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## 5 Diffusion Equations on Graph.

### ⊛ Background : Heat diffusion equation.

↳ Informally, diffusion describes the movement of substances from higher to lower concentration. For example, the heat diffused from a hot surface to a cold surface.

↳ (Diffusion Equation) Let $x(t)$ denote a family of scalar-valued function on $\Omega \times [0,\infty)$ representing distribution of some property (in this case, temperature). According the Fourier's law of heat conduction, the heat flux:

$$\rightarrow \quad h \propto -\nabla x \Rightarrow h = -g \nabla x$$

↳ g is refered to as the diffusitivity of substance.

Conservation conditn → $\dfrac{\partial x(u,t)}{\partial t} = -\operatorname{div}(h)$

(No heat created/disappear).

↳ In an idealized homogeneous setting, we assume g to be a constant throughout $\Omega$. More generally, the diffusitivity is position dependent. So g can be either a scalar-valued or a matrix-valued function:

$$⊛ \rightarrow \boxed{\frac{\partial x(u,t)}{\partial t} = \operatorname{div}\left[g(u, x(u,t), t)\,\nabla x(u,t)\right]}$$

↳ Depending on the choice of diffusitivity equation, we will have.

① $\dfrac{\partial x}{\partial t} = c \Delta x$

Homogeneous isotropic (Diffusion is the same everywhere).

② $\dfrac{\partial x}{\partial t} = \operatorname{div}[a \nabla x]$ (position dependent)

Non-homo isotropic (In GRAND a is learned as an attention function).

③ $\dfrac{\partial x}{\partial t} = \operatorname{div}[A \nabla x]$ (position & diffusion dependn.)

Non-homo Anisotropic

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## (*) Diffusion equation on graph.

↳ The message passing on a graph is nothing but diffusion in discrete domain.

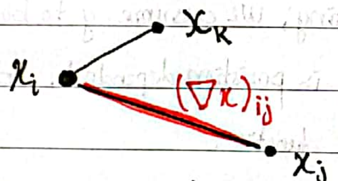
↳ So how to get from the continuous PDE - diff eqution to graph?

## (*) Spatial discretisation.

↳ Let $G = (V, E)$ be an undirected graph with $|V| = n$ nodes and $|E| = e$ edges. Let $x$ and $X$ define features defined on nodes and edges respectively.

↳ denotes $w_{ij}$ as the adjacency of $G$ : $w_{ij} = w_{ji} = 1$ if $(i,j) \in E$. We tactically assume that the edge field is alternating => $X_{ij} = -X_{ji}$ and no self-edges (i.e $(i,i) \notin E \ \forall \ 1 \leq i \leq |V|$).

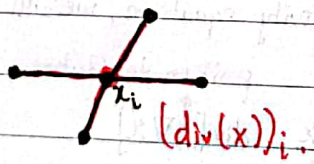
↳ ① The gradient $(\nabla x)_{ij}$.




(*) $$\boxed{(\nabla x)_{ij} = -(x_i - x_j)}$$

→ The gradient $(\nabla x)_{ij}$ assigns edge $(i,j) \in E$ the difference between its endpoints.

↳ ② The divergence $(\mathrm{div}(X))_i$




(*) $$\boxed{(\mathrm{div}(X))_i = \sum_{j=1}^{n} w_{ij} X_{ij}}$$

→ Similarly, the divergence $(\mathrm{div}(X))_i$ assigns node $i$ with the sum of all the edges that it shares.

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Diffusion equation on graphs.

We consider the following diffusion equation on graph:

How to get here?

$$\frac{\partial}{\partial t} x(t) = \mathrm{div}\left[G(x(t),t)\,\nabla x(t)\right]$$

Where $G$ is an $e \times e$ diagonal matrix $G = \mathrm{diag}(a(x_i(t), x_j(t), t))$ and $a$ is some function that computes the similarity between node $j$ and $i$.

We can rewrite the diffusion equation as:

$$\frac{\partial}{\partial t} x(t) = (A(x(t)) - I)\,x(t) = \bar{A}(x(t))\,x(t)$$

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