Graph Learning
5. Heat Diffusion

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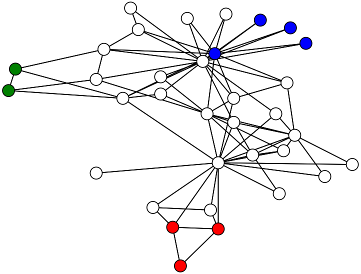
Motivation

Classification

(semi-supervised learning)



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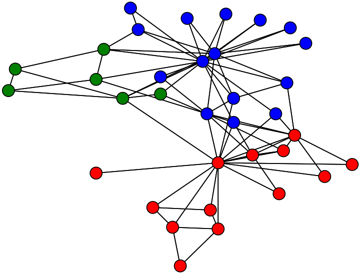
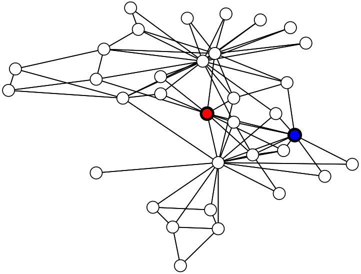


Motivation

Contrastive ranking



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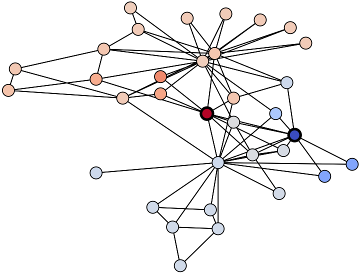
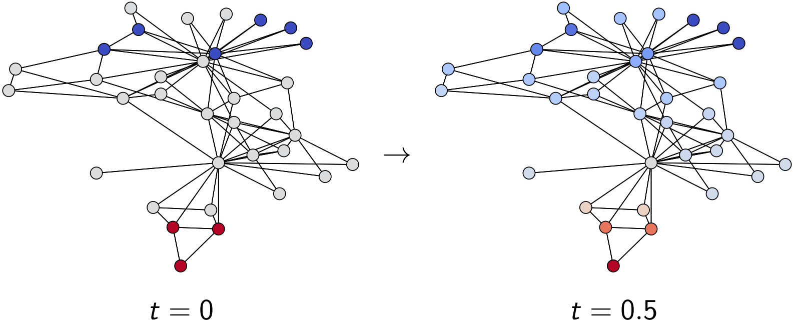


Outline

Heat diffusion (continuous time)

Evolution of the **temperature** T_i of each node i :

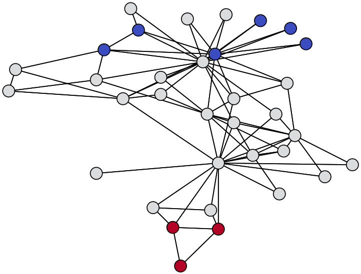
$$\boxed{\frac{\mathrm{d}T_i}{\mathrm{d}t} = \sum_j A_{ij}(T_j - T_i)}$$



Heat equation (continuous time)

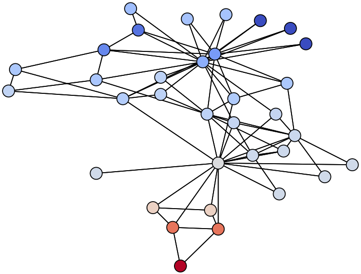
Vectorial representation:

$$\boxed{\frac{\mathrm{d}T}{\mathrm{d}t} = -\underbrace{(D - A)}_{L}\, T}$$



$t = 0$

$\rightarrow$



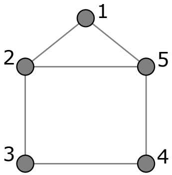
$t = 0.5$

Laplacian matrix

Definition

$$L = D - A \quad \text{with} \quad D = \mathrm{diag}(A\mathbf{1})$$

Example:



$$L = \begin{bmatrix} 2 & -1 & & & -1 \\ -1 & 3 & -1 & & -1 \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ -1 & -1 & & -1 & 3 \end{bmatrix}$$

Laplacian matrix

Definition

$$L = D - A$$

Properties

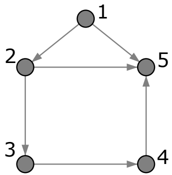
- Symmetric
- Positive semi-definite
- Discrete differential operator

$$\boxed{L = \nabla^T \nabla}$$

with ∇ the $m \times n$ **incidence matrix** of the graph

Incidence matrix

Given some arbitrary direction of the edges:



$$\nabla = \begin{bmatrix} -1 & 1 & & & \\ -1 & & & & 1 \\ & -1 & 1 & & \\ & -1 & & & 1 \\ & & -1 & 1 & \\ & & & -1 & 1 \end{bmatrix}$$

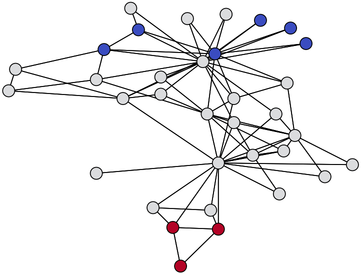
The incidence matrix applied to the vector T gives the temperature **difference** over the edges:

$$\boxed{\nabla T = [T_j - T_i]_{i \to j}}$$

Heat diffusion (continuous time)

Solution to the heat equation:

$$\boxed{\frac{\mathrm{d}T}{\mathrm{d}t} = -LT} \quad \rightarrow \quad \boxed{T(t) = \underbrace{e^{-Lt}}_{\text{heat kernel}} \; T(0)}$$



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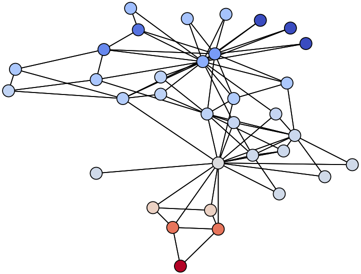


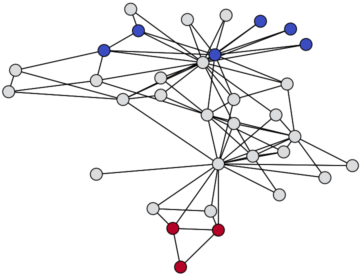
$t = 0$ $\qquad$ $t = 0.5$

Heat diffusion (continuous time)

At equilibrium,

$$\boxed{\frac{\mathrm{d}T}{\mathrm{d}t} = 0} \quad \rightarrow \quad \boxed{\nabla T = 0}$$

This is **Laplace's equation**



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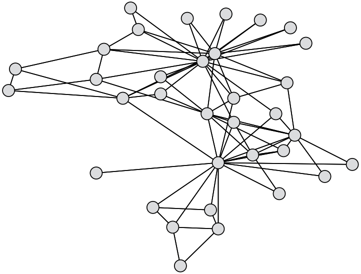


$t = 0$ $\qquad$ $t \rightarrow +\infty$

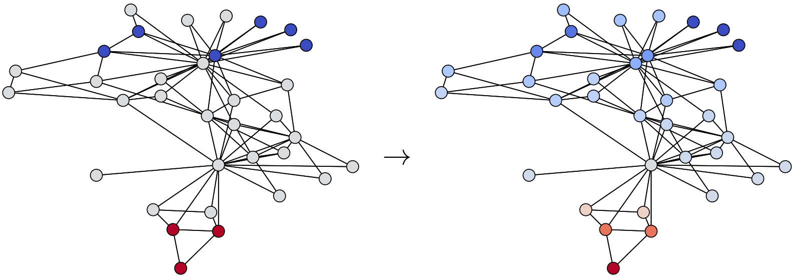
Conservation (continuous time)

The **average** temperature is constant:

$$\boxed{\forall t \geq 0, \quad \bar{T}(t) = \bar{T}(0)}$$

where

$$\bar{T}(t) = \frac{1}{n} \sum_{i=1}^{n} T_i(t)$$

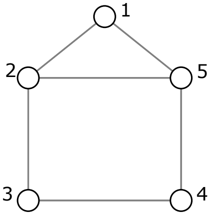


$t = 0$ $\rightarrow$ $t = 0.5$

Exercise

Give the **ranking** of nodes in terms of temperatures at time $t = 0^+$ after heat diffusion in continuous time

The initial vector of temperatures is $T(0) = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$



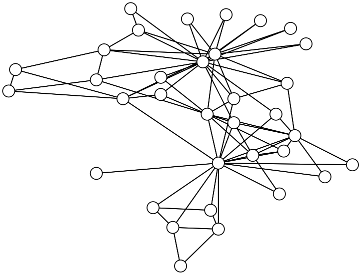
Hint: $e^{-Lt} = I - Lt + o(t)$

Spectral analysis

Spectral decomposition of the **Laplacian** matrix:

$$\boxed{L = U \Lambda U^T}$$

with $U^T U = I$, $\Lambda = \mathrm{diag}(\lambda_1, \dots, \lambda_n)$, $\lambda_1 = 0 \leq \lambda_2 \leq \dots \leq \lambda_n$



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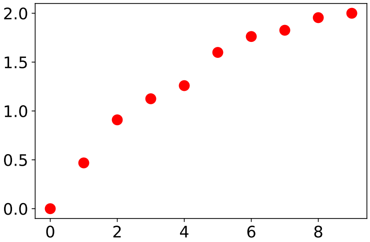
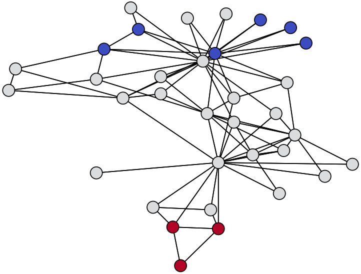


$$\lambda_1 = 0 \leq \lambda_2 \leq \dots \leq \lambda_{10} \leq \dots$$

Convergence (continuous time)

If the graph is connected, then $0 = \lambda_1 < \lambda_2$ and the convergence is **exponential** at rate λ_2:

$$\boxed{e^{-Lt} = Ue^{-\Lambda t}U^T \to \frac{11^T}{n}}$$



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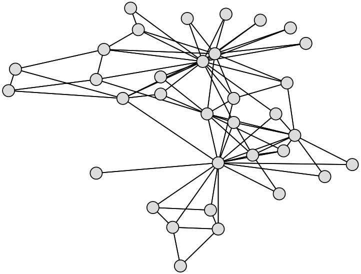


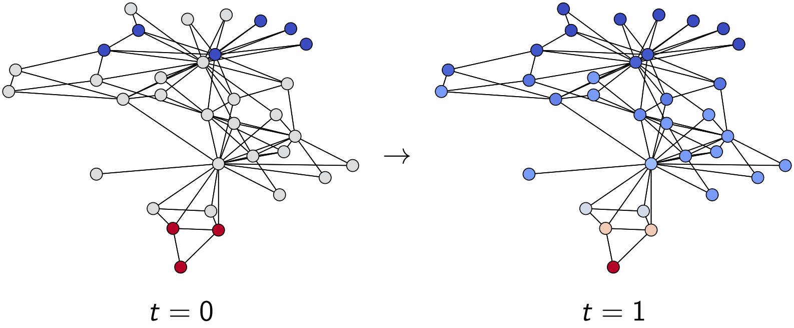
$t = 0$ $\qquad$ $t \to +\infty$

Heat diffusion (discrete time)

Evolution of **temperature** T_i of each node i:

$$\boxed{\forall t = 0, 1, 2, \dots \quad T_i(t+1) = (1-\alpha) T_i(t) + \frac{\alpha}{d_i} \sum_j A_{ij} T_j(t)}$$

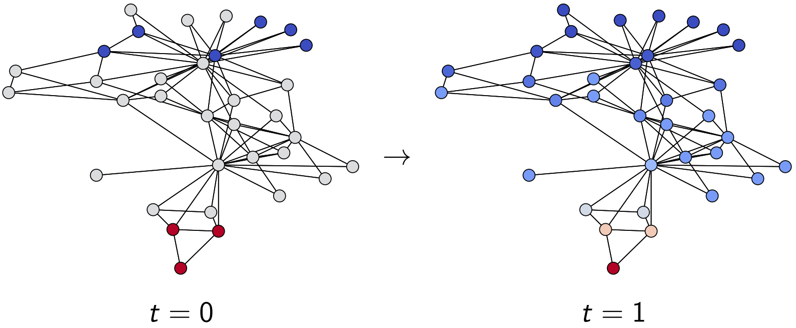
where $\alpha \in (0, 1)$ is some **damping factor**



Heat diffusion (discrete time)

Equivalently,

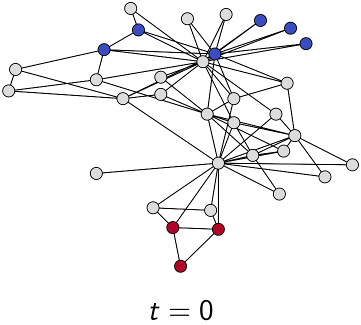
$$\boxed{\forall t = 0, 1, 2, \ldots \quad T_i(t+1) - T_i(t) = \frac{\alpha}{d_i} \sum_j A_{ij}(T_j(t) - T_i(t))}$$



Heat equation (discrete time)

Vectorial representation:

$$\boxed{\forall t = 0, 1, 2, \ldots \quad T(t+1) = ((1-\alpha)I + \alpha \underbrace{D^{-1}A}_{P})T(t)}$$

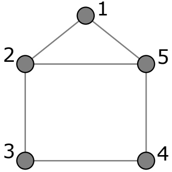


Transition matrix

Definition

$$P = D^{-1}A \quad \text{with} \quad D = \operatorname{diag}(A\mathbb{1})$$

Example:



$$P = \begin{bmatrix} & \frac{1}{2} & & & \frac{1}{2} \\ \frac{1}{3} & & \frac{1}{3} & & \frac{1}{3} \\ & \frac{1}{2} & & \frac{1}{2} & \\ & & \frac{1}{2} & & \frac{1}{2} \\ \frac{1}{3} & \frac{1}{3} & & \frac{1}{3} & \end{bmatrix}$$

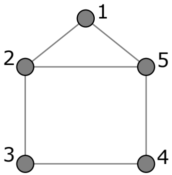
Impact of damping factor

Principle: Walk with probability α, stop with probability $1-\alpha$

New transition matrix

$$P^{(\alpha)} = (1-\alpha)I + \alpha P$$

Example: $\alpha = \frac{1}{2}$

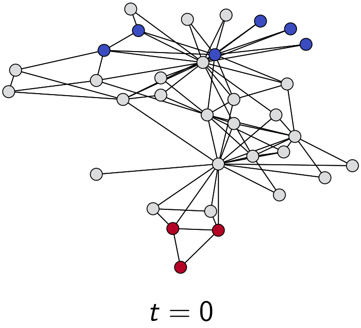


$$P^{(\alpha)} = \begin{bmatrix} \frac{1}{2} & \frac{1}{4} & & & \frac{1}{4} \\ \frac{1}{6} & \frac{1}{2} & \frac{1}{6} & & \frac{1}{6} \\ & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & \\ & & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ \frac{1}{6} & \frac{1}{6} & & \frac{1}{6} & \frac{1}{2} \end{bmatrix}$$

Heat diffusion (discrete time)

Solution to the heat equation:

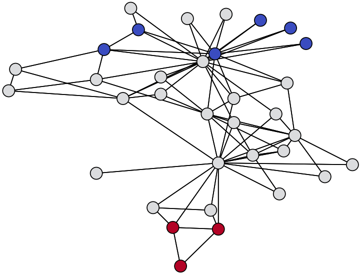
$$\boxed{T(t) = ((1-\alpha)I + \alpha P)^t\, T(0)}$$



Heat diffusion (discrete time)

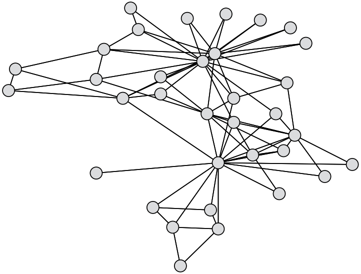
At equilibrium,

$$\boxed{((1-\alpha)I+\alpha P)T = T} \quad \rightarrow \quad PT = T \quad \rightarrow \quad \boxed{\nabla T = 0}$$



$t = 0$

$\rightarrow$



$t \rightarrow +\infty$

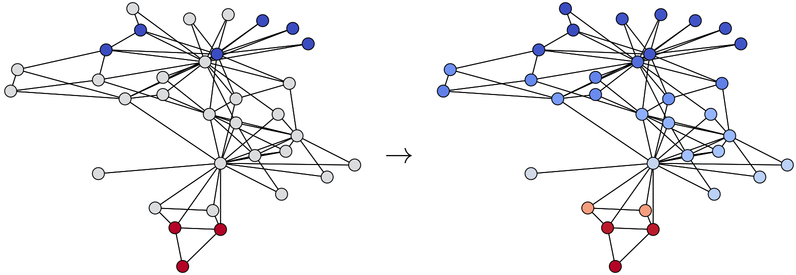
Conservation (discrete time)

The **weighted average** temperature is constant:

$$\boxed{\forall t \geq 0, \quad \tilde{T}(t) = \tilde{T}(0)}$$

where

$$\tilde{T}(t) = \frac{\sum_i d_i T_i(t)}{\sum_i d_i}$$

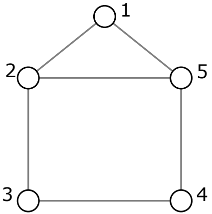


$t = 0$ $\rightarrow$ $t = 2$

Exercise

Give the **ranking** of nodes in terms of temperatures at time $t = 1$ after heat diffusion in discrete time, with $\alpha = \frac{1}{2}$

The initial vector of temperatures is $T(0) = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$

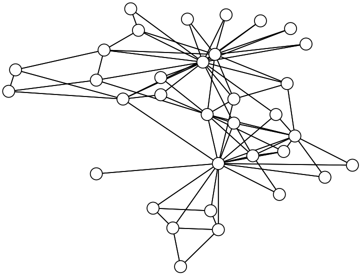


Spectral analysis

Spectral decomposition of the **transition** matrix:

$$\boxed{P = V \Gamma V^T D}$$

with $V^T D V = I$, $\Gamma = \mathrm{diag}(\gamma_1, \ldots, \gamma_n)$, $\gamma_1 = 1 \geq \gamma_2 \geq \ldots \geq \gamma_n$



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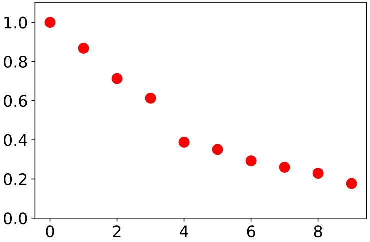
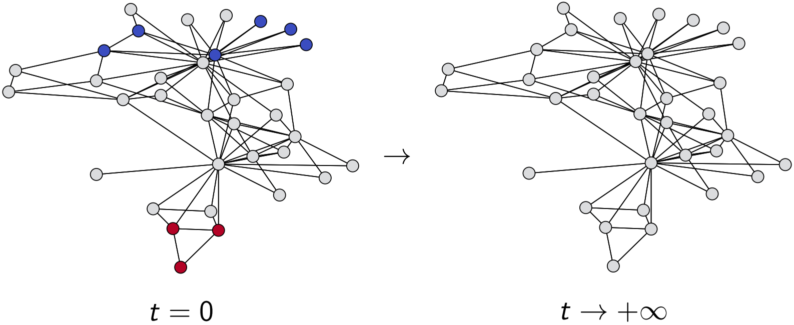


$\gamma_1 = 1 \geq \gamma_2 \geq \ldots \geq \gamma_{10} \geq \ldots$

Convergence (discrete time)

If the graph is connected and not bipartite,
$\gamma_1 = 1 > \gamma_2 \geq \ldots \geq \gamma_n > -1$ and the convergence is **geometric**:

$$\boxed{((1-\alpha)I + \alpha P)^t = V((1-\alpha)I + \alpha\Gamma)^t V^T D \propto_{t\to\infty} 11^T D}$$



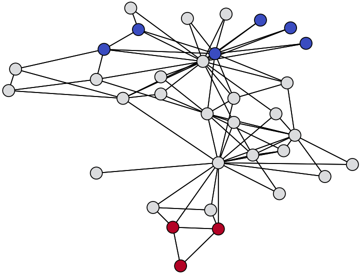
Outline

1. Heat diffusion
2. **Dirichlet problem**
3. Applications
4. Extensions

Diffusion with a boundary

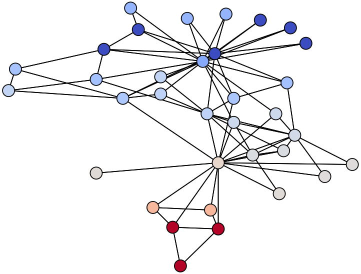
Heat equation with **boundary** conditions:

$$\boxed{\forall i \text{ free}, \quad \frac{\mathrm{d}T_i}{\mathrm{d}t} = -(LT)_i}$$



$t = 0$

$\rightarrow$

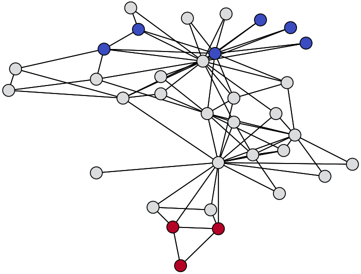


$t = 0.5$

Dirichlet problem

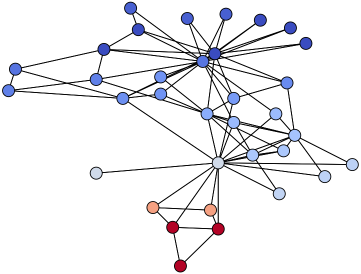
Equilibrium with **boundary** conditions:

$$\boxed{\forall i \text{ free}, \quad (LT)_i = 0}$$



$t = 0$

$\rightarrow$



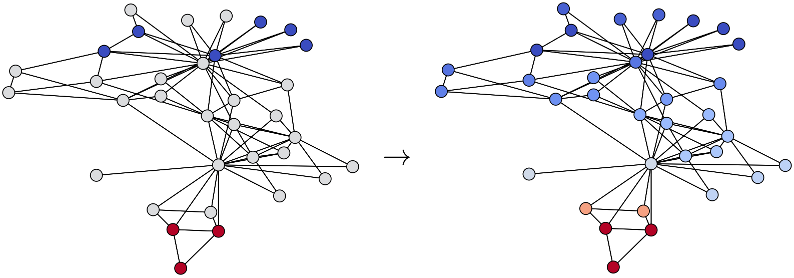
$t \rightarrow +\infty$

Dirichlet problem

At equilibrium, the temperature of each free node is the **average** of the temperatures of its neighbors:

$$\boxed{\forall i \text{ free}, \quad T_i = (PT)_i}$$

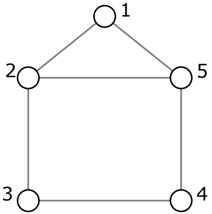
Note: Same solution in discrete time



$t = 0$ $\quad\to\quad$ $t \to +\infty$

Exercise

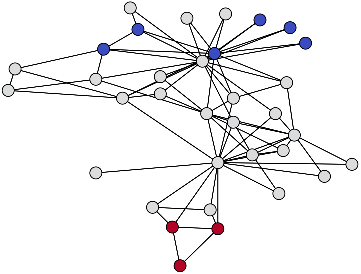
Solve the Dirichlet problem with $T_1 = 0$ and $T_4 = 1$.

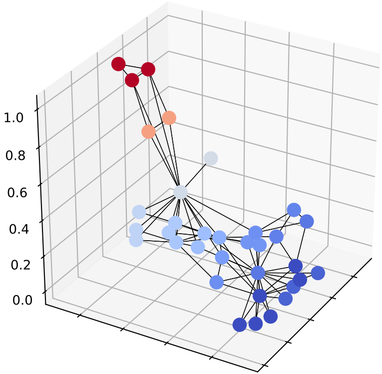


A regression problem

The solution minimizes the **Dirichlet energy**:

$$\boxed{E = \frac{1}{2} T^T L T = \frac{1}{2} ||\nabla T||^2}$$

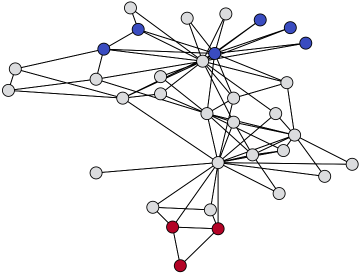




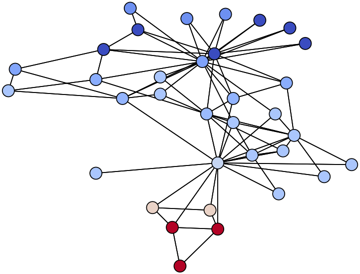
Computation

Power iteration with boundary condition:

$$\boxed{\forall i \text{ free}, \quad T_i \leftarrow (PT)_i}$$



$t = 0$



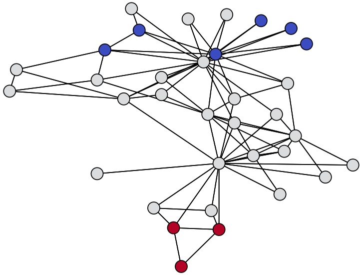
$t = 1$

Random walk

Consider a **random walk** starting from free node i

$$\boxed{T_i = \sum_j P_{i \to j} T_j}$$

where $P_{i \to j}$ is the probability to reach the boundary in j first

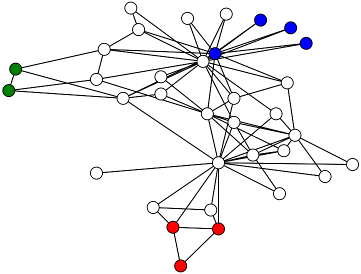


Outline

1. Heat diffusion
2. Dirichlet problem
3. **Applications**
4. Extensions

Classification

Given some nodes with **known labels**, how to **predict** the labels of the other nodes?



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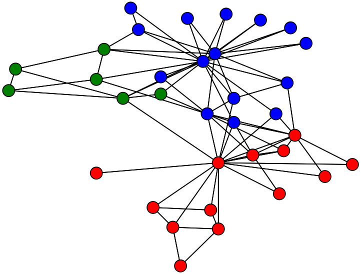
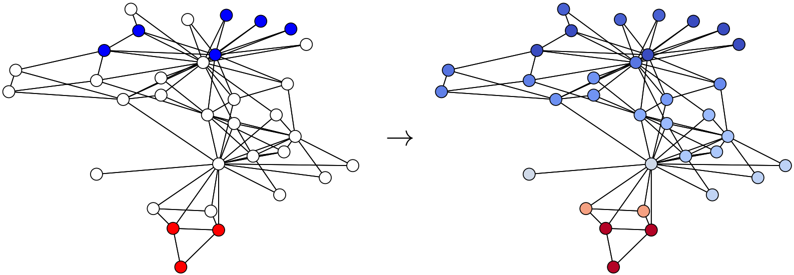


Binary classification

Binary classification by diffusion

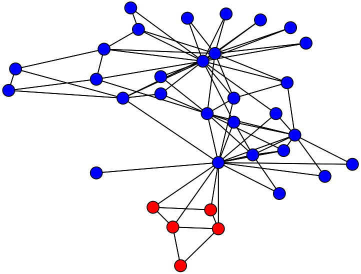
1. Solve the **Dirichlet problem** with boundary given by nodes with known labels
2. Classify nodes by some suitable **threshold** θ



Threshold

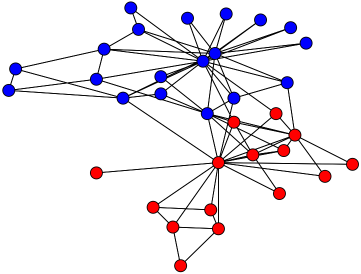
1. **Fixed** threshold

$$\boxed{\theta = \frac{1}{2}}$$



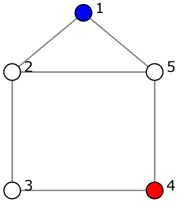
2. **Adaptive** threshold

$$\boxed{\theta = \bar{T} \equiv \frac{1}{n}\sum_{i=1}^{n} T_i}$$



Exercise

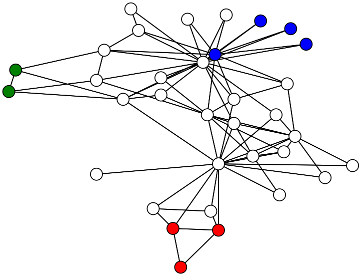
Give the labels of nodes 2, 3, 5 as predicted by diffusion.



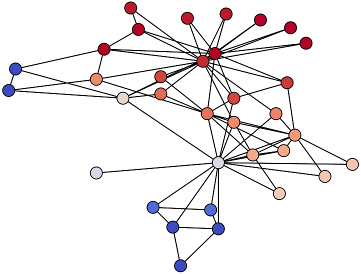
General case

Classification by diffusion

1. Solve one Dirichlet problem **per label** (one-against-others)
2. Classify nodes by selecting the solution of **highest** temperature



$\rightarrow$

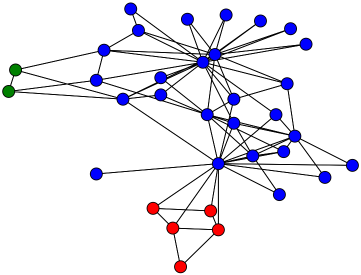


• against •,•

Centering

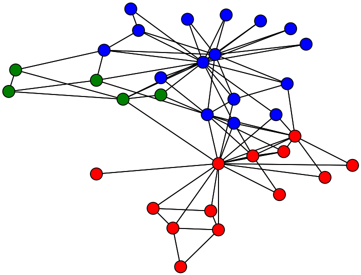
1. **Without** centering

$$\boxed{\arg\max_k T_i^{(k)}}$$



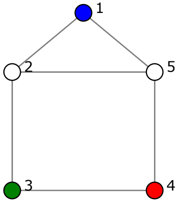
2. **With** centering

$$\boxed{\arg\max_k (T_i^{(k)} - \bar{T}^{(k)})}$$



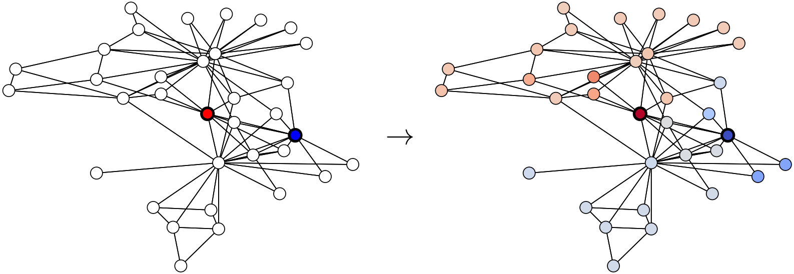
Exercise

Give the labels of nodes 2, 5 as predicted by diffusion.



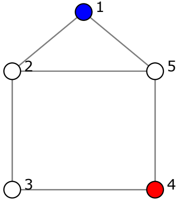
Contrastive ranking

How to rank nodes in the presence of **hot** nodes and **cold** nodes?
$\rightarrow$ solution to the Dirichlet problem



Exercise

Give the ranking of nodes with 1 hot source (node 4) and 1 cold source (node 1).



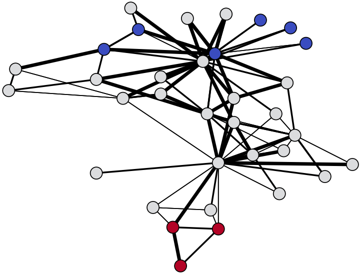
Outline

1. Heat diffusion
2. Dirichlet problem
3. Applications
4. **Extensions**

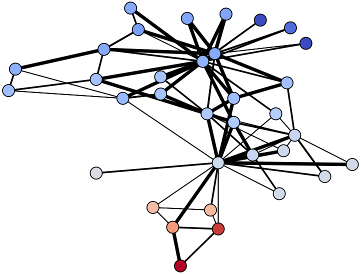
Case of weighted graphs

Evolution of **temperature** T_i of each node i :

$$\boxed{\frac{\mathrm{d}T_i}{\mathrm{d}t} = \sum_j A_{ij}(T_j - T_i)}$$



$\rightarrow$



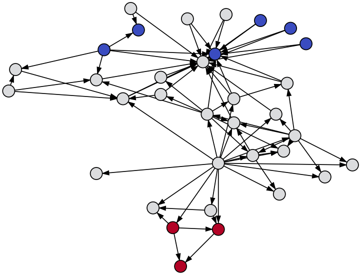
$t = 0$ $\qquad$ $t = 0.5$

Case of directed graphs

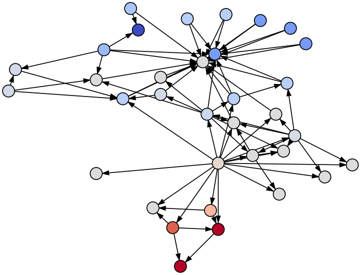
Evolution of **temperature** T_i of each node i:

$$\boxed{\frac{\mathrm{d}T_i}{\mathrm{d}t} = \sum_j A_{ij}(T_j - T_i)}$$

Note: Heat is propagated in **backward** direction



$\rightarrow$



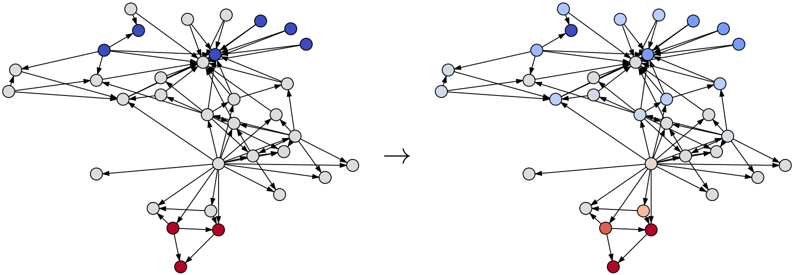
$t = 0$ $t = 0.5$

Heat equation (continuous time)

Evolution of the **vector** of temperatures:

$$\boxed{\frac{\mathrm{d}T}{\mathrm{d}t} = -(D^+ - A)T}$$

Note: The temperatures of **sinks** are constant.



$t = 0$ $\rightarrow$ $t = 0.5$

Summary

Heat diffusion

- **Heat diffusion** $\frac{\mathrm{d}T}{\mathrm{d}t} = -LT$
- The **Dirichlet problem**
- Application to **classification** and **ranking**
- Applicable to **weighted**, **directed** and **bipartite** graphs