical systems. They showed that the long-term behavior of a diffusion processes X_t generated by the SDE

$$dX_t = b(X_t)dt + \sqrt{2\varepsilon}dW_t$$

can be effectively modeled by a Markov chain whose states correspond to the stable attractors of $\dot{x}_t = b(x_t)$.

To estimate the exponential factor U_{ij}, they described the large deviations of X_t from the deterministic trajectory $\dot{x}_t = b(x_t)$ by introducing the *action functional*

$$I_T(\phi) = \frac{1}{2}\int_0^T \|\dot{\phi}(t) - b(\phi(t))\|^2 dt$$

defined on the space of absolute continuous paths ϕ, and the *quasi-potential*

$$U_{ij} = \inf\{I_T(\phi) \mid \phi(0) \in K_i,\ \phi(T) \in K_j,\ T > 0\}$$

which characterizes the difficulty of the passage from attractor i to attractor j. Here K_i and K_j are two compact sets corresponding to the two distinct attractors.

Long-term dynamics and spectral decomposition

The long-term dynamics of such a Markov chain is largely governed by the spectral properties of the generator.

- $\lambda_0 = 0$ is a simple eigenvalue, the corresponding right eigenvector is $\varphi_0 = \mathbf{1}$ (every entry equals to 1), and the left eigenvector is $\psi_0 = \pi$ (the invariant distribution).
- Let $\lambda_1, \lambda_2, \cdots, \lambda_{n-1}$ be the nonzero eigenvalues of $-L$ s.t. $|\lambda_1| \leq |\lambda_2| \leq \cdots \leq |\lambda_{n-1}|$, then $\mathrm{Re}(\lambda_k) > 0$, and they are exponentially small.
- In the case that all λ_k's are real and distinct, one can write the *probability distribution* $p(t)$, governed by the Fokker-Planck equation $dp^T/dt = p^T L$, in the following form

$$p(t) = \pi + \sum_{k=1}^{n-1} e^{-\lambda_k t} p(0)^T \varphi_k \psi_k.$$

Let $t(\varepsilon)$ be a timescale satisfying $\lim_{\varepsilon \to 0} \varepsilon \ln \lambda_{\hat{k}}^{-1} < \lim_{\varepsilon \to 0} \varepsilon \ln t(\varepsilon) < \lim_{\varepsilon \to 0} \varepsilon \ln \lambda_{\hat{k}-1}^{-1}$, for some $\hat{k}$ between 2 and $n-1$, then

$$\lim_{\varepsilon \to 0} \lambda_k t(\varepsilon) = \begin{cases} 0, & 1 \leq k \leq \hat{k}-1, \\ \infty, & \hat{k} \leq k \leq n-1. \end{cases} \text{ Hence, } \lim_{\varepsilon \to 0} p(t(\varepsilon)) = \lim_{\varepsilon \to 0} \left(\pi + \sum_{k=1}^{\hat{k}-1} (p(0)^T \phi_k) \psi_k \right).$$

That is to say, the kth eigen-component of the probability distribution $p(t)$ will not be significant after the timescale surpasses λ_k^{-1}.

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The essence of the main results

- There is a sequence of exponentially increasing characteristic timescales which are associated with two types of events: exits and rotations.

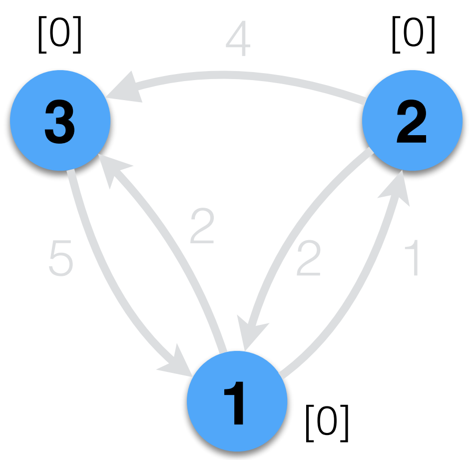
- Exits from metastable* classes occur on timescales that are asymptotically equivalent to the inverses of eigenvalues. Asymptotic estimates of eigenvalues can be expressed in terms of optimal W-graphs (Wentzell).

- Rotations within metastable classes can be described by Freidlin's cycles. Through propagating weights on vertices, we can estimate quasi-invariant distributions on metastable classes, which can then be used to construct asymptotic eigenvectors.

- Optimal W-graphs and Freidlin's cycles can be unified under the hierarchy of typical transitions graphs, which we can construct in a single sweep.

*In physics, metastability is a stable state of a dynamical system other than the system's state of least energy. The system will spontaneously leave any other state of higher energy to eventually reach (after a sequence of transitions) the least energetic state.

A simple example to demonstrate the main results

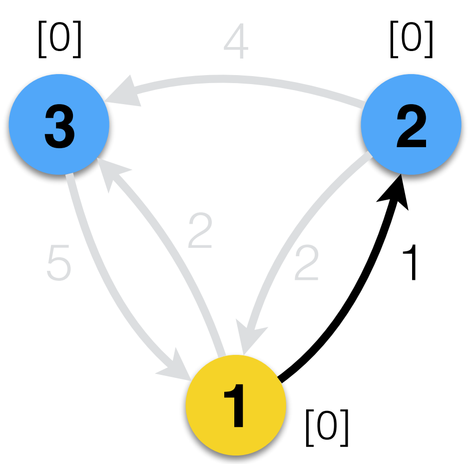


$t = 0$

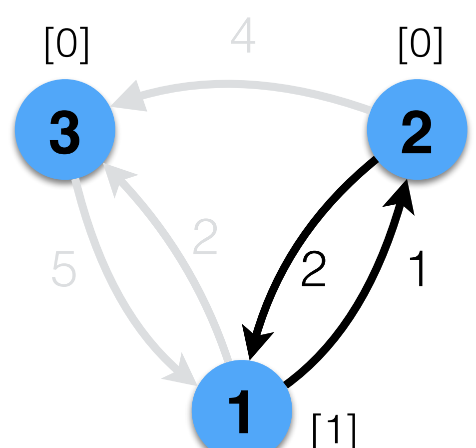
$$L \asymp \begin{bmatrix} -(e^{-1/\varepsilon} + e^{-2/\varepsilon}) & e^{-1/\varepsilon} & e^{-2/\varepsilon} \\ e^{-2/\varepsilon} & -(e^{-2/\varepsilon} + e^{-4/\varepsilon}) & e^{-4/\varepsilon} \\ e^{-5/\varepsilon} & 0 & -e^{-5/\varepsilon} \end{bmatrix}$$

$$0 = \lambda_0 < \lambda_1 < \lambda_2 \text{ are eigenvalues of } -L.$$

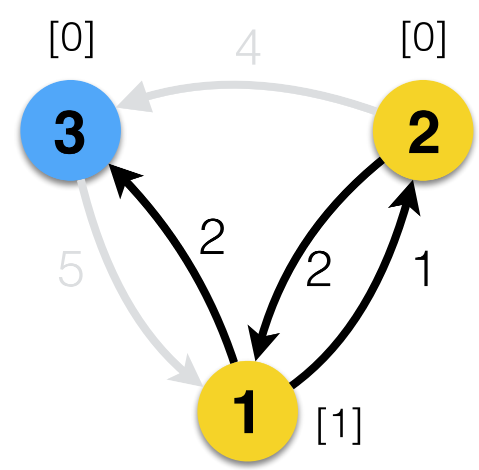
The hierarchy of typical transitions graphs



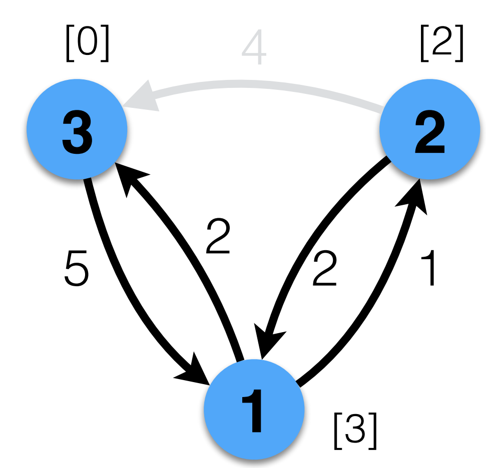
$t \asymp e^{1/\varepsilon}$



$t \asymp e^{2/\varepsilon}$



$t \asymp e^{3/\varepsilon}$



$t \asymp e^{5/\varepsilon}$

Exit: $1 \to 2$
Rate: $L_{12} \asymp e^{-1/\varepsilon} \asymp \lambda_2$
Right: $\varphi_2 \asymp [1, 0, 0]^T$
Left: $\psi_2 \asymp [1, -1, 0]^T$

Rotation: $1 \leftrightarrow 2$
Rate: $e^{-2/\varepsilon}$
$\pi_{1,2} \asymp [e^{-1/\varepsilon}, 1]^T$

Exit: $\{1, 2\} \to 3$
Rate: $\pi_{1,2}(1) L_{13} \asymp e^{-3/\varepsilon} \asymp \lambda_1$
Right: $\varphi_1 \asymp [1, 1, 0]^T$
Left: $\psi_1 \asymp [e^{-1/\varepsilon}, 1, -1]^T$

Rotation: $\{1 \leftrightarrow 2\} \leftrightarrow 3$
Rate: $e^{-5/\varepsilon}$
$\pi_{1,2,3} \asymp [e^{-3/\varepsilon}, e^{-2/\varepsilon}, 1]^T$

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Wentzell's result on asymptotic estimates of eigenvalues

In 1972, Wentzell established the following asymptotic estimates of the real parts of eigenvalues in terms of optimal W-graphs.

Theorem 1. *(Wentzell, 1972) Let* $0, -\lambda_1, -\lambda_2, \cdots, -\lambda_{n-1}$ *be the eigenvalues of a generator matrix* L *with off-diagonal entries* $L_{ij} \asymp \exp(-U_{ij}/\varepsilon)$*, indexed so that* $0 < |\lambda_1| \le |\lambda_2| \le \cdots \le |\lambda_{n-1}|$*. Then as* $\varepsilon \to 0$*,*

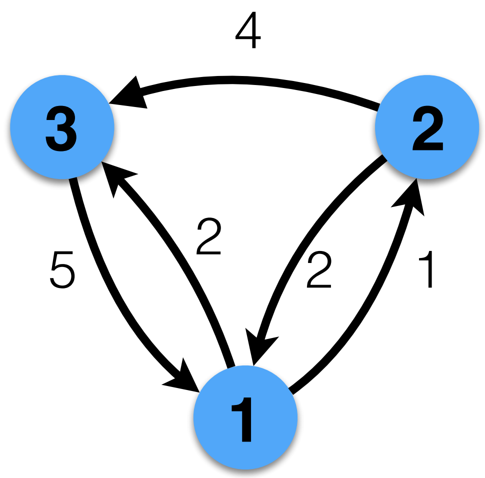
$$Re(\lambda_k) \asymp \exp(-\Delta_k/\varepsilon),$$

where $\Delta_k = \sum_{(i \to j) \in g_k^*} U_{ij} - \sum_{(i \to j) \in g_{k+1}^*} U_{ij}$

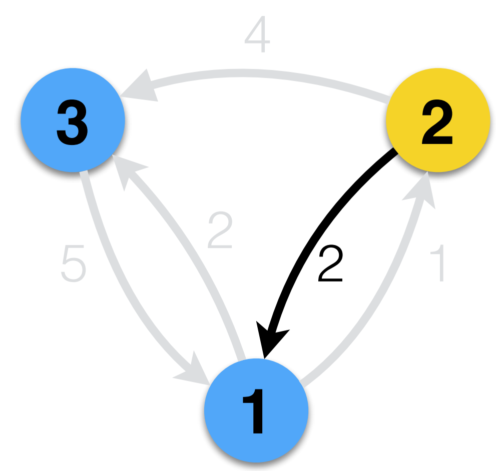
- g_k^* is an optimal W-graph with k sinks, which is a minimum spanning forest of G with k in-trees. In each in-tree, there is a unique directed path from any vertex to the root (sink), Hence, each non-sink vertex emits exactly one arrow and there are no cycles.
- Reversibility is not required in Wentzell's result.

Theorem 1 implies that $\Delta_1 \ge \Delta_2 \ge \cdots \ge \Delta_{n-1}$.

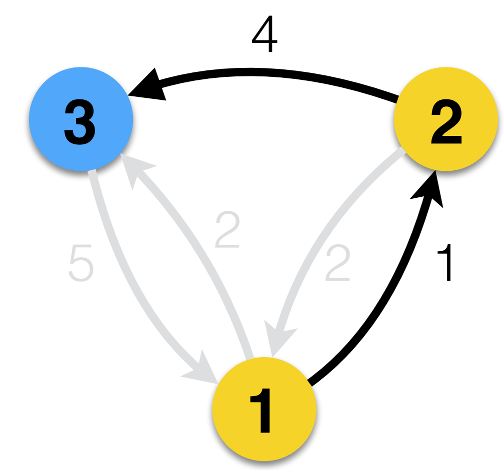
A simple example to demonstrate Wentzell's result



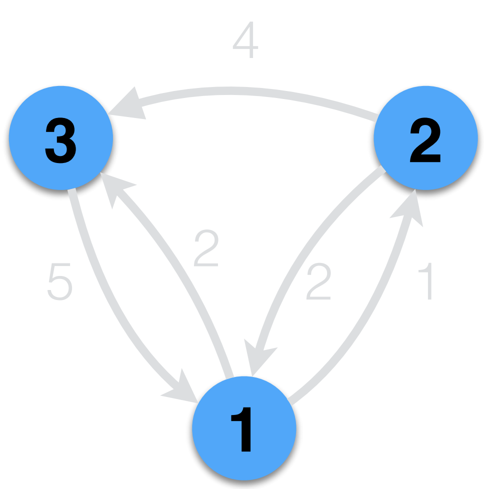
G



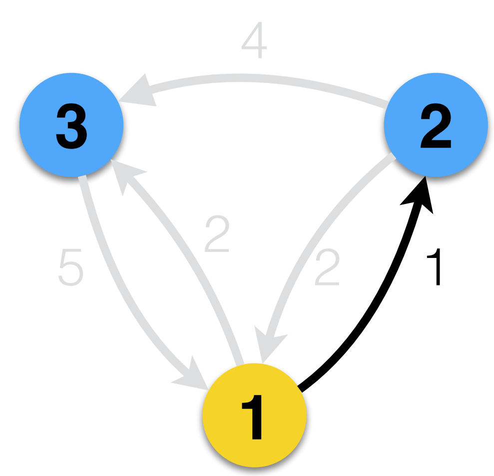
A W-graph with 2 sinks



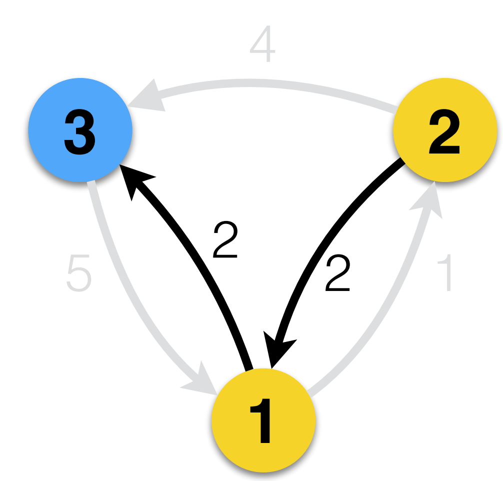
A W-graph with 1 sink



g_3^*



g_2^*



g_1^*

$$\mathcal{V}(g_3^*) = 0 \xrightarrow[\lambda_2 \asymp \exp(-1/\varepsilon)]{\Delta_2 = 1} \mathcal{V}(g_2^*) = 1 \xrightarrow[\lambda_1 \asymp \exp(-3/\varepsilon)]{\Delta_1 = 3} \mathcal{V}(g_1^*) = 4$$

Refined asymptotic estimates of eigenvalues

Assumption: All optimal W-graphs g_k^* are unique (*nondegenerate*).

Under the above Assumption, Δ_k's are strictly decreasing, i.e., $\Delta_1 > \Delta_2 > \cdots > \Delta_{n-1}$. Hence, for ε sufficiently small, all λ_k's are real and distinct. In addition, if pre-factors of transition rates are known, then refined estimates of eigenvalues can be obtained.

Theorem 2. *Assume all optimal W-graphs are unique. Let* $0 > -\lambda_1 > -\lambda_2 > \cdots > -\lambda_{n-1}$ *be the eigenvalues of a generator matrix* L *with off-diagonal entries* $L_{ij} = \kappa_{ij} \exp(-U_{ij}/\varepsilon)(1+o(1))$*. Then*

$$\lambda_k = \alpha_k \exp(-\Delta_k/\varepsilon)\,(1+o(1))\,,$$

where $\Delta_k = \sum_{(i\to j)\in g_k^*} U_{ij} - \sum_{(i\to j)\in g_{k+1}^*} U_{ij}$*, and* $\alpha_k = \dfrac{\prod_{(i\to j)\in g_k^*} \kappa_{ij}}{\prod_{(i\to j)\in g_{k+1}^*} \kappa_{ij}}$.

The key to proving Theorem 2 lies in identifying the connection between the coefficients of the characteristic polynomial of L and the sets of W-graphs with the corresponding number of sinks.

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How to construct optimal W-graphs?

- Prove a weak nested property of optimal graphs.
- Borrow the ideas of contraction and expansion of cycles from Chu-Liu/Edmonds' algorithm for finding optimal branching (the directed analog of the minimum spanning tree problem).

Chu-Liu/Edmonds' algorithm can be used to find the optimal W-graph with one sink. However, we want the full hierarchy of optimal W-graphs, in other words, we need to solve a sequence of combinatoric optimization problems. The beauty here is that when the ideas of contraction and expansion fuse with the weak nested property, constructing the hierarchy of optimal W-graphs can be done in a single sweep, from bottom up.

- The algorithm is *conceptually recursive*. (However, it can be implemented more efficiently in a non-recursive fashion.)
  - Every time a cycle is encountered during the construction, it gets contracted into a super-vertex, resulting in a coarser Markov chain represented by a smaller graph.
  - The optimal W-graphs of the smaller graph can then be expanded recursively to obtain the optimal W-graphs of the original graph G.

Weak nested property of optimal W-graphs

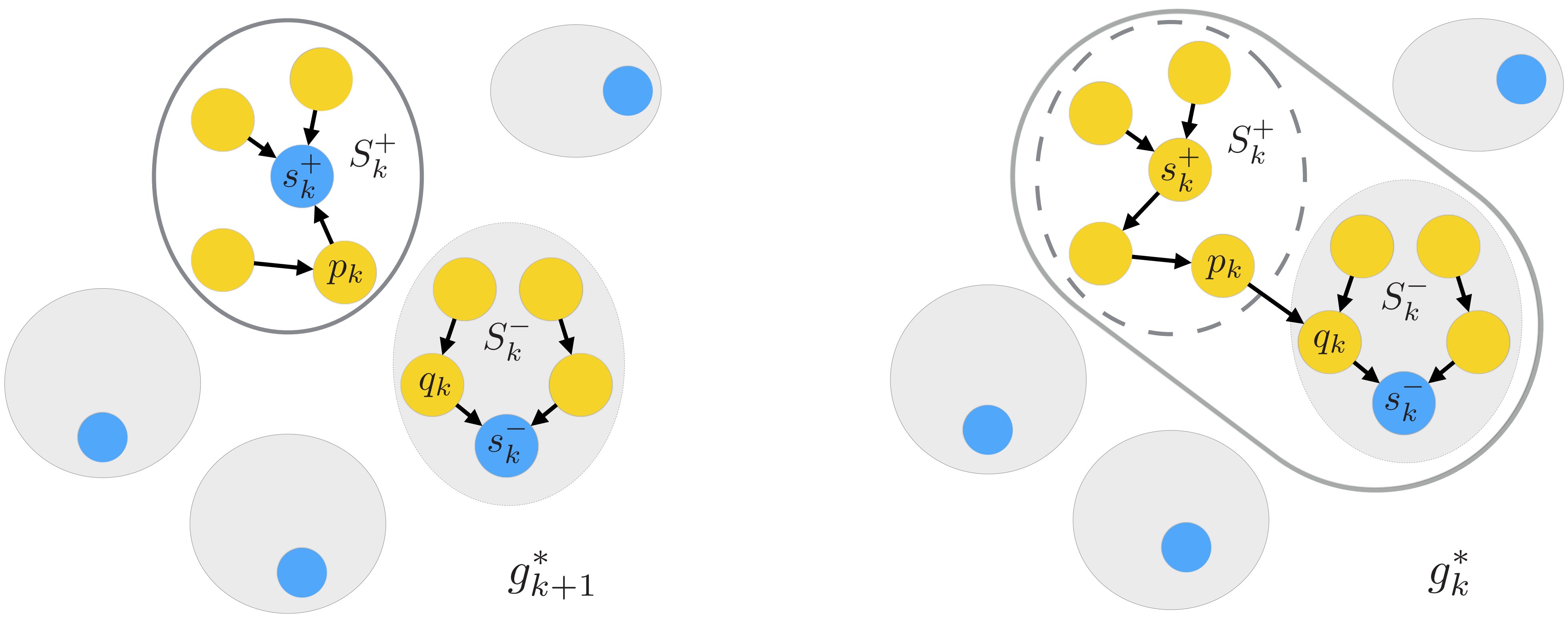
Theorem 3. *Assume all optimal W-graphs are unique. The collection of optimal W-graphs* $\{g_k^*\}_{k=1}^n$ *is a hierarchy satisfying the following properties:*

(i) There is a unique component S_k^+ *of* g_{k+1}^* *whose sink* s_k^+ *is not a sink of* g_k^*.

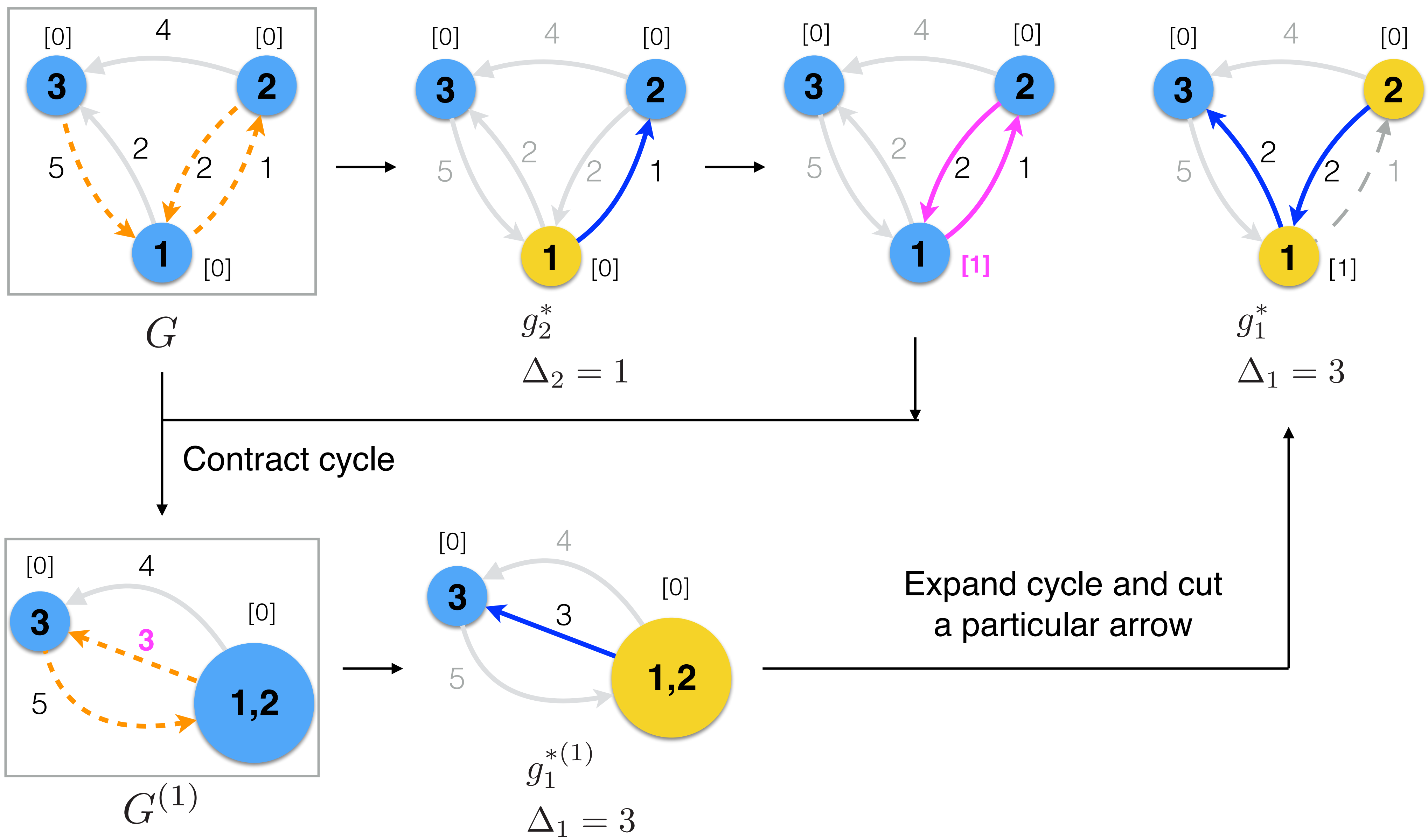
(ii) All the arrows of g_k^* *with tails not in* S_k^+ *are inherited from* g_{k+1}^**, however, arrows with tails in* S_k^+ *can be different.*

(iii) In g_k^**, there is a single arrow* $(p_k \to q_k)$ *with tail* p_k *in* S_k^+ *of* g_{k+1}^* *and head* q_k *in another component* S_k^- *of* g_{k+1}^*.

The main technique involved in proving Theorem 3 is the swapping of subsets of arrows.



A simple example to demonstrate the algorithm



- $U^1_{\{1,2\},3} = v_1 + U_{13} = (\max_{\{1\leftrightarrow 2\}} U - U_{12}) + U_{13} = (2-1) + 2 = 3$
  Exit from $\{1 \leftrightarrow 2\}$ via $1 \to 3$ with rate $e^{-U^1_{\{1,2\},3}/\varepsilon} \asymp \pi_{1,2}(1) L_{13}$
- $U^2_{\{1,2\},3} = v_2 + U_{23} = (\max_{\{1\leftrightarrow 2\}} U - U_{21}) + U_{23} = (2-2) + 4 = 4$
  Exit from $\{1 \leftrightarrow 2\}$ via $2 \to 3$ with rate $e^{-U^2_{\{1,2\},3}/\varepsilon} \asymp \pi_{1,2}(2) L_{23}$

Quasi-invariant distribution on the cycle {1, 2}

$$L_{\{1\leftrightarrow 2\}} \asymp \begin{bmatrix} -e^{-U_{12}/\varepsilon} & e^{-U_{12}/\varepsilon} \\ e^{-U_{21}/\varepsilon} & -e^{-U_{21}/\varepsilon} \end{bmatrix}$$

$$\begin{aligned}
\pi_{1,2} &\asymp \left[\frac{e^{U_{12}/\varepsilon}}{e^{U_{12}/\varepsilon} + e^{U_{21}/\varepsilon}}, \frac{e^{U_{21}/\varepsilon}}{e^{U_{12}/\varepsilon} + e^{U_{21}/\varepsilon}} \right]^T \\
&\asymp \left[e^{-(\max_{\{1\leftrightarrow 2\}} U - U_{12})/\varepsilon}, e^{-(\max_{\{1\leftrightarrow 2\}} U - U_{21})/\varepsilon} \right]^T \\
&\asymp \left[e^{-v_1/\varepsilon}, e^{-v_2/\varepsilon} \right]^T
\end{aligned}$$

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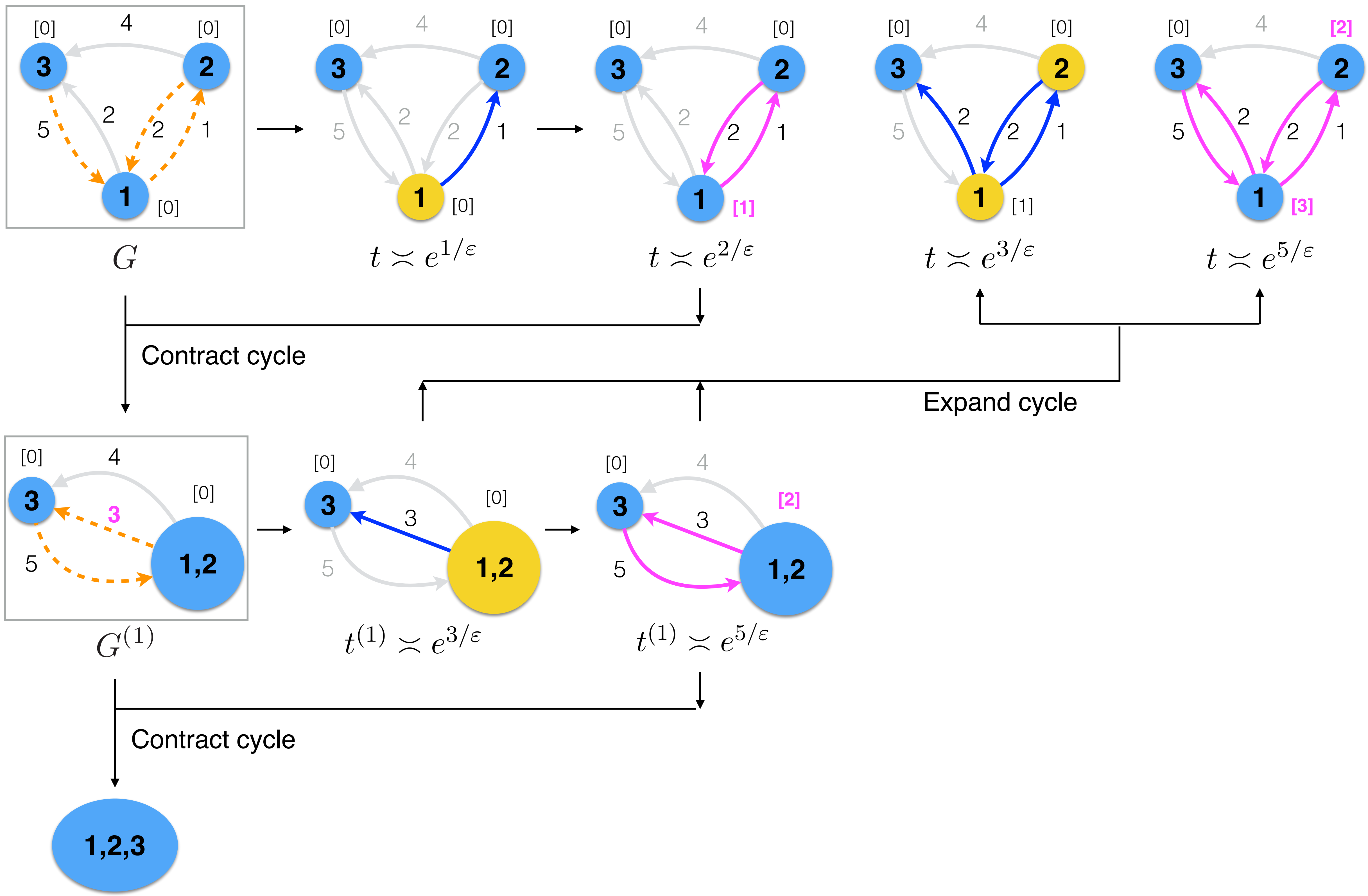
What if we preserve all arrows in expansions?

- The result is a (strongly nested) hierarchy of graphs consisting of typical transitions (exponentially dominating) for each characteristic timescale.
- The closed communicating classes (recurrent) in each typical transitions graph are the metastable classes for the corresponding timescale.
- Weights on the vertices can be used to construct quasi-invariant distributions on the metastable classes.
- The cycles encountered during the constructions coincide with Friedlin's cycles. Freidlin's cycles are constructed rank by rank, with cycles of the same rank partitioning the state-space, while they do not necessarily respect the order of timescales.

Typical transitions graphs



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Result on asymptotic estimates of eigenvectors

Theorem 4. *Assume all optimal W-graphs are unique. In the typical transitions graph corresponding to the characteristic timescale just prior to λ_k^{-1}, identify the two metastable classes $C_k^+ \subset S_k^+$ and $C_k^- \subset S_k^-$, such that the component S_k^+ collapses into S_k^- on the timescale λ_k^{-1}. Let $\mu_{C_k^+}$ and $\mu_{C_k^-}$ be the quasi-invariant distributions, respectively. Define $\tilde{\psi}_k$ and $\tilde{\varphi}_k$ as follows ($k = 1, \cdots, n-1$):*

$$\tilde{\varphi}_k(i) = \begin{cases} 1, & i \in S_k^+, \\ 0, & i \in S \setminus S_k^+, \end{cases} \qquad \tilde{\psi}_k(i) = \begin{cases} \mu_{C_k^+}(i) \asymp e^{-v_i/\varepsilon}, & i \in C_k^+, \\ -\mu_{C_k^-}(i) \asymp -e^{-v_i/\varepsilon}, & i \in C_k^-, \\ 0, & i \in S \setminus (C_k^+ \cup C_k^-). \end{cases}$$

Then

(i) $\tilde{\psi}_k^T \tilde{\varphi}_{k'} = \mathbf{1}_{\{k=k'\}} + o(1)$;

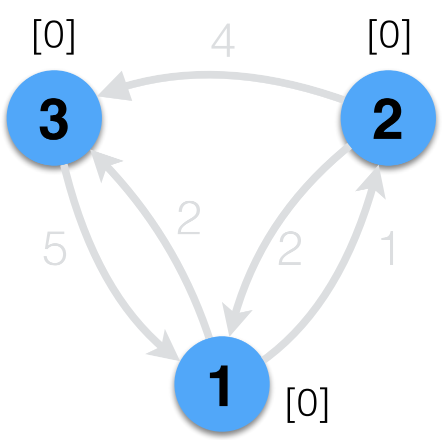
(ii) *(a)* $\tilde{\psi}_k^T L \tilde{\varphi}_k = -\lambda_k (1 + o(1))$;

(b) *If* $k > k'$, *then* $\lim\limits_{\varepsilon \to 0} \varepsilon \ln(|\tilde{\psi}_k^T L \tilde{\varphi}_{k'}|) < -\Delta_k$;

(c) *If* $k < k'$, *then* $\lim\limits_{\varepsilon \to 0} \varepsilon \ln(|\tilde{\psi}_k^T L \tilde{\varphi}_{k'}|) \leq -\Delta_{k'}$.

The proof of Theorem 4 makes use of the weak nested property of optimal W-graphs.

A simple example to demonstrate the asymptotic eigenvectors

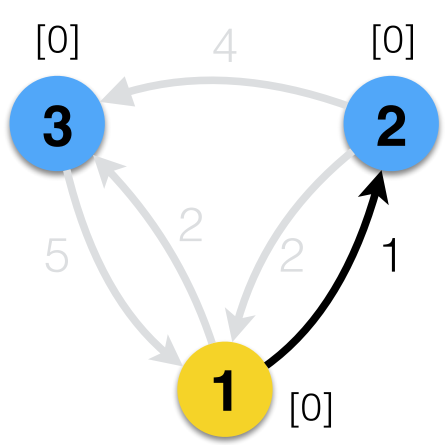


$t = 0$

$S_2^+ = \{1\}$, $C_2^+ = \{1\}$
$S_2^- = \{2\}$, $C_2^- = \{2\}$

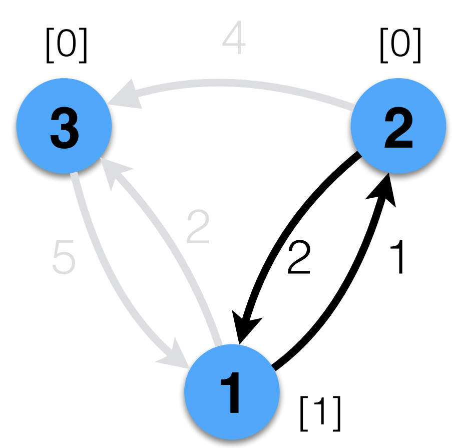
$$L \asymp \begin{bmatrix} -(e^{-1/\varepsilon} + e^{-2/\varepsilon}) & e^{-1/\varepsilon} & e^{-2/\varepsilon} \\ e^{-2/\varepsilon} & -(e^{-2/\varepsilon} + e^{-4/\varepsilon}) & e^{-4/\varepsilon} \\ e^{-5/\varepsilon} & 0 & -e^{-5/\varepsilon} \end{bmatrix}$$

$0 = \lambda_0 < \lambda_1 < \lambda_2$ are eigenvalues of $-L$.



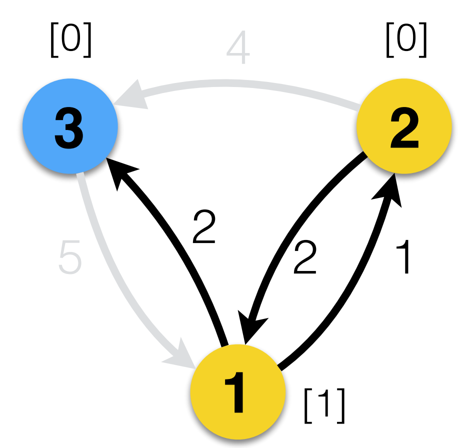
$t \asymp e^{1/\varepsilon}$

Exit: $1 \to 2$
$\lambda_2 \asymp e^{-1/\varepsilon}$
Right: $\varphi_2 \asymp [1, 0, 0]^T$
Left: $\psi_2 \asymp [1, -1, 0]^T$



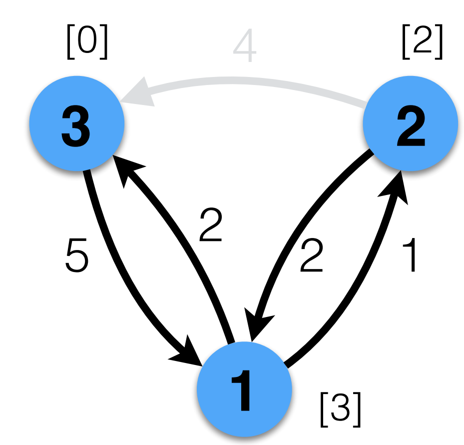
$t \asymp e^{2/\varepsilon}$

$S_1^+ = \{1, 2\}$, $C_1^+ = \{1, 2\}$
$S_1^- = \{3\}$, $C_1^- = \{3\}$



$t \asymp e^{3/\varepsilon}$

Exit: $\{1, 2\} \to 3$
$\lambda_1 \asymp e^{-3/\varepsilon}$
Right: $\varphi_1 \asymp [1, 1, 0]^T$
Left: $\psi_1 \asymp [e^{-1/\varepsilon}, 1, -1]^T$



$t \asymp e^{5/\varepsilon}$

Rotation: $\{1 \leftrightarrow 2\} \leftrightarrow 3$
$\pi_{1,2,3} \asymp [e^{-3/\varepsilon}, e^{-2/\varepsilon}, 1]^T \asymp \pi$

Compare the asymptotic estimates with numerical results

$$L \asymp \begin{bmatrix} -(e^{-1/\varepsilon}+e^{-2/\varepsilon}) & e^{-1/\varepsilon} & e^{-2/\varepsilon} \\ e^{-2/\varepsilon} & -(e^{-2/\varepsilon}+e^{-4/\varepsilon}) & e^{-4/\varepsilon} \\ e^{-5/\varepsilon} & 0 & -e^{-5/\varepsilon} \end{bmatrix}$$

Asymptotic estimates

$$\lambda \asymp \begin{bmatrix} e^{-1/\varepsilon} & e^{-3/\varepsilon} & 0 \end{bmatrix}$$

$$\varphi \asymp \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\psi \asymp \begin{bmatrix} 1 & e^{-1/\varepsilon} & e^{-3/\varepsilon} \\ -1 & 1 & e^{-2/\varepsilon} \\ 0 & -1 & 1 \end{bmatrix}$$

Numerical results (set $e^{-1/\varepsilon} = 0.1$)

$$\lambda = \begin{bmatrix} 0.1192 & 0.0009 & 0 \end{bmatrix}$$

$$\varphi = \begin{bmatrix} 0.9958 & -0.6755 & 0.5774 \\ -0.0913 & -0.7374 & 0.5774 \\ -0.0001 & 0.0073 & 0.5774 \end{bmatrix}$$

$$\psi = \begin{bmatrix} 0.7357 & -0.0618 & 0.0009 \\ -0.6745 & -0.6742 & 0.0090 \\ -0.0612 & 0.7360 & 1.0000 \end{bmatrix}$$

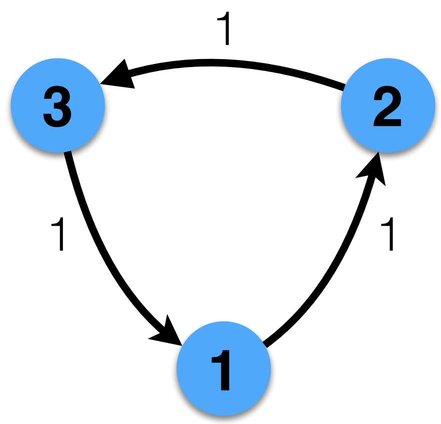
Outline

What if optimal W-graphs are not unique?

- Good news: We can still construct asymptotic estimates of eigenvalues from the hierarchy of typical transitions graphs. An event of exit is associated with a decrease in the number of connected components.

- Bad news: When there is symmetry, asymptotic estimates of eigenvectors can no longer be constructed simply by using the weights on vertices.

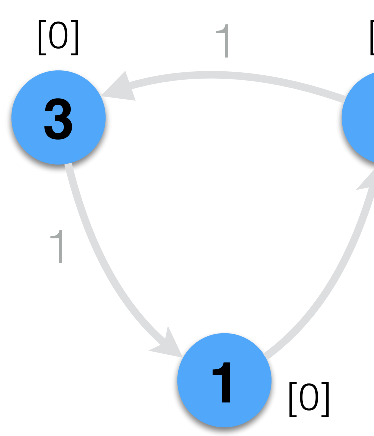
A simple example with symmetry



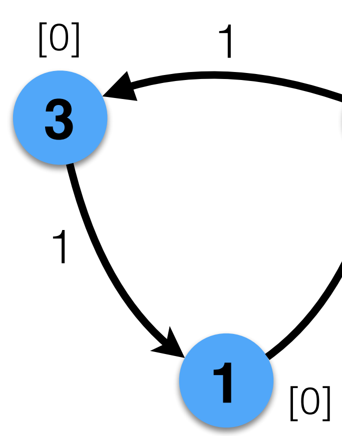
G

$$L \asymp \begin{bmatrix} -e^{-1/\varepsilon} & e^{-1/\varepsilon} & 0 \\ 0 & -e^{-1/\varepsilon} & e^{-1/\varepsilon} \\ e^{-1/\varepsilon} & 0 & -e^{-1/\varepsilon} \end{bmatrix}$$

$0, \lambda_1, \lambda_2$ are the eigenvalues of $-L$.



$t = 0$



$t \asymp e^{1/\varepsilon}$

From $t = 0$ to $t \asymp e^{1/\varepsilon}$, the number of connected components in the typical transitions graphs decreases by two, thus releasing two eigenvalues, and $\mathrm{Re}(\lambda_{1,2}) \asymp e^{-1/\varepsilon}$.

Numerical results (set $e^{-1/\varepsilon} = 0.1$)

$$L = \begin{bmatrix} -0.1000 & 0.1000 & 0 \\ 0 & -0.1000 & 0.1000 \\ 0.1000 & 0 & -0.1000 \end{bmatrix}$$

$$\lambda = \begin{bmatrix} 0.0000 + 0.0000i & 0.1500 + 0.0866i & 0.1500 - 0.0866i \end{bmatrix}$$

$$\varphi = \begin{bmatrix} -0.5774 + 0.0000i & 0.5774 + 0.0000i & 0.5774 + 0.0000i \\ -0.5774 + 0.0000i & -0.2887 - 0.5000i & -0.2887 + 0.5000i \\ -0.5774 + 0.0000i & -0.2887 + 0.5000i & -0.2887 - 0.5000i \end{bmatrix}$$

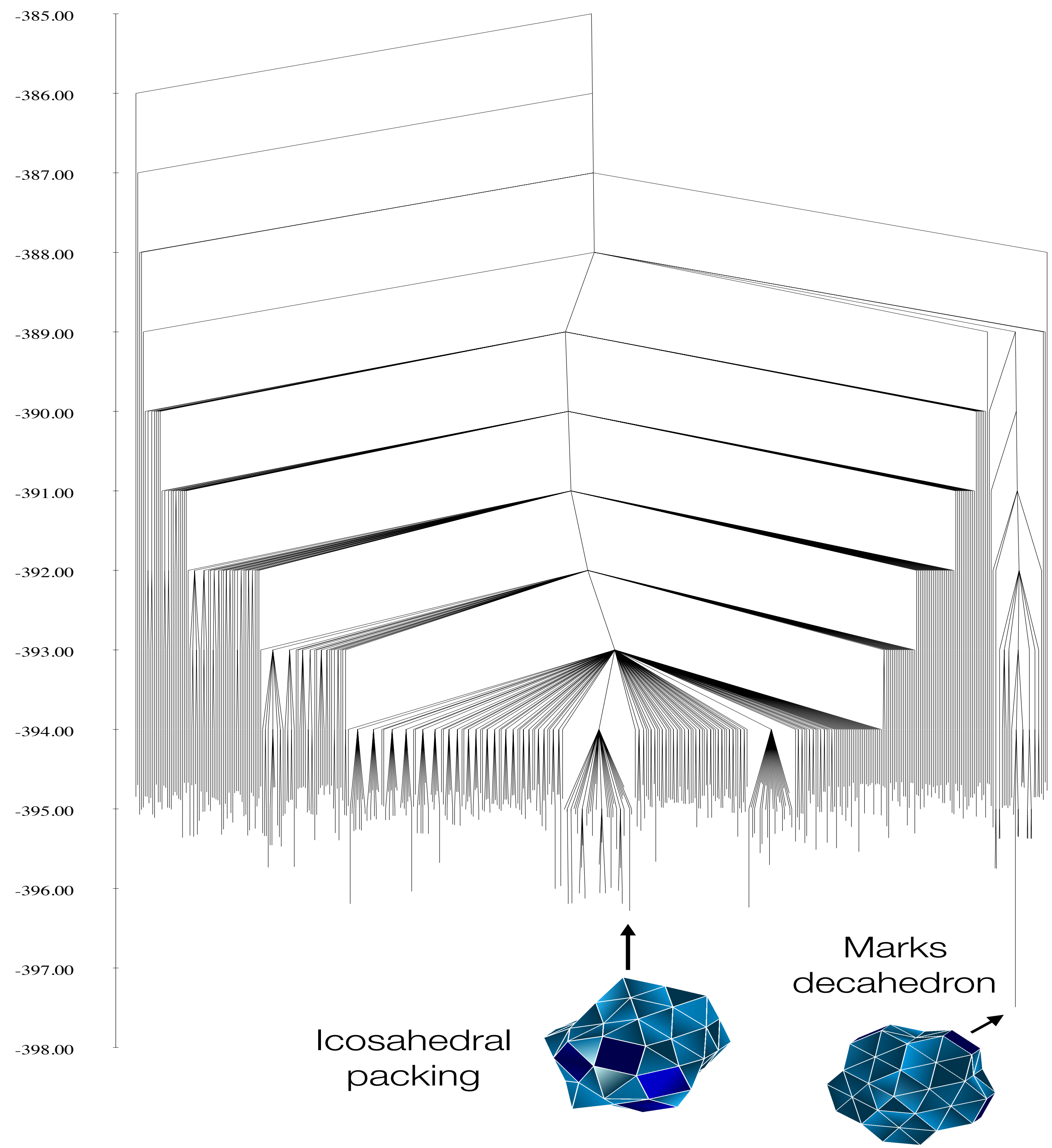
$$\psi = \begin{bmatrix} -0.5774 + 0.0000i & 0.2887 - 0.5000i & 0.2887 + 0.5000i \\ -0.5774 + 0.0000i & -0.5774 + 0.0000i & -0.5774 + 0.0000i \\ -0.5774 + 0.0000i & 0.2887 + 0.5000i & 0.2887 - 0.5000i \end{bmatrix}$$

Outline

- The problem
- Backgrounds and motivations
- The essence of the main results
- Optimal W-graphs and asymptotic eigenvalues
- The construction of optimal W-graphs
- Typical transitions graphs and the rediscovery of Freidlin's cycles
- Asymptotic estimates of eigenvectors
- What if optimal W-graphs are not unique?
- An application to LJ75 network
- Conclusion

Lennard-Jones cluster of 75 atoms

- Lennard-Jones clusters have become a much-studied test system for global optimization methods designed for configurational problems.
- Lennard-Jones potential energy plays a key role in determining the stability of crowed and highly branched molecules such as proteins.
- The energy landscape of Lennard-Jones cluster of 75 atoms* has a double funnel structure. The global minimum is a Marks decahedron, lying at the bottom of the deep and narrow funnel. The second lowest minimum is icosahedral, locating at the wide and shallow funnel. This causes the system to enter the wider icosahedral on relaxation from high energy.



*The data for the LJ 75 network were kindly provided by Professor D. Wales, Cambridge University, UK.

Zero-temperature asymptotic analysis of the LJ75 Network

- Vertices in the LJ75 network correspond to local potential minima, while arrows represent transition states (potential barriers) between them.

- The largest connected component containing the two deepest minima has 169,523 vertices and 452,754 arrows.

- Transition rates:

$$L_{ij} = \frac{O_i(\Pi_+\nu_i)^{1/2}}{O_{ij}(\Pi_+\nu_{ij})^{1/2}} \exp\left(-\frac{V_{ij}-V_i}{T}\right). \qquad \text{Here } U_{ij} = V_{ij} - V_i \text{ and } \varepsilon = T.$$

∗ O_i and O_{ij} are the point group orders of the local minimum i and the transition state (ij) separating the local minima i and j respectively, while $\Pi_+\nu_i$ and $\Pi_+\nu_{ij}$ are the products of the positive eigenvalues of the Hessian matrices of the potential V at the minimum i and the transition state (ij) respectively, and V_i and V_{ij} are the values of the potential at i and (ij) respectively.

- The process of physical interest is the transition from the second lowest minimum to the global minimum at very low temperature. We apply the proposed algorithm to

  (1) estimate the asymptotic exit rate;

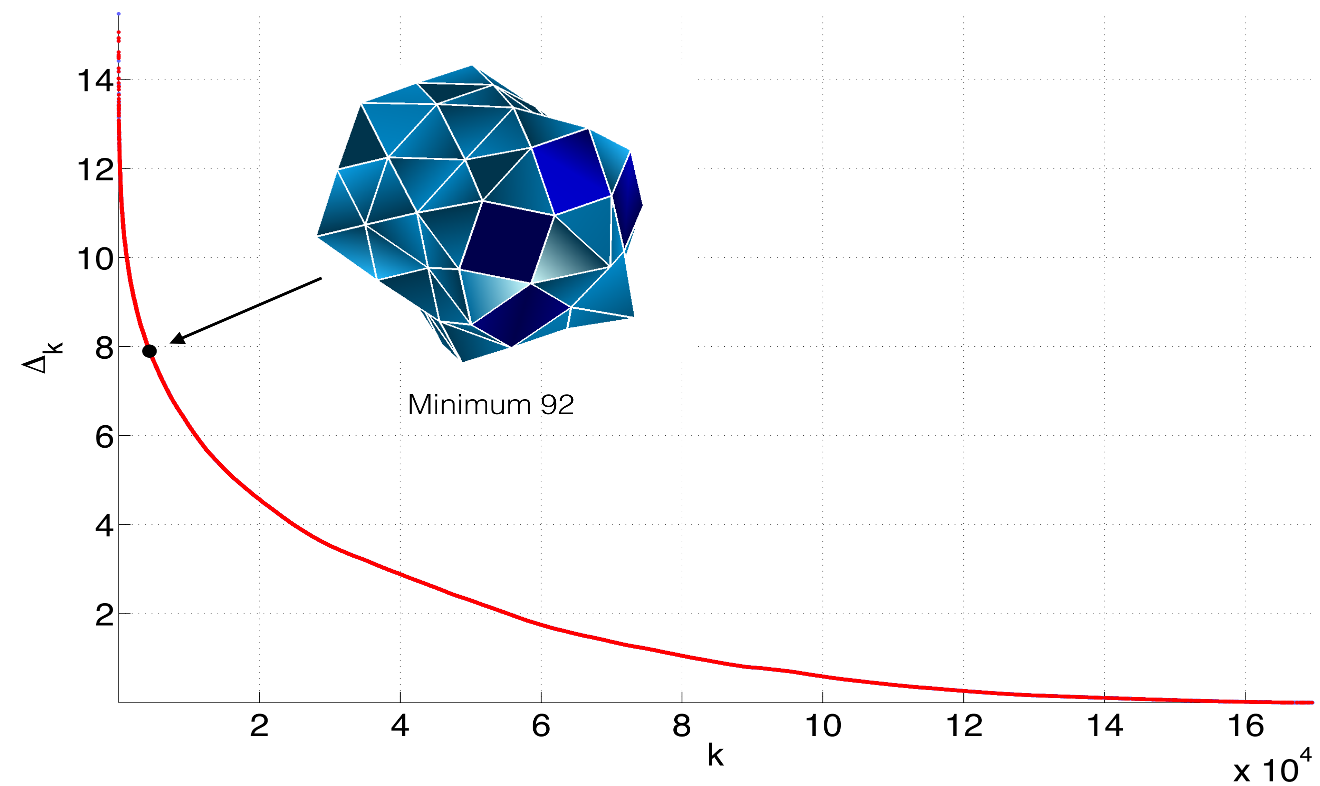
  (2) identify the most likely zero-temperature transition path.

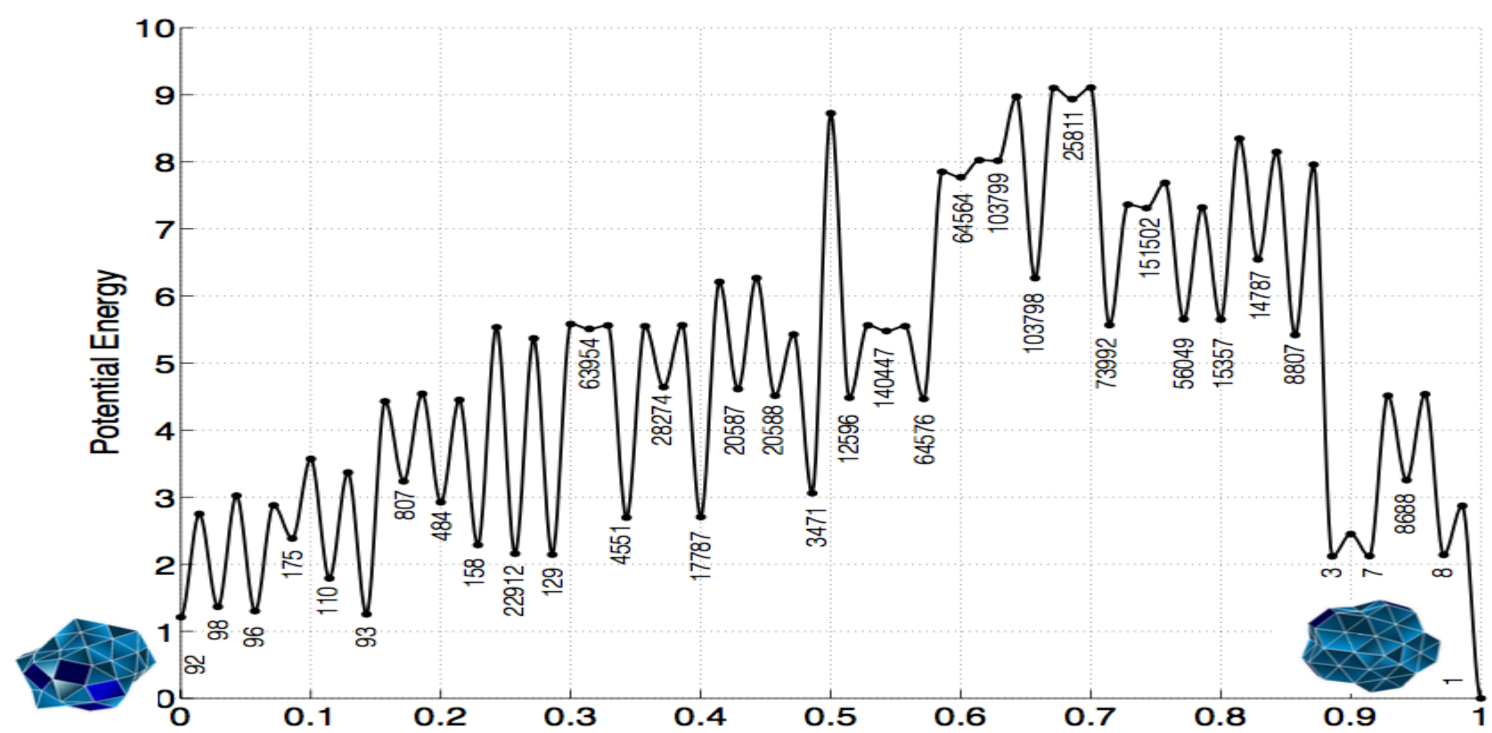
Zero-temperature asymptotic analysis of the LJ75 Network

- The Δ_k corresponding to the escape process is extracted at k = 4395, and

  $$\lambda_{4395} \approx 147.2 \exp(-7.897/T).$$

- The "bridge" $(p_{4395} \to q_{4395})$ is found to be $(25811 \to 73992)$.
- The "collapsing" component S^+_{4395} has 92883 vertices and its closed communicating class C^+_{4395} has 28032 vertices.
- Most likely zero-temperature transition path $\to$





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Concluding remarks

- We are interested in continuous-time Markov chains with exponentially small transition rates $L_{ij} \asymp \exp(-U_{ij}/\varepsilon)$, and study their long-term dynamics through asymptotic spectral decomposition of the generators.

- We propose an efficient algorithm to compute the asymptotic estimates of eigenvalues and eigenvectors of the generator via constructing a hierarchy of typical transitions graphs.

- Future work:

    - Try using this methodology to study metastability in stochastic lattice systems, such as the Ising model with Glauber dynamics?