Wavelets and Applications

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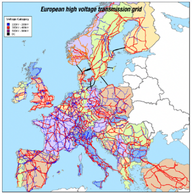
M2 MSIAM & Ensimag 3A MMIS

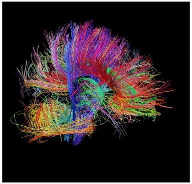
January 21, 2022

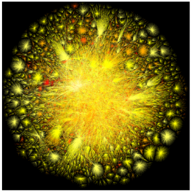
The Laplacian and graph Fourier transform

What is a graph signal ?



Why graph signal processing ?





Credits: N. Tremblay

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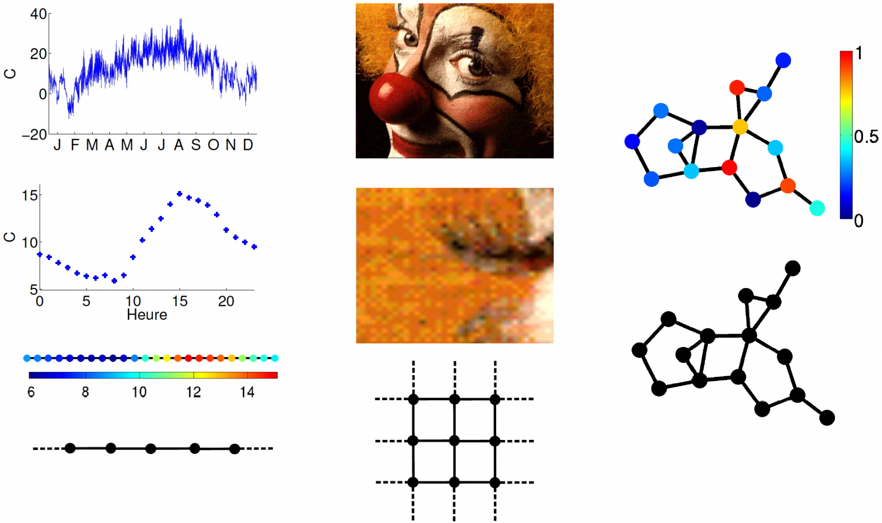

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Basic concepts in Graph Theory

Definition of a Graph

A **graph** $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ consists of two finite sets:

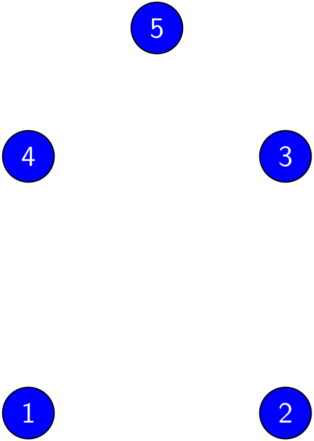
- $\mathcal{V}$ – the **vertex set** of a graph is a nonempty set of elements called **vertices** or **nodes**.
- $\mathcal{E}$ – the **edge set** of a graph is a possibly empty set of elements called **edges** or **links**.

Conceptually a graph is formed by vertices and edges connecting them.

- $|\mathcal{V}| = n$ is the number of vertices known as **order** of a graph
- $|\mathcal{E}| = m$ is the number of edges known as **size** of a graph

A **weighted graph** $\mathcal{G} = (\mathcal{V}, \mathcal{E}, w)$ has in addition a weight function $w : \mathcal{E} \to \mathbb{R}^+$ which assign a positive value to each edge.

The adjacency matrix $\mathbf{A} = (a_{ij})_{1 \leqslant i,j \leqslant n}$



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$\mathcal{V} = \{1, 2, 3, 4, 5\}$, $|\mathcal{V}| = 5$

$\mathcal{E} = \{\}$

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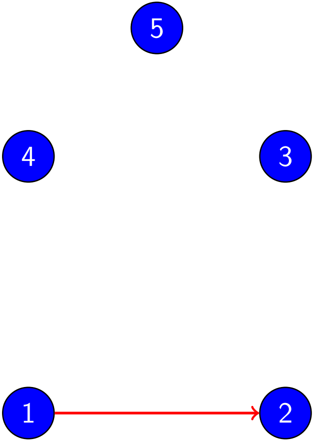

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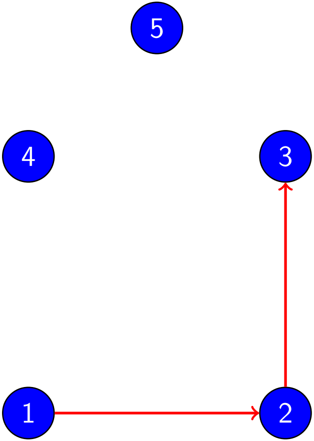

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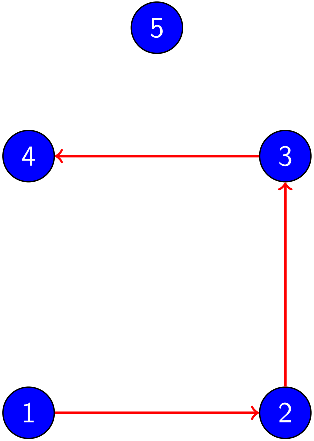

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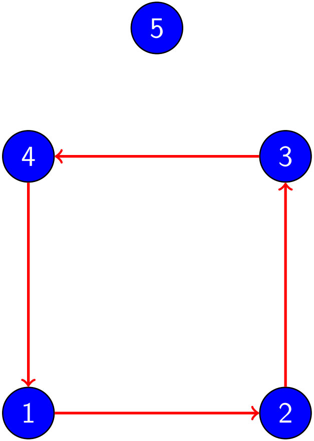

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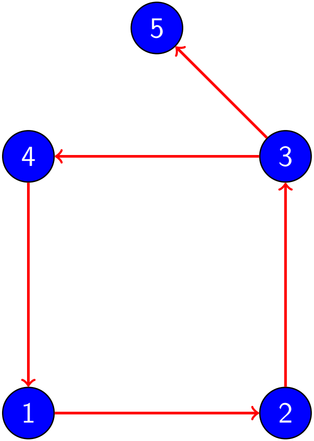

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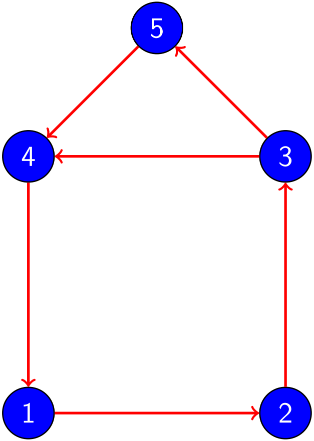

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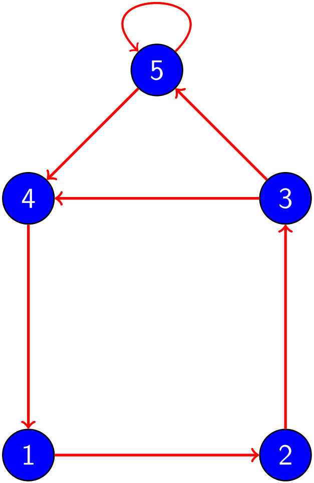

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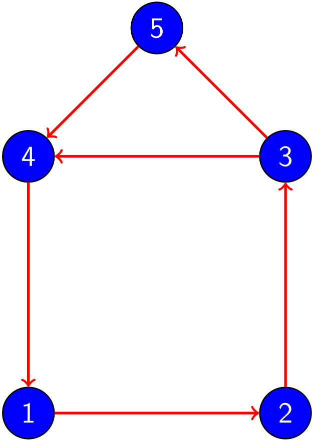

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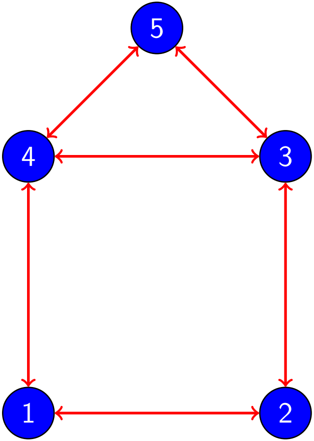

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$\mathbf{A} \leftarrow \mathbf{A} + \mathbf{A}^{\mathrm{T}}$ (directed $\rightarrow$ undirected)

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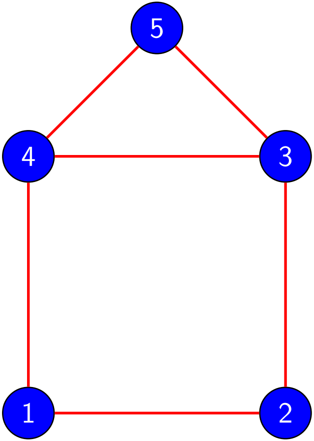

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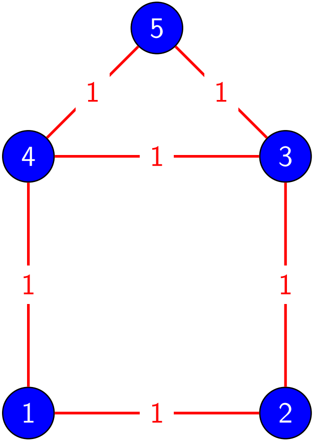
The weighted adjacency matrix $\mathbf{W} = (w_{ij})_{1 \leqslant i,j \leqslant n}$



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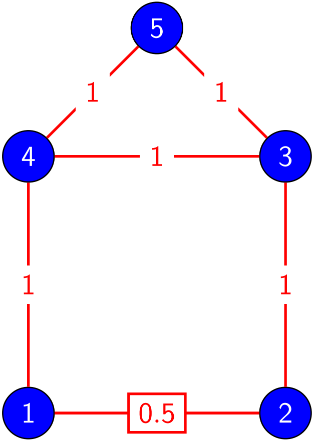

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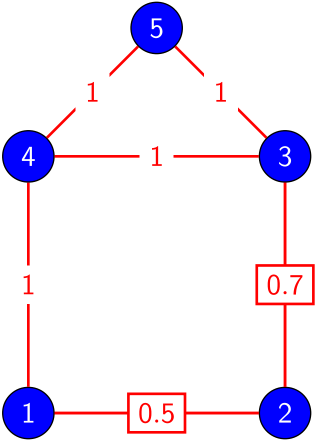

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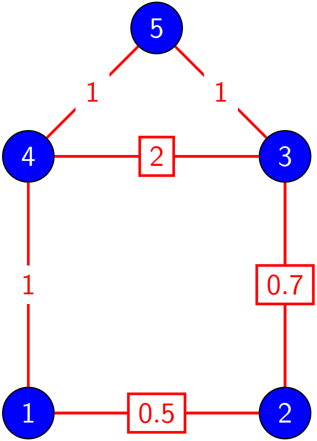

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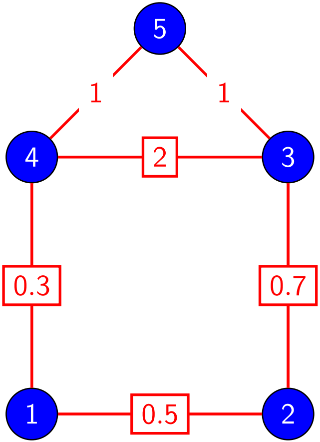

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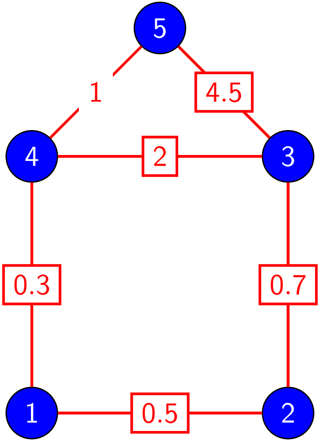

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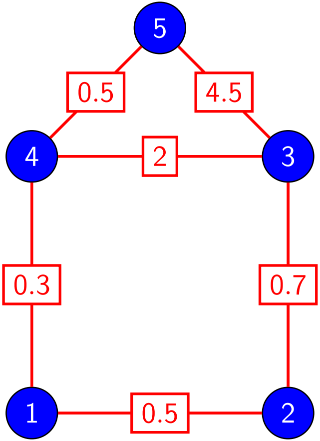

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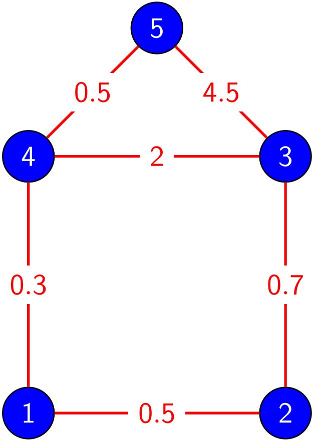
The weighted degree matrix $\mathbf{D} = (d_{ij})_{1\leqslant i,j\leqslant n}$



$$d_{ij} = d_i\delta_{ij} = \sum_{j=1}^{n} w_{ij}\delta_{ij}$$

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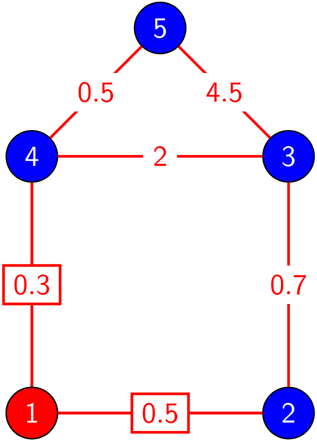
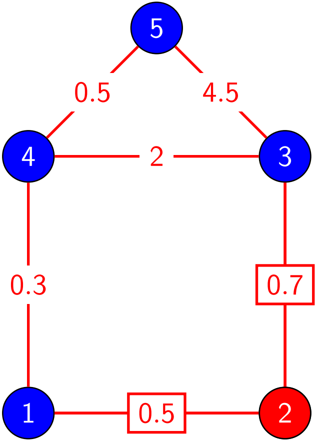


$$d_{ij} = d_i \delta_{ij} = \sum_{j=1}^{n} w_{ij} \delta_{ij}$$

$$\mathbf{W} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \begin{array}{c} \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{pmatrix} 0 & \boxed{0.5} & 0 & \boxed{0.3} & 0 \\ 0.5 & 0 & 0.7 & 0 & 0 \\ 0 & 0.7 & 0 & 2 & 4.5 \\ 0.3 & 0 & 2 & 0 & 0.5 \\ 0 & 0 & 4.5 & 0.5 & 0 \end{pmatrix} \end{array}$$

$$\mathbf{D} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \begin{array}{c} \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{pmatrix} \boxed{0.8} & & & & \\ & d_2 & & & \\ & & d_3 & & \\ & & & d_4 & \\ & & & & d_5 \end{pmatrix} \end{array}$$

The weighted degree matrix $\mathbf{D} = (d_{ij})_{1 \leqslant i,j \leqslant n}$



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$$\mathbf{D} = \begin{array}{c c} & \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} & \begin{pmatrix} 0.8 & & & & \\ & \boxed{1.2} & & & \\ & & d_3 & & \\ & & & d_4 & \\ & & & & d_5 \end{pmatrix} \end{array}$$

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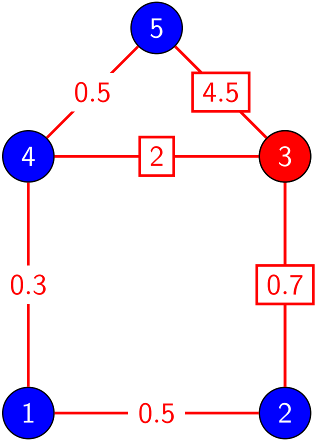

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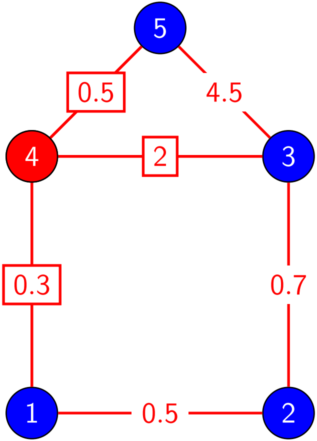
$$\mathbf{D} = \begin{array}{c} \\ 1 \\ 2 \\ 2 \\ 4 \\ 5 \end{array} \begin{array}{c} \begin{matrix} 1 & 2 & 3 & 4 & 5 \end{matrix} \\ \begin{pmatrix} 0.8 & & & & \\ & 1.2 & & & \\ & & \boxed{7.2} & & \\ & & & d_4 & \\ & & & & d_5 \end{pmatrix} \end{array}$$

The weighted degree matrix $\mathbf{D} = (d_{ij})_{1\leqslant i,j\leqslant n}$

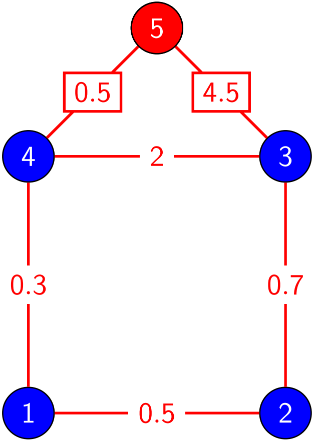


$$d_{ij} = d_i\delta_{ij} = \sum_{j=1}^{n} w_{ij}\delta_{ij}$$

$$\mathbf{W} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \begin{array}{c} \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{pmatrix} 0 & 0.5 & 0 & 0.3 & 0 \\ 0.5 & 0 & 0.7 & 0 & 0 \\ 0 & 0.7 & 0 & 2 & 4.5 \\ \boxed{0.3} & 0 & \boxed{2} & 0 & \boxed{0.5} \\ 0 & 0 & 4.5 & 0.5 & 0 \end{pmatrix} \end{array}$$

$$\mathbf{D} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \begin{array}{c} \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{pmatrix} 0.8 & & & & \\ & 1.2 & & & \\ & & 7.2 & & \\ & & & \boxed{2.8} & \\ & & & & d_5 \end{pmatrix} \end{array}$$

The weighted degree matrix $\mathbf{D} = (d_{ij})_{1 \leqslant i,j \leqslant n}$



$$d_{ij} = d_i \delta_{ij} = \sum_{j=1}^{n} w_{ij} \delta_{ij}$$

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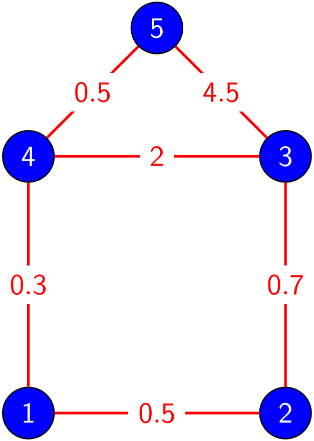
The weighted degree matrix $\mathbf{D} = (d_{ij})_{1 \leqslant i,j \leqslant n}$



$$d_{ij} = d_i \delta_{ij} = \sum_{j=1}^{n} w_{ij} \delta_{ij}$$

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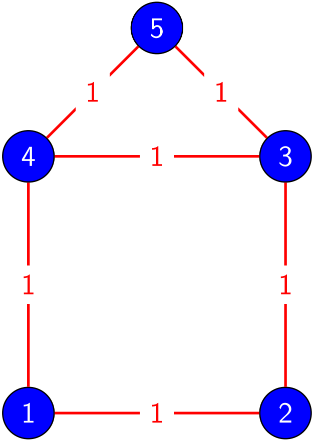
$$\mathbf{D} = \begin{array}{cc} & \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} & \begin{pmatrix} 0.8 & & & & \\ & 1.2 & & & \\ & & 7.2 & & \\ & & & 2.8 & \\ & & & & 5 \end{pmatrix} \end{array}$$

The unweighted degree matrix $\mathbf{D} = (d_{ij})_{1 \leqslant i,j \leqslant n}$



$$\mathbf{A} = \begin{array}{c c} & \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} & \begin{pmatrix} 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{pmatrix} \end{array}$$

$$\mathbf{D} = \begin{array}{c c} & \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} & \begin{pmatrix} 2 & & & & \\ & 2 & & & \\ & & 3 & & \\ & & & 3 & \\ & & & & 2 \end{pmatrix} \end{array}$$

$$d_i = \sum_{j=1}^{n} a_{ij} = \sharp\{j : \{i,j\} \in \mathcal{E}\}$$

Graph signals

Definition

A graph signal is a mapping $f : \mathcal{V} \to \mathbb{R}$ that associates a value $f(v)$ to each node $v \in \mathcal{V}$ of a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, w)$.

The function f can be represented as a vector

$$\mathbf{f} = [f(v_1), \ldots, f(v_n)] \in \mathbb{R}^n$$

where $n = |\mathcal{V}|$ is the number of nodes in the graph.

Hilbert space of functions on vertices

▶ Let $\mathcal{H}(\mathcal{V})$ denote the Hilbert space of real-valued functions on the nodes of a weighted graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, w)$.

By analogy with functional analysis on continuous spaces, the integral of a function $f \in \mathcal{H}(\mathcal{V})$ over the set of nodes $\mathcal{V}$ is defined as:

$$\int_{\mathcal{V}} f = \sum_{v \in \mathcal{V}} f(v)$$

The space $\mathcal{H}(\mathcal{V})$ is endowed with the inner product:

$$\langle f, g \rangle_{\mathcal{H}(\mathcal{V})} = \sum_{v \in \mathcal{V}} f(v) g(v), \quad f, g \in \mathcal{H}(\mathcal{V})$$

▶ Similarly, let $\mathcal{H}(\mathcal{E})$ be the space of real-valued functions defined on the edges of a weighted graph $\mathcal{G}$. It is endowed with the inner product:

$$\langle F, G \rangle_{\mathcal{H}(\mathcal{E})} = \sum_{u \in \mathcal{V}} \sum_{v \sim u} F(u, v) G(u, v), \quad F, G \in \mathcal{H}(\mathcal{E})$$

Difference operator

- The **difference operator**, noted $d : \mathcal{H}(\mathcal{V}) \to \mathcal{H}(\mathcal{E})$, applied to a function $f \in \mathcal{H}(\mathcal{V})$ gives a function $df \in \mathcal{H}(\mathcal{E})$ defined on edges $e = (u, v) \in \mathcal{E}$ by:

$$(df)(e) = \sqrt{w(e)}(f(v) - f(u))$$

- The **directional derivative** (or edge derivative) of f at a node $v \in \mathcal{V}$ along an edge $e = (u, v)$ is defined as:

$$\left.\frac{\partial f}{\partial e}\right|_u = \partial_v f(u) = (df)(u, v)$$

$\Rightarrow$ This is *consistent* with the continuous definition of the derivative:

- $\partial_v f(u) = -\partial_u f(v)$
- $\partial_v f(v) = 0$
- $f(u) = f(v) \Longrightarrow \partial_v f(u) = 0$

Adjoint of the difference operator

The **adjoint of the difference operator**, noted $d^* : \mathcal{H}(\mathcal{E}) \to \mathcal{H}(\mathcal{V})$ is a linear operator defined by:

$$\langle df, G \rangle_{\mathcal{H}(\mathcal{E})} = \langle f, d^* G \rangle_{\mathcal{H}(\mathcal{V})}$$

for any function $f \in \mathcal{H}(\mathcal{V})$ and $G \in \mathcal{H}(\mathcal{E})$.

The adjoint of the difference operator can be expressed as follows:

$$(d^* G)(u) = \sum_{v \sim u} \sqrt{w(u, v)} (G(v, u) - G(u, v))$$

Adjoint of the difference operator

Proof.

$$
\begin{aligned}
\langle df, G\rangle_{\mathcal{H}(\mathcal{E})} &= \sum_{(u,v)\in\mathcal{E}} (df)(u,v)G(u,v) \\
&= \sum_{(u,v)\in\mathcal{E}} \sqrt{w(u,v)}(f(v)-f(u))G(u,v) \\
&= \sum_{(u,v)\in\mathcal{E}} \sqrt{w(u,v)}f(v)G(u,v) - \sum_{(u,v)\in\mathcal{E}} \sqrt{w(u,v)}f(u)G(u,v) \\
&= \sum_{u\in v}\sum_{v\sim u} \sqrt{w(v,u)}f(u)G(v,u) - \sum_{u\in v}\sum_{v\sim u} \sqrt{w(u,v)}f(u)G(u,v) \\
&= \sum_{u\in v} f(u)\sum_{v\sim u} \sqrt{w(u,v)}(G(v,u)-G(u,v)) \\
&= \langle f, d^*G\rangle_{\mathcal{H}(\mathcal{V})} \equiv \sum_{u\in\mathcal{V}} f(u)(d^*G)(u)
\end{aligned}
$$

$\square$

Divergence operator

The **divergence operator** is defined by $-d^*$ and measures the network outflow of a function in $\mathcal{H}(\mathcal{E})$ at each node of the graph.

Proposition

Each function $G \in \mathcal{H}(\mathcal{E})$ has a null divergence over the entire set of nodes

$$\sum_{u \in \mathcal{V}} (d^* G)(u) = 0$$

Proof. Given the previous expression, we have a sum of terms

$$\sqrt{w(v,u)}(G(v,u) - G(u,v)) + \sqrt{w(u,v)}(G(u,v) - G(v,u)) = 0$$

since w is symmetric. $\square$

Gradient operator

The **weighted gradient operator** of a function $f \in \mathcal{H}(\mathcal{V})$ at a node $u \in \mathcal{V}$ is the column vector of dimension $d(u)$ (the *degree* of the node u) defined by:

$$\nabla_w f(u) = (\partial_v f(u) \, : \, v \sim u)^T = (\partial_{v_1} f(u), \ldots, \partial_{v_k} f(u))^T, \quad \forall (u, v_i) \in \mathcal{E}$$

- The L_2 norm of this vector represents the local variation of the function f at node u of the graph:

$$\|\nabla_w f(u)\|_2 = \sqrt{\sum_{v \sim u} (\partial_v f(u))^2} = \sqrt{\sum_{v \sim u} w(u, v)(f(v) - f(u))^2}$$

- The local variation is a seminorm and can be viewed as a **measure of the regularity** of a function around a node.

Laplace operator

The **weighted Laplace operator** of a function $f \in \mathcal{H}(\mathcal{V})$, noted $\Delta_w : \mathcal{H}(\mathcal{V}) \rightarrow \mathcal{H}(\mathcal{V})$ is defined by:

$$\Delta_w f \overset{\text{def}}{=} \frac{1}{2} d^*(df) : u \mapsto \sum_{v \sim u} w(u,v)(f(u) - f(v))$$

Proof. Using the previous expressions of df and d^*G:

$$\begin{aligned}
\Delta_w f(u) &= \frac{1}{2}(d^* df)(u) \\
&= \frac{1}{2} \sum_{v \sim u} \sqrt{w(u,v)}(df(v,u) - df(u,v)) \\
&= \frac{1}{2} \sum_{v \sim u} w(u,v)[(f(u) - f(v)) - (f(v) - f(u))] \\
&= \sum_{v \sim u} w(u,v)(f(u) - f(v))
\end{aligned}$$

$\square$

NB. Note that $\Delta_w f(u) = \frac{1}{2} \sum_{v \sim u} \frac{\partial}{\partial e} \left(\frac{\partial f}{\partial e} \right)\Big|_u = \frac{1}{2} \nabla_w \cdot \nabla_w f \quad$ (*i.e* div(grad))

Laplacian matrix

The Laplace operator $\Delta_w f$ is also called the combinatorial Laplacian matrix $\mathbf{L}$, since one has the following link:

Proposition

$$\Delta_w f(u) = (\mathbf{Lf})[u] \quad \text{with} \quad \mathbf{L} = \mathbf{D} - \mathbf{W}$$

Proof.

$$\begin{aligned}
\Delta_w f(u) &= \sum_{(u,v)\in\mathcal{E}} w(u,v)(f(u) - f(v)) \\
&= d(u)f(u) - \sum_{(u,v)\in\mathcal{E}} w(u,v)f(v) \\
&= (\mathbf{Df})[u] - (\mathbf{Wf})[u] \\
&= ((\mathbf{D} - \mathbf{W})\mathbf{f})[u] \\
&\stackrel{\text{def}}{=} (\mathbf{Lf})[u]
\end{aligned}$$

$\square$

The indicidence matrix of a graph

Let say by convention $e_{ij} = (v_i, v_j)$ with $i < j$ is oriented from v_i to v_j.

The **incidence matrix** $\triangledown_w$[1] of a graph is the $|\mathcal{V}| \times |\mathcal{E}|$ $(n \times m)$

$$(\triangledown_w)_{ve} = \begin{cases} -\sqrt{w(e)} & \text{if } v \text{ is the initial vertex of } e = (v, \cdot) \\ +\sqrt{w(e)} & \text{if } v \text{ is the terminal vertex of } e = (\cdot, v) \\ 0 & \text{otherwise} \end{cases}$$

Then $(\triangledown_w \mathbf{f})_e = (df)(e)$ and the Laplacian matrix can be factorized as:

$$\mathbf{L} = \triangledown_w \triangledown_w^T$$

Proof. Given $u, v \in \mathcal{V}$ and $e \in \mathcal{E}$ it is easy to check that:

$$(\triangledown_w)_{ue}(\triangledown_w^T)_{ev} = \begin{cases} -w(u, v) & \text{if } u \neq v \text{ and } e = (u, v) \\ w(u, s) & \text{if } u = v \text{ and } e = (u, s) \\ 0 & \text{otherwise} \end{cases}$$

By summing up over all edges of the graph the proposition follows $\square$

[1] The matrix $\triangledown_w$ should not be confused with the gradient operator ∇_w.

The Laplacian quadratic form

Proposition

The Laplacian quadratic form of a weighted graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, w)$ is

$$\mathbf{f}^T \mathbf{L} \mathbf{f} = \sum_{v \sim u} w(u, v)(f(v) - f(u))^2$$

Proof. Since $\mathbf{L} = \bigtriangledown_w \bigtriangledown_w^T$ it implies

$$\langle \mathbf{f}, \mathbf{L}\mathbf{f} \rangle = \langle \mathbf{f}, \bigtriangledown_w \bigtriangledown_w^T \mathbf{f} \rangle = \langle \bigtriangledown_w^T \mathbf{f}, \bigtriangledown_w^T \mathbf{f} \rangle = \sum_{e \in \mathcal{E}} (\bigtriangledown_w^T \mathbf{f})_e^2 = \sum_{u \sim v} w(u, v)(f(u) - f(v))^2$$

- This form measures the *smoothness* of the function f. This quantity is small if the function f does not jump too much over any connected edges.
- $\mathbf{L}$ is symmetric and positive semi-definite
- $\mathbf{L}$ has n non-negative, real-valued eigenvalues $0 \leqslant \lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_n$

Dirichlet energy

- The mapping $\mathbf{f} \longrightarrow \nabla_w^T \mathbf{f}$ is known as the **co-boundary mapping** of the graph. It sends functions from space of vertices to edges.
- The Dirichlet energy of a graph signal f is defined by:

$$\mathscr{E}(f) = \sum_{u \sim v} w(u,v)(f(u) - f(v))^2 = \|\nabla_w^T \mathbf{f}\|^2_{\ell^2(\mathcal{E})} = \mathbf{f}^T \mathbf{L} \mathbf{f}$$

- To compute the **gradient of the functional** $\mathscr{E}$ one can look at:

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} \|\nabla_w^T(\mathbf{f} + t\mathbf{g})\|^2_{\ell^2}$$

Since $\nabla_w^T(\mathbf{f} + t\mathbf{g}) = \nabla_w \mathbf{f} + t \nabla_w \mathbf{g}$ and $\|\nabla_w^T \mathbf{h}\|^2 = \langle \nabla_w^T \mathbf{h} \mid \nabla_w^T \mathbf{h} \rangle$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} \|\nabla_w^T(\mathbf{f} + t\mathbf{g})\|^2_{\ell^2} = \langle \nabla_w^T \mathbf{g} \mid \nabla_w^T \mathbf{f} \rangle = \langle \mathbf{g} \mid \nabla_w \nabla_w^T \mathbf{f} \rangle$$

hence $\mathbf{L}\mathbf{f} = \nabla_w \nabla_w^T \mathbf{f}$ is the gradient of $\mathscr{E}$ at the "point" $\mathbf{f}$.

- Functions that minimize the Dirichlet energy are the eigenvectors of the Laplacian matrix $\mathbf{L}$

Spectrum of a graph

Let be an undirected graph, such that its Laplacian matrix is real symmetric, thus **diagonalizable** in an orthonormal eigenbasis

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

where $\mathbf{U} = (\mathbf{u}_1 | \dots | \mathbf{u}_n) \in \mathbb{R}^{n \times n}$ is the matrix of orthonormal eigenvectors and $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \dots, \lambda_n)$ whose eigenvalues give the graph spectrum

$$\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$$

Evaluating the Laplacian quadratic from with $\mathbf{f} = \mathbf{u}_k$ and $\mathbf{L}\mathbf{u}_k = \lambda_k \mathbf{u}_k$:

$$\lambda_k = \mathbf{u}_k^T \mathbf{L} \mathbf{u}_k = \sum_{i \sim j} w_{ij} (u_k(i) - u_k(j))^2$$

such that eigenvectors associated to low eigenvalues tend to be smooth with respect to any path in the network. In block-structured graphs, this usually means quasi-constant within each block.

Laplacian of a graph with one connected component

- Let denote the one vector $\mathbf{1}_n = [1, \ldots, 1]^\top$ and remark that $\mathbf{L}\mathbf{1}_n = \mathbf{0}_n$ that is $\lambda_1 = 0$ is the smallest eigenvalue.
- Besides,
$$0 = \mathbf{u}^T \mathbf{L} \mathbf{u} = \sum_{i \sim j} w_{ij}(u(i) - u(j))^2$$
so if any two vertices are connected by a path, then
$$\mathbf{u} = [u(1), \ldots, u(n)]^\top$$
needs to be constant at all vertices such that the quadratic form vanishes.

$\Rightarrow$ A graph with one connected component has the constant vector $\mathbf{u}_1 = \mathbf{1}_n$ as the only eigenvector associated to eigenvalue 0.

Laplacian of a graph with k connected components

- The k connected components have their own associated Laplacian $\mathbf{L}_k$ (with an eigenvalue 0 with multiplicity 1), such that the matrix $\mathbf{L}$ can be written as a block diagonal matrix formed from the k submatrices $\mathbf{L}_k$.
- The spectrum of $\mathbf{L}$ is the union of the spectra of the $\mathbf{L}_k$, so the eigenvalue $\lambda_1 = 0$ has multiplicity k

Fiedler vector

- The first non-zero eigenvalue λ_{k+1} is called the **Fiedler value** (whose multiplicity is always equal to 1) and represents the *algebraic connectivity of the graph*. The greater value, the more connected graph.
- The corresponding eigenvector $\mathbf{u}_{k+1}$ is called the **Fiedler vector**

Eigenvectors of a connected graph

$\mathbf{u}_1 = \mathbf{1}_n$ and $\mathbf{u}_2$ is the Fiedler vector.

For any eigenvector $\mathbf{u}_k = (u_k(v_1), \ldots, u_k(v_n))^\top$ with $2 \leqslant k \leqslant n$

- The eigenvectors form an orthonormal basis $\mathbf{u}_k^\top \mathbf{u}_l = \delta_{kl}$
- $|u_k(v_i)| < 1$
- Its mean is null

$$\mathbf{u}_k^\top \mathbf{1}_n = 0 \Longleftrightarrow \sum_{i=1}^{n} u_k(v_i) = 0$$

Manifold unfolding problem

Given a set of points in a high dimensional Euclidian space but along a manifold $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathcal{M} \subset \mathbb{R}^d$, we want to find another set of vectors in a low-dimensional Euclidien space $\mathbf{y}_1, \ldots, \mathbf{y}_n \in \mathbb{R}^k$ with $k \ll d$ and such that $\mathbf{y}_i$ "represents" $\mathbf{x}_i$.

1. **Build a neighborhood graph** $G = (\mathcal{V}, \mathcal{E})$ from the given data $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathcal{M} \subset \mathbb{R}^d$ by connecting only "nearby" points:
   - connecting a point to its k-nearest neighbors (kNN graph),
   - connecting a point to all points closer than ϵ (in some measure);
2. **Associate a weight to each existing edge**. In general, we want that the closer a pair of points, the larger the weight on the associated edge. A classical option is to use the Gaussian kernel to define the similarity graph:

$$w_{ij} = w(v_i, v_j) = \mathrm{d}(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\sigma^{-2} \|\mathbf{x}_i - \mathbf{x}_j\|_2^2)$$

3. Consider an embedding $f : \mathcal{V} \to \mathbb{R}^k$ and denote by $\mathbf{y}_i = f(i) \in \mathbb{R}^k$ the coordinates of node i in the embedding space.

Laplacian Eigenmaps on a line

Let consider the problem of mapping the graph to a line (1D dimension reduction $k = 1$) in such a way *close nodes will still be close on the line*.

$\Rightarrow$ Laplacian eigenmaps will preserve the local geometry.

Let $\mathbf{f} = [f(v_1), \ldots, f(v_n)]^T$ with $f(v_i) \in \mathbb{R}$ represent the 1D embedding of the nodes. Then, we want to solve:

$$\mathbf{f}^\star = \underset{\mathbf{f} \in \mathbb{R}^n}{\arg\min} \sum_{i \sim j} w_{ij} (f_i - f_j)^2 = \underset{\mathbf{f} \in \mathbb{R}^n}{\arg\min}\, \mathbf{f}^\top \mathbf{L} \mathbf{f}$$

Interpretation:

- If w_{ij} is large (close to 1, meaning $\mathbf{x}_i$ and $\mathbf{x}_j$ are originally close) then f_i and f_j must still be close.
- If w_{ij} is small (close to 0, meaning $\mathbf{x}_i$ and $\mathbf{x}_j$ are originally very far) then there is much flexibility in putting f_i and f_j on the line.

Laplacian Eigenmaps on a line

- To make the objective function scaling invariant in $\mathbf{f}$ (and also to get rid of the trivial solution 0 and constant vector), we add additional constraint leading to the Rayleight quotient:

$$\mathbf{f}^\star = \underset{\substack{\mathbf{f} \neq \mathbf{0} \in \mathbb{R}^n \\ \mathbf{f}^\top \mathbf{1}_n = 0}}{\arg\min} \frac{\mathbf{f}^\top \mathbf{L} \mathbf{f}}{\mathbf{f}^\top \mathbf{f}}$$

- The minimizer of this new problem is given by the second smallest eigenvector of the Laplacian matrix $\mathbf{L}$ that is the **Fiedler vector**:

$$\mathbf{f}^\star = \mathbf{u}_2$$

and the minimum value of the Rayleight quotient is λ_2.

NB. $\mathbf{u}_2$ is the normalized vector that minimizes local variation and that has zero average. Similarly, $\mathbf{u}_3$ is the normalized vector that minimizes local variation and that is orthogonal both to $\mathbf{u}_1$ and $\mathbf{u}_2$, etc.
Spectral clustering takes advantage of this property.