In the lectures, we introduced the Graph Laplacian as $L = D - W$, or with unweighted edges $L = D - A$ where A is the adjacency matrix.

Interestingly, L can be seen as a kind of "derivative" for functions defined on the graph.

Laplace operator

Lets first take a step back into the "real-valued" world! Given a scalar field $f(\vec{x})$, its gradient is given by $\vec{\nabla} f(\vec{x}) = \begin{pmatrix} \partial_{x_i} f(\vec{x}) \\ \vdots \end{pmatrix}$.

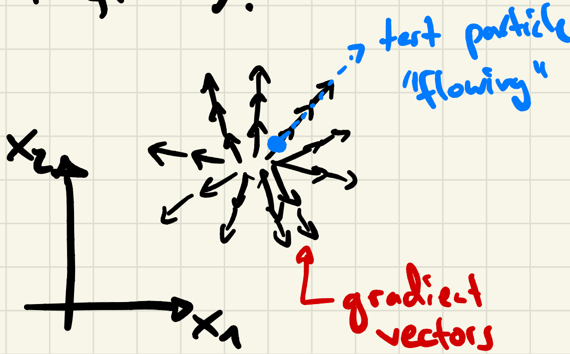
This gives us the direction of "steepest" ascend.
The Laplacian is defined as

$$\Delta f = \vec{\nabla} \cdot \vec{\nabla} f(\vec{x}) = \mathrm{div}(\mathrm{grad}\, f)$$
$$= \sum_i \partial_{x_i}^2 f$$

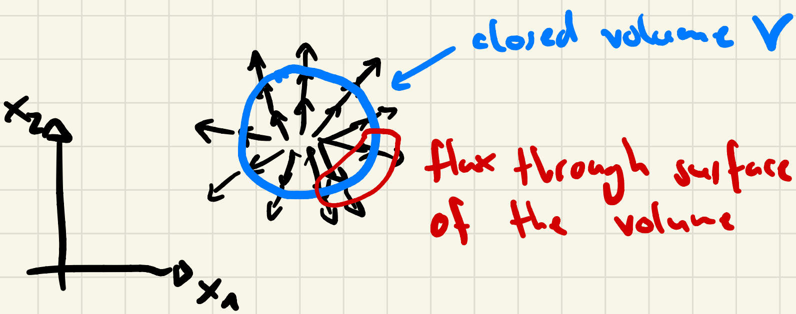
which is the sum of second derivatives!

What does this mean?

Consider little particles that follow the gradients (a "gradient flow").



If we integrate the Laplacian over a given closed volume, this tells us "how much" flows in or out of that volume (Gauss's theorem).



$\longrightarrow$ $\int_V \Delta f > 0$ flow outwards
(the volume contains a "source")

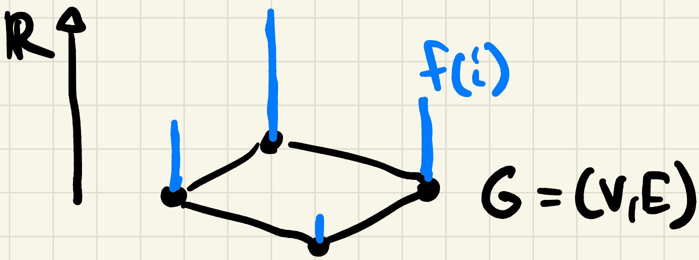
$\int_V \Delta f < 0$ flow inward
(the volume contains a "sink")

$\int_V \Delta f = 0$ "no" flow on average

What does this have to do with graphs?

We can define the same operator for functions on graphs, which will turn out to be L!

First, we define a function that assigns every node i a real value: $f: V \rightarrow \mathbb{R}$ where V is the set of all graph nodes.



The edges kinda represent "different directions", although its non-Euclidean.

As before, lets define the gradient per edge:

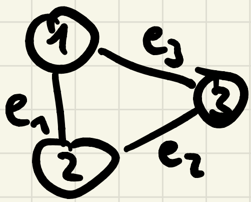
$$\text{grad}_e f = f(i) - f(j) \text{ for } e = \underbrace{(i,j)}_{\substack{\text{edge between} \\ \text{node } i \text{ and } j}}$$

We can write this with the incidence matrix $K \in \mathbb{R}^{|V| \times |E|}$:

$$K_{ue} = \begin{cases} 1 & \text{if } \exists v' \in V \text{ s.t. } e = (u, v') \\ -1 & \text{if } \exists v' \in V \text{ s.t. } e = (v', u) \\ 0 & \text{otherwise} \end{cases}$$

With this, we can write $\text{grad} f = K^T f$.

<u>Example:</u>



$$\longrightarrow \quad K = \begin{pmatrix} 1 & 0 & 1 \\ -1 & 1 & 0 \\ 0 & -1 & -1 \end{pmatrix}$$

$$K^T = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ 1 & 0 & -1 \end{pmatrix}$$

$$\Rightarrow K^T f = \begin{pmatrix} f_1 - f_2 \\ f_2 - f_3 \\ f_1 - f_3 \end{pmatrix} \left.\vphantom{\begin{pmatrix} a \\ b \\ c \end{pmatrix}}\right\} \text{for every edge! } \hat{=} \text{ every "direction"}$$

With this, we can calculate the "Laplacian":

$$L = K K^T \quad \hat{=} \quad \text{div}(\text{grad}) = \vec{\nabla} \cdot \vec{\nabla}$$

which then represents the divergence of the "gradient flow" on the graph (same idea as in the continuous case!).

Lets look at it!

$$L_{ac} = (KK^T)_{ac} = \sum_b K_{ab} K^T_{bc} = \sum_b K_{ab} K_{cb}$$

<u>case 1:</u> $a=c$: $L_{aa} = \sum_b K_{ab}^2$ = # edges connecting to node a = D_{aa} ← degree matrix

$=1$ if b is an edge of a

<u>case 2:</u> $a \neq c$: $L_{ac} = \sum_b K_{ab} K_{cb}$

$$= \begin{cases} -1 & \text{if } \exists b' : b' = (a,c) \\ 0 & \text{otherwise} \end{cases}$$

$= -A_{ac}$ ← adj. matrix

$$\Rightarrow L = KK^T = D - A$$ $\hat{=}$ discrete version of continuous Laplace operator