Signal Processing on Graphs

ACMS 80770: Deep Learning with Graphs

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  - Probabilistic graph models
  - Graph isomorphism test
  - Graph signal processing

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- The concept of signal processing on graphs can define **convolutions** on graphs from a **spectral perspective**.

Convolution

- Classical **convolution** operation on the continuous Euclidean space is defined as

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- To perform this, one
  - **Maps** the filter and the signal to the Fourier domain
  - **Performs** the convolution in the Fourier domain
  - **Transforms** the result **back** to the Euclidean space.

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- This transform is performed by **expanding** the data in Fourier bases.
- Mathematically put

$$\begin{aligned}\mathcal{F}(f(t)) = \hat{f}(s) &:= \langle f, e^{2\pi ist} \rangle \\ &= \int_{\mathbb{R}} f(t) e^{-2\pi ist} dt\end{aligned}$$

where $e^{2\pi ist}$ represents the **Fourier bases**.

Inverse Fourier transform

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- This can be done using the **inverse Fourier transform**.
- Given the Fourier coefficient of a function, one can reconstruct the original data by **projecting** the resulted Fourier coefficients back to the Euclidean domain using inverse Fourier transform.
- **Inverse Fourier transform** is formulated as

$$\mathcal{F}^{-1}(\hat{f}(s)) = f(t) := \int_{\mathbb{R}} \hat{f}(s) e^{2\pi i s t} ds$$

Convolution

- As discussed earlier, we can use this notion to define **convolution**.
- Convolution of the two signals in the Fourier domain is represented by **element-wise** (Hadamard) **product**.

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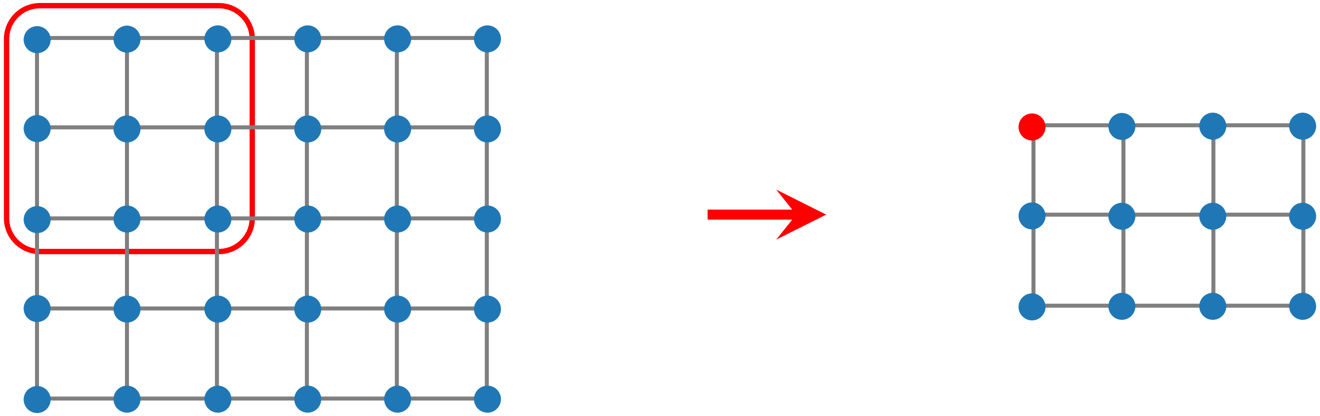
- Using **Fourier transform**, we can define convolution as

$$\begin{aligned}(f * h)(t) &= \mathcal{F}^{-1}\left(\mathcal{F}\left(f(t)\right) \odot \mathcal{F}\left(h(t)\right)\right) \\ &= \mathcal{F}^{-1}\left(\hat{f}(s) \odot \hat{h}(s)\right)\end{aligned}$$

- This operation filters the signal f using the filter h, such that it **amplifies** or **reduces** the contribution of some basis functions.

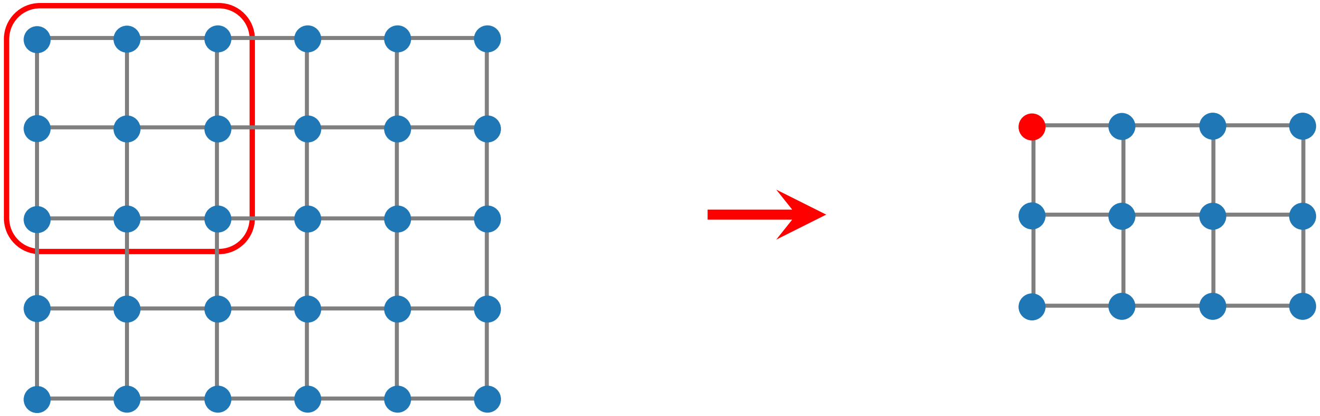
Convolution

- Convolutional neural networks are one of the most successful deep learning models, that use **convolution** operation.



Convolution

- Convolutional neural networks are one of the most successful deep learning models, that use **convolution** operation.
- CNN models operate on data defined over **discrete grids**.
- Therefore, the transformations above need to be reformulated for the data defined on **discrete** mesh.



Discrete Fourier transform

- For the case of a finite 1D grid $t \in \{0, \ldots N-1\}$, the **Fourier transform** is derived as

$$\hat{\mathbf{f}}_\ell = \frac{1}{\sqrt{N}} \sum_{t=0}^{N-1} \mathbf{f}_t e^{-i\frac{2\pi}{N}kt}$$

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- In essence, this decomposition represents the signal $\mathbf{f}$ as **weighted sum** of the Fourier bases.

- Analogously, the **inverse Fourier transform** is defined as

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Shift and Difference

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- **Shift equivariance** implies that

$$f(t+a) * g(t) = f(t) * g(t+a) = (f*g)(t+a)$$

- In other words, as a result of shift equivariance of the convolution operation, convolving a translated signal is equal to translating a convolved signal.

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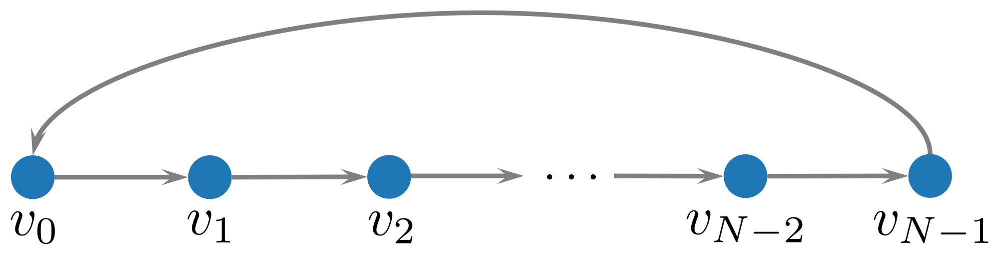
- To motivate these definitions, we rely on the **ring graphs**.

Ring Graph

- A **cycle** graph, **circular** graph, or **ring graph** is a graph consisting of a single cycle.
- All nodes of the graph are connected through this closed cycle.



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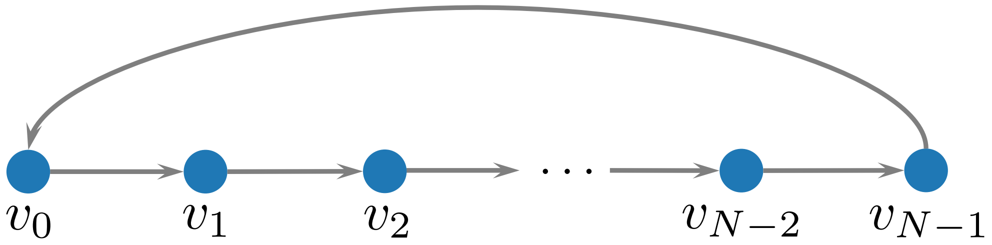
- In this representation, each **time** t is represented by **node** v_t of the ring graph
- Thus, function f's **value at time** t is represented by signal value $f(t)$ residing on **node** v_t.

Ring Graph

- In other words, $\mathbf{f}$ is represented on the graph, such that $\mathbf{f}_t$ is signal value corresponding to node v_t.



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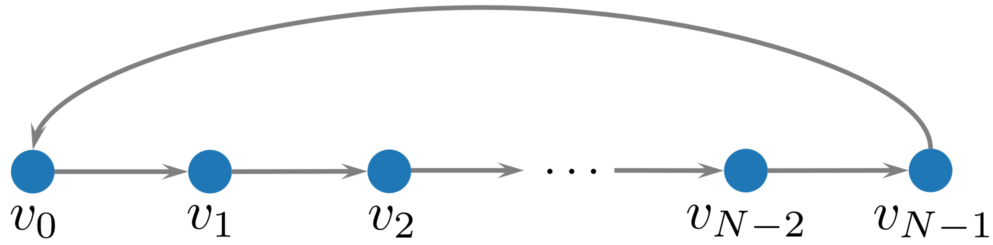
- In other words, $\mathbf{f}$ is represented on the graph, such that $\mathbf{f}_t$ is signal value corresponding to node v_t.
- Using this representation, the shift operator is represented by the **circulant adjacency** matrix

$$[\mathbf{A}_c]_{i,j} = \begin{cases} 1 & \text{if } j = (i+1) \mod N \\ 0 & \text{otherwise} \end{cases}$$



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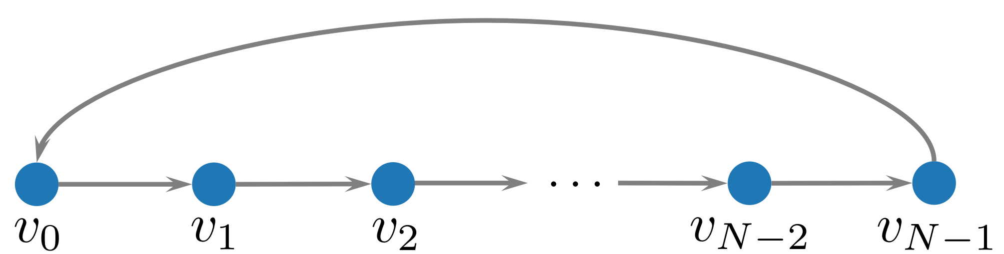

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- Intuitively, applying **shift** in signal $\mathbf{f}$ residing on graph G **propagates information** from one node to the other.

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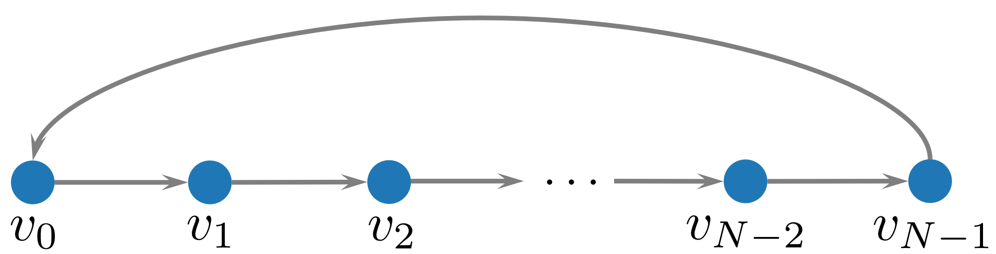
- On the other hand, the difference operator is defined using the **circulant Laplace** matrix

$$\mathbf{L}_c = \mathbf{I} - \mathbf{A}_c$$



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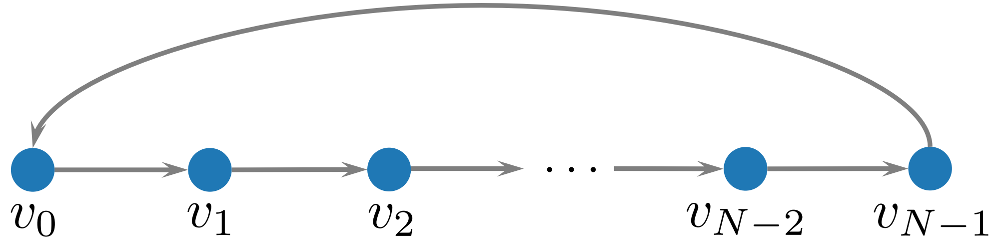
- Using $\mathbf{L}_c$, one can apply **difference operation** on signal $\mathbf{f}$ as

$$[\mathbf{L}_c \mathbf{f}]_t = \mathbf{f}_t - \mathbf{f}_{(t+1) \bmod N}$$

- In this equation, applying the difference operator computes the difference between $\mathbf{f}$ at node v_t with its neighbors.



Convolution on Chain Graph

- Given a convolution matrix $\boldsymbol{Q}$ of filter function h, we can perform **convolution** on signals on **graph** using the matrix product

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- In the matrix form, we can represent that as

  - **Shift equivariance**

$$\mathbf{A}_c \mathbf{Q}_h = \mathbf{Q}_h \mathbf{A}_c$$

  - **Difference equivariance**

$$\mathbf{L}_c \mathbf{Q}_h = \mathbf{Q}_h \mathbf{L}_c$$

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- In other words, $\boldsymbol{Q}_h$ should be **commutative** with respect to $\mathbf{A}_c$ and $\mathbf{L}_c$.
- One can show that defining the matrix $\boldsymbol{Q}_h$ as a **polynomial function** of the **circular adjacency** $\mathbf{A}_c$ matrix would satisfy shift and difference equivariance.

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$$\mathbf{Q}_h = p_N\left(\mathbf{A}_c\right) = \sum_{i=0}^{N-1} \alpha_i \mathbf{A}_c^i$$

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- One can generalize the idea defined on cycle graph to perform **convolution** on **arbitrary graphs**.

Spatial Graph Convolution

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- Using the adjacency $\mathbf{A}$, we can define convolution filter matrices as

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- We recall that $\mathbf{A}^n$ represents neighbors of node v_i that are within $\boldsymbol{n}$ **−hop** distance from the node.
- Therefore, performing convolution $\boldsymbol{Q}_h$ on signal $f \in \mathbb{R}^{|V|}$ in the **nodal domain** will collect information from an N −hop neighborhood of each node $v_i \in V$.

Spatial Graph Convolution

- Thus, $\boldsymbol{Q}_h\mathbf{f}$ contains information from different $\boldsymbol{n}$ **−hop** neighborhoods,

$$\mathbf{Q}_h\mathbf{f} = \alpha_0\mathbf{I}\mathbf{f} + \alpha_1\mathbf{A}\mathbf{f} + \alpha_2\mathbf{A}^2\mathbf{f} + \ldots + \alpha_N\mathbf{A}^N\mathbf{f}$$

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- While $\boldsymbol{Q}_h$ defined for chain graphs are commutative with both adjacency and Laplacian matrices, this **does not** always **extend** to general graphs.

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- While $\boldsymbol{Q}_h$ defined for chain graphs are commutative with both adjacency and Laplacian matrices, this **does not** always **extend** to general graphs.

- In addition to the Laplace and adjacency matrices, one can use **normalized variants** of them to define the convolution matrix,

$$\mathbf{L}_{\text{sym}} = \mathbf{D}^{-\frac{1}{2}}\mathbf{L}\mathbf{D}^{-\frac{1}{2}} \qquad \mathbf{A}_{\text{sym}} = \mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}}$$

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- Choosing **which matrix** to use is a matter of **trade-off** between the pros and cons of each method.
  - We can define **bounds** for the spectrum of the normalized Laplacian and Adjacency matrixes, which results in numerical stability.
  - Another plausible property of the normalized variants is that **commutativity** with respect to one will indicate commutativity with respect to the other one.

Graph Fourier Transform

- So far, we have relied on the notion of **convolution** in the **nodal domain**.
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- One can leverage tools from graph signal processing to define convolution in the **graph spectral domain**.
- To do so, we need to redefine the **building block** of signal processing tools, namely Fourier transform, on graph domain.
- In the earlier slides, we presented **Fourier transform** as

$$\mathcal{F}(f(t)) = \int_{\mathbb{R}} f(t) e^{-2\pi i s t} dt$$

where we expand the signal in Fourier **bases** $e^{2\pi i s t}$.

Graph Fourier Transform

- We recall that the **Laplace operator** is defined as

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  - For s far larger than zero, the associated exponential component **oscillates more rapidly**.

Graph Fourier Transform

- Recall from earlier lecture that **Laplacian matrix** is analogue of the multivariate **Laplace operator** in the graph domain.
- One can exploit this analogy and define the **Fourier bases** for the **graph domain**.

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- Recall from earlier lecture that **Laplacian matrix** is analogue of the multivariate **Laplace operator** in the graph domain.
- One can exploit this analogy and define the **Fourier bases** for the **graph domain**.
- Since the Laplace matrix is a positive semi-definite matrix, it has a set of orthonormal **eigenvectors** $\{u_\ell\}_{\ell=0,\ldots,N-1}$ and associated real non-negative **eigenvalues** $\{\lambda_\ell\}_{\ell=0,\ldots,N-1}$ that satisfy

$$\mathbf{L}u_\ell = \lambda_\ell u_\ell$$

for $\ell = 0, \ldots, N-1$.

Graph Fourier Transform

- In the matrix form

$$\mathbf{L} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^\top$$

where $\mathbf{U}$ is the **eigenvector matrix** and $\boldsymbol{\Lambda}$ is a **diagonal matrix** with eigenvalues λ_ℓ of $\mathbf{L}$ as its diagonal elements.

- The set of eigenvalues

$$\sigma(\mathbf{L}) = \{\lambda_0, \lambda_1, \ldots, \lambda_{N-1}\}$$

is the **spectrum** of graph G, where we assume

$$0 = \lambda_0 < \lambda_1 \leq \cdots \leq \lambda_{N-1} \leq \lambda_{\max}$$

Graph Fourier Transform

- Using the eigenvectors U as Fourier bases, we can define the **Fourier transform** of a signal $\mathbf{f} \in \mathbb{R}^N$ in the **graph domain** as

$$\hat{f}(\lambda_\ell) := \langle f, u_\ell \rangle = \sum_{i=1}^{N} f(i) u_\ell(i)$$

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- Analogously, one can define the **inverse graph Fourier transform** as

$$f(i) = \sum_{\ell=0}^{N-1} \hat{f}\left(\lambda_\ell\right) u_\ell(i)$$

- In the matrix notation

$$\mathbf{f} = \mathbf{U}\hat{\mathbf{f}}$$

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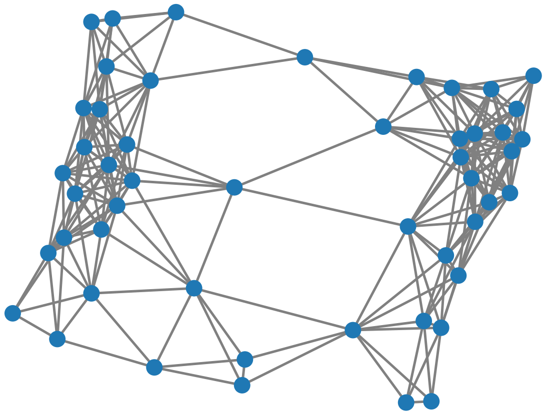
Graph Fourier Transform

- Consider the graph G below:



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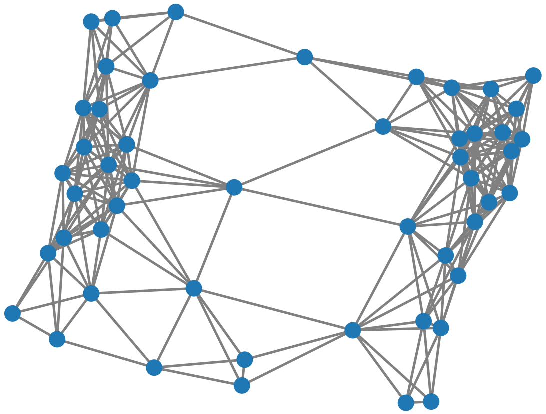

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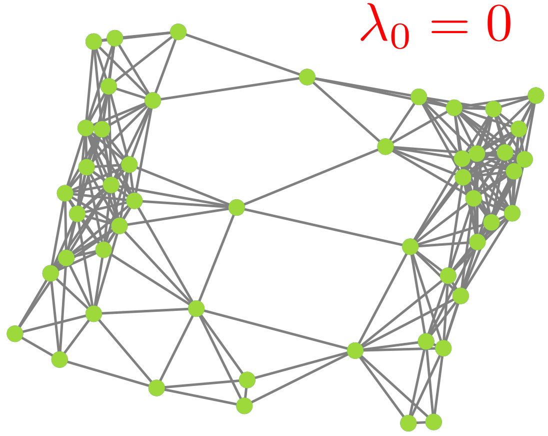

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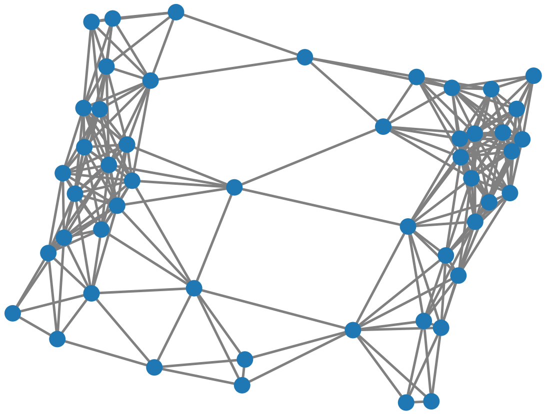

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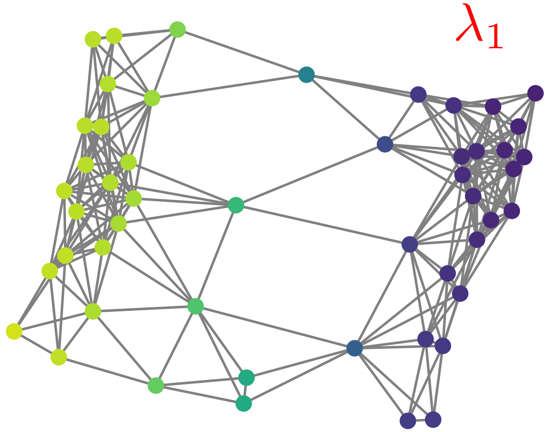

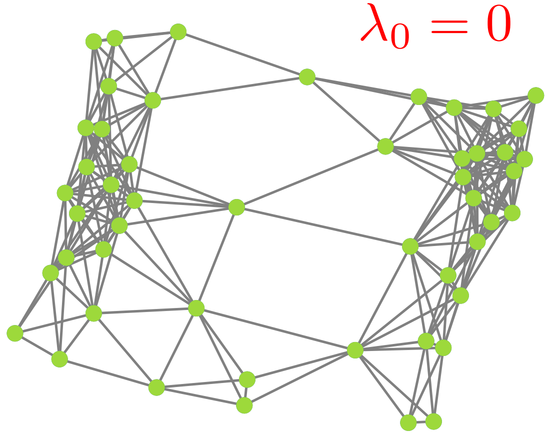

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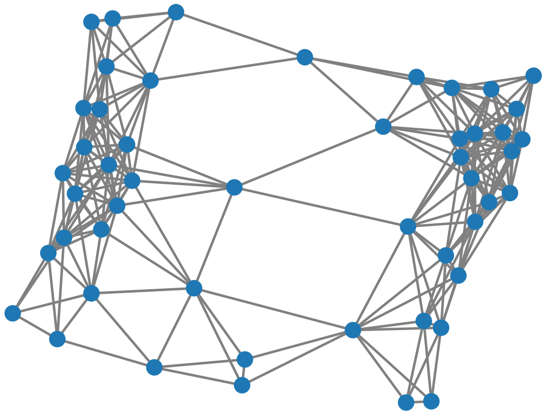

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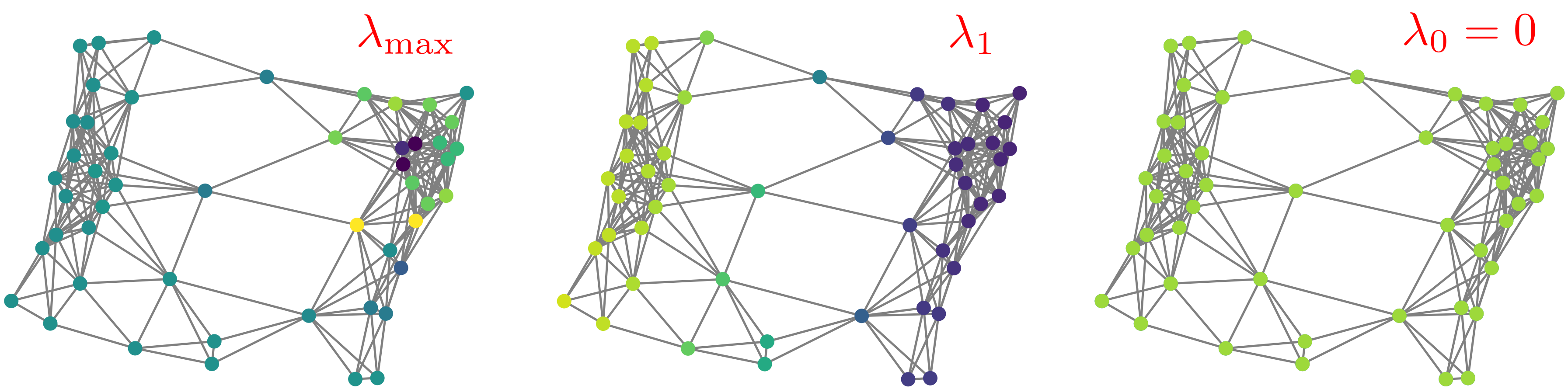

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- So far, we have used **graph Laplacian matrix** to construct graph Fourier bases.
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- One alternative is **normalized** graph Laplacian $\tilde{\mathbf{L}}$, in which elements $\mathbf{A}_{ij}$ are normalized by $\frac{1}{\sqrt{d_i d_j}}$.
- However, the eigenvalues associated with the smallest eigenvalue $\tilde{\lambda}_0$ does **not** have **constant elements** anymore.

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- However, the eigenvalues associated with the smallest eigenvalue $\tilde{\lambda}_0$ does **not** have **constant elements** anymore.
- Another approach is to use the **stochastic matrix**

$$P := \mathrm{D}^{-1}\mathbf{A}$$

where each element $\boldsymbol{P}_{ij}$ is the probability of going from v_i to v_j in one step.

Summary

- Signal Processing on Graphs
- Convolution
- Fourier transform
- Discrete Fourier transform
- Shift and Difference
- Chain Graph
- Shift and Difference on Chain Graph
- Convolution on Chain Graph
- Graph Convolution
- Graph Fourier Transform