Graphs in Machine Learning

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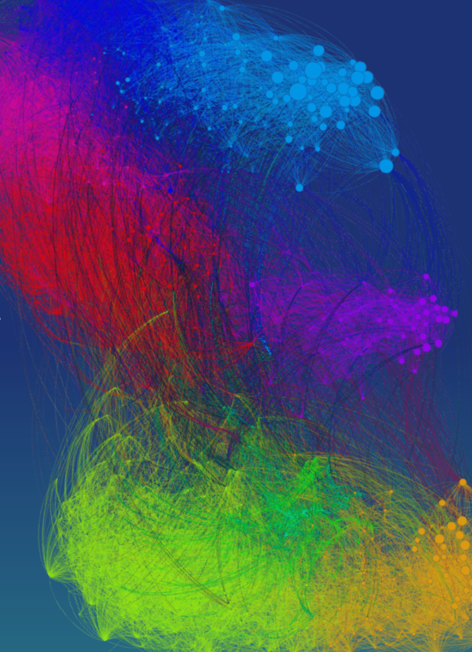
Based on material by: Petar Veličković, Marc Lelarge

https://petar-v.com/communications.html

https://dataflowr.github.io



Message passing GNNs

recapping

A recipe for graph neural networks

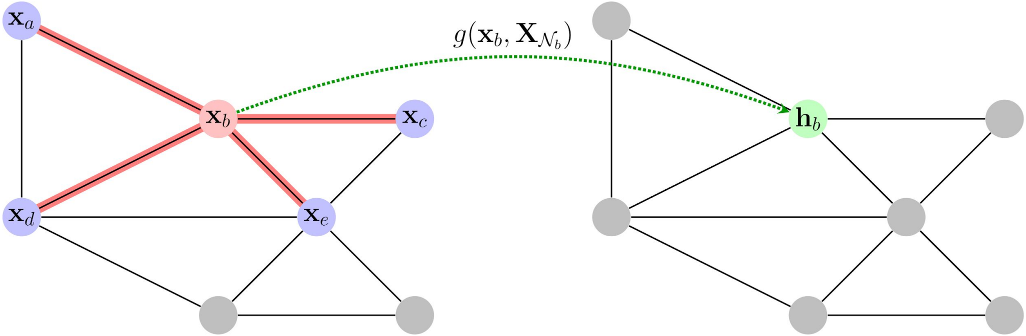
$X \in \mathbb{R}^{n \times d}$ $\quad n = |V|$

We can construct permutation equivariant functions $f(\mathbf{X}, \mathbf{A})$ by appropriately applying an invariant g over all local neighbourhoods:

features with dim d $\quad$ adjacency matrix

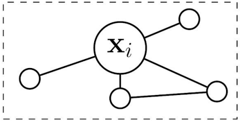
$$f(\mathbf{X}, \mathbf{A}) = \begin{bmatrix} — & g(\mathbf{x}_1, \mathbf{X}_{\mathcal{N}_1}) & — \\ — & g(\mathbf{x}_2, \mathbf{X}_{\mathcal{N}_2}) & — \\ & \vdots & \\ — & g(\mathbf{x}_n, \mathbf{X}_{\mathcal{N}_n}) & — \end{bmatrix}$$

A recipe for graph neural networks, visualised



$$\mathbf{X}_{\mathcal{N}_b} = \{\!\{\mathbf{x}_a, \mathbf{x}_b, \mathbf{x}_c, \mathbf{x}_d, \mathbf{x}_e\}\!\}$$

General blueprint for learning on graphs



Inputs
$(\mathbf{X}, \mathbf{A})$

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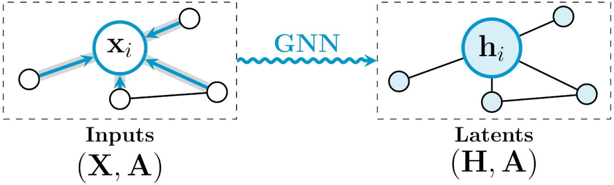

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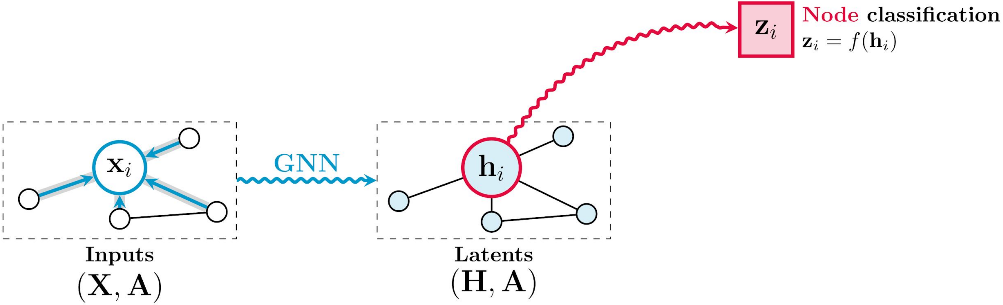

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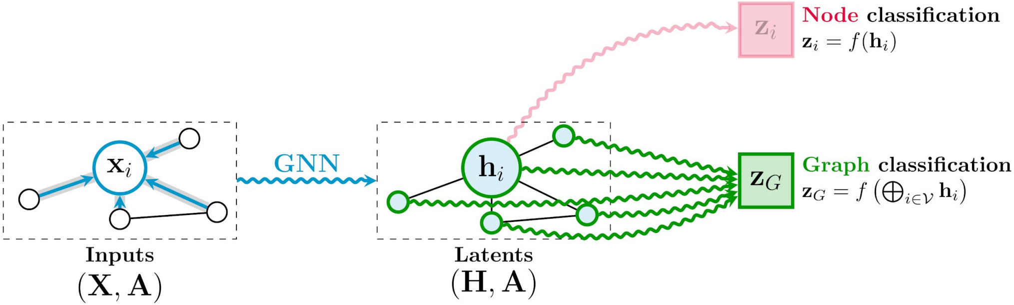

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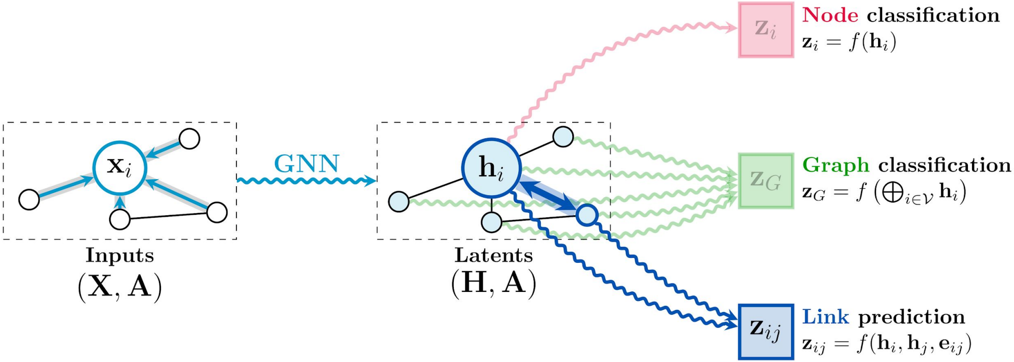
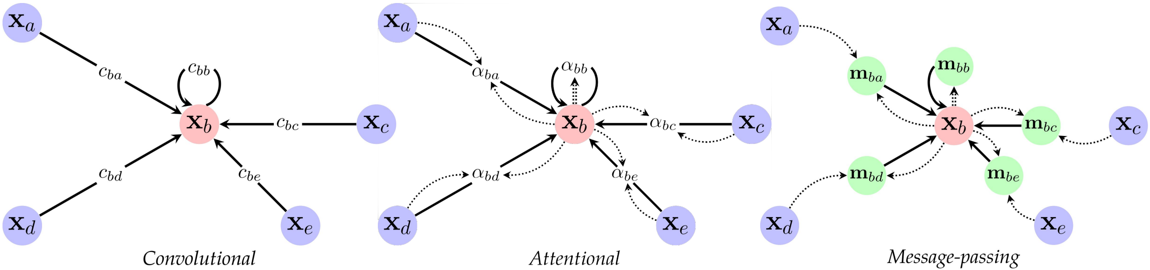


The three "flavours" of GNN layers



$$\mathbf{h}_i = \phi\left(\mathbf{x}_i, \bigoplus_{j\in\mathcal{N}_i} c_{ij}\psi(\mathbf{x}_j)\right) \qquad \mathbf{h}_i = \phi\left(\mathbf{x}_i, \bigoplus_{j\in\mathcal{N}_i} a(\mathbf{x}_i,\mathbf{x}_j)\psi(\mathbf{x}_j)\right) \qquad \mathbf{h}_i = \phi\left(\mathbf{x}_i, \bigoplus_{j\in\mathcal{N}_i} \psi(\mathbf{x}_i,\mathbf{x}_j)\right)$$

Spectral GNNs

the Laplacian strikes back

Convolutions on a graph

GCNs start from convolution, but then replaces it with permutation $\{$in,equ$\}$ivariance

$\hookrightarrow$ how far can we take vanilla convolutions in graph ML?

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The convolution theorem defines a very attractive identity:

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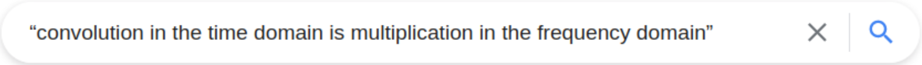
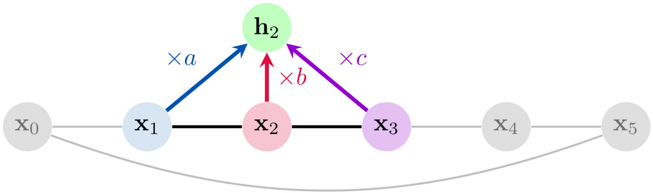


Convolutions on a graph

For special graphs (e.g., direct cycle) we can directly define a convolution over it:



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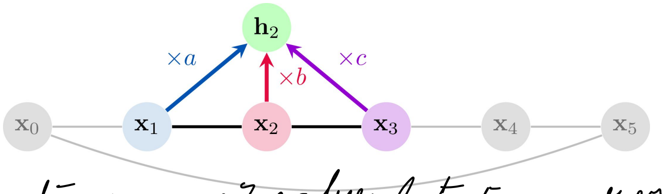

circulant matrix : same 3 values but at every row, move right

This convolution can be represented using a **circulant** matrix $C([b, c, 0, \dots, 0, a])$

$$f(\mathbf{X}) = \begin{bmatrix} b & c & & & a \\ a & b & c & & \\ & \ddots & \ddots & \ddots & \\ & & a & b & c \\ c & & & a & b \end{bmatrix} \begin{bmatrix} — & \mathbf{x}_0 & — \\ — & \mathbf{x}_1 & — \\ & \vdots & \\ — & \mathbf{x}_{n-2} & — \\ — & \mathbf{x}_{n-1} & — \end{bmatrix}$$

Properties of circulants, and their eigenvectors

Circulant matrices commute: $C(\mathbf{a})C(\mathbf{b})\mathbf{X} = C(\mathbf{b})C(\mathbf{a})\mathbf{X}$, for any parameters $\mathbf{a}$, $\mathbf{b}$
$\hookrightarrow$ matrices that commute are jointly **diagonalisable**

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↳ the eigenvectors of circulants are the discrete Fourier basis!

$$\phi = \frac{1}{\sqrt{n}}\left(1, e^{\frac{2\pi il}{n}}, e^{\frac{2\pi i\cdot 2\cdot l}{n}}, \ldots, e^{\frac{2\pi i\cdot(n-1)\cdot l}{n}}\right)$$

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If we stack these Fourier basis vectors ϕ into a matrix $\mathbf{\Phi}$ we recover the discrete Fourier transform (DFT) as multiplication by $\mathbf{\Phi}^*$ (adjoint).

Properties of circulants, and their eigenvectors

We can now eigendecompose any circulant as $C(\boldsymbol{\theta}) = \boldsymbol{\Phi}\boldsymbol{\Theta}\boldsymbol{\Phi}^*$
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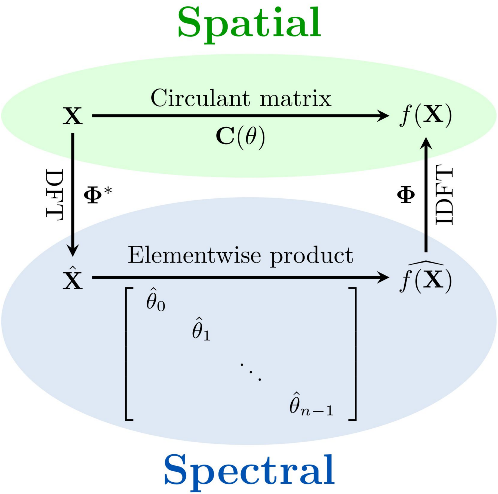
The convolution theorem naturally follows:

$$f(\mathbf{x}) = C(\boldsymbol{\theta})\mathbf{X} = \boldsymbol{\Phi}\boldsymbol{\Theta}\boldsymbol{\Phi}^* = \boldsymbol{\Phi}\begin{bmatrix}\widehat{\boldsymbol{\theta}}_0 & & \\ & \ddots & \\ & & \widehat{\boldsymbol{\theta}}_n\end{bmatrix}\boldsymbol{\Phi}^{*\mathbf{X}} = \boldsymbol{\Phi}(\widehat{\boldsymbol{\theta}} \cdot \widehat{\mathbf{X}})$$

and as long as we know $\boldsymbol{\Phi}$ we can express convolutions as multiplications in $\widehat{\boldsymbol{\theta}}$.

The spectral CNN blueprint



From spectral CNN to spectral GNN

For which convolutions we know $\mathbf{\Phi}$?
↳ cycle $\rightarrow$ DFT

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grid $\rightarrow$ n-way DFT

general graph $\rightarrow$????

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general graph $\rightarrow$ eigenvectors of Laplacian! ↳ captures the structure of the graph

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This allows us to re-express $\mathbf{L} = \mathbf{\Phi}\mathbf{\Theta}\mathbf{\Phi}^{\mathsf{T}}$, as before

↳ changing the eigenvalues in $\mathbf{\Theta}$ expresses any operation that commutes with $\mathbf{L}$

commonly referred to as the graph Fourier transform (Bruna et al., ICLR'14)

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To convolve with some feature matrix $\mathbf{X}$ we do as usual (the diagonal can be **learned**):

$$f(\mathbf{x}) = \boldsymbol{\Phi} \begin{bmatrix} \widehat{\boldsymbol{\theta}}_0 & & \\ & \ddots & \\ & & \widehat{\boldsymbol{\theta}}_n \end{bmatrix} \boldsymbol{\Phi}^* \mathbf{X} = \boldsymbol{\Phi}(\widehat{\boldsymbol{\theta}} \cdot \widehat{\mathbf{X}})$$

Spectral GNNs in practice

Directly learning the eigenvalues is typically inappropriate
$\hookrightarrow$ Not localised, doesn't transfer to other graphs, computationally expensive, ...

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↳ i.e., $f(\mathbf{X}) = \mathbf{\Phi} p_k(\mathbf{\Theta})\mathbf{\Phi}^\intercal = p_k(\mathbf{L})\mathbf{X}$
↳ Cubic splines (Bruna et al., ICLR'14)
Chebyshev polynomials (Defferrard et al., NeurIPS'16)
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This is equivalent to some **conv-GNN!**
↳ Most efficient spectral approaches "spatialise" themselves in similar ways
The "spatial-spectral" divide is often *not really a divide* but a **design tool!**

The Transformer positional encodings and beyond

Transformers signal that the input is a sequence of words by using positional embeddings

$$PE_{(pos,2i)} = \sin(pos/10000^{2i/d_{\mathsf{model}}}), \qquad PE_{(pos,2i+1)} = \cos(pos/10000^{2i/d_{\mathsf{model}}}),$$

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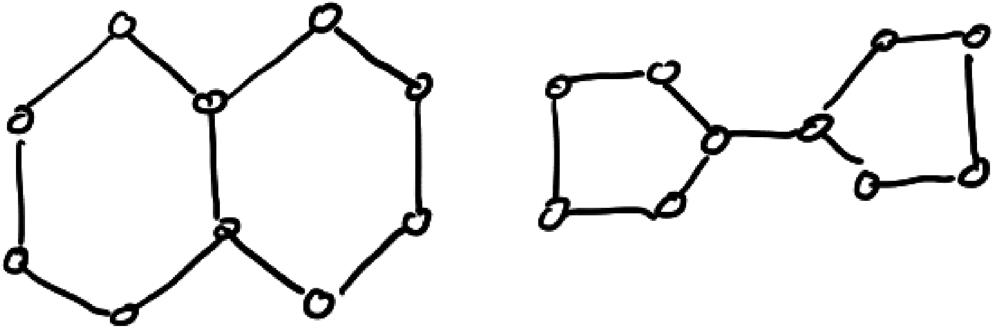
↳ Another flavor of Graph Transformers! (Dwivedi & Bresson, 2021)

GNNs’ expressiveness

and new architectural directions

https://dataflowr.github.io/website/modules/graph3/

A problematic pair of graphs



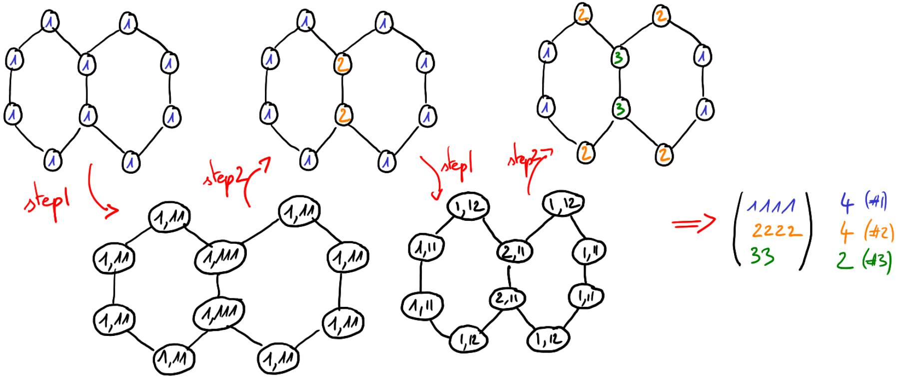
Separating power

Let $\mathcal{F}$ be a set of functions $f : \mathcal{X} \to \mathbb{R}$, then $\mathcal{F}$'s equivalence relation $\rho(\mathcal{F})$ on $\mathcal{X}$ is:

$$(\mathbf{x}, \mathbf{x}') \in \rho(\mathcal{F}) \iff \forall f \in \mathcal{F}, f(\mathbf{x}) = f(\mathbf{x}').$$

Given two sets of functions $\mathcal{F}$ and $\mathcal{H}$, $\mathcal{F}$ is more separating than $\mathcal{H}$ if $\rho(\mathcal{F}) \subset \rho(\mathcal{H})$.

2-Weisfeiler-Lehman test



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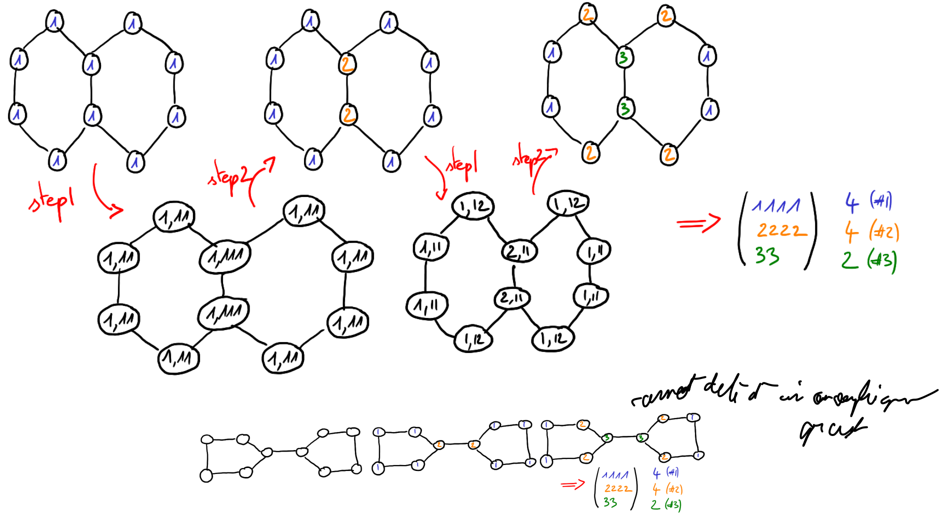
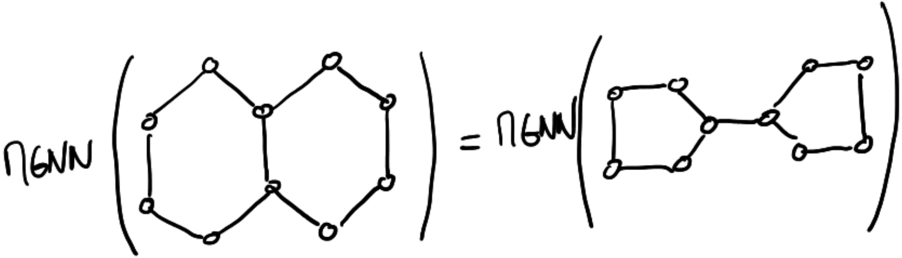
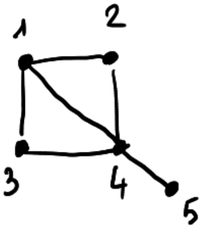


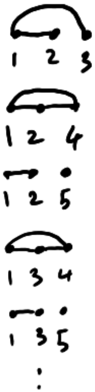
How Powerful Are Graph Neural Networks?, Xu et al., ICLR 2019

Message Passing GNNs are as powerful as 2-Weisfeiler-Lehman test



On the Universality of Invariant Networks, Maron et al., ICML 2019





(1,2,3)	[1 1 0]
(1,2,4)	[1 1 1]
(1,2,5)	[1 0 0]
(1,3,4)	[1 1 1]
(1,3,5)	[1 0 0]
⋮	⋮

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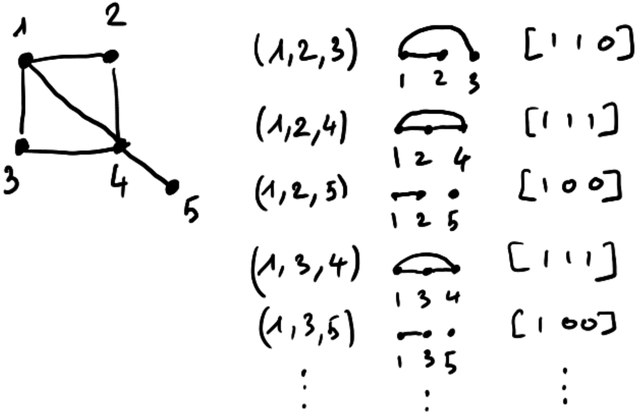

Minimal required order is $k \geq n^2$ to be able to approximate any invariant function.

Provably Powerful Graph Networks, Maron et al., NeurIPS 2019

Folklore GNN (FGNN)

$$\mathbf{h}'_{i\to j} = g\left(\mathbf{h}_{i\to j}, \sum_{k\in\mathcal{V}} \psi(\mathbf{h}_{i\to k}) \odot \psi(\mathbf{h}_{k\to j})\right)$$

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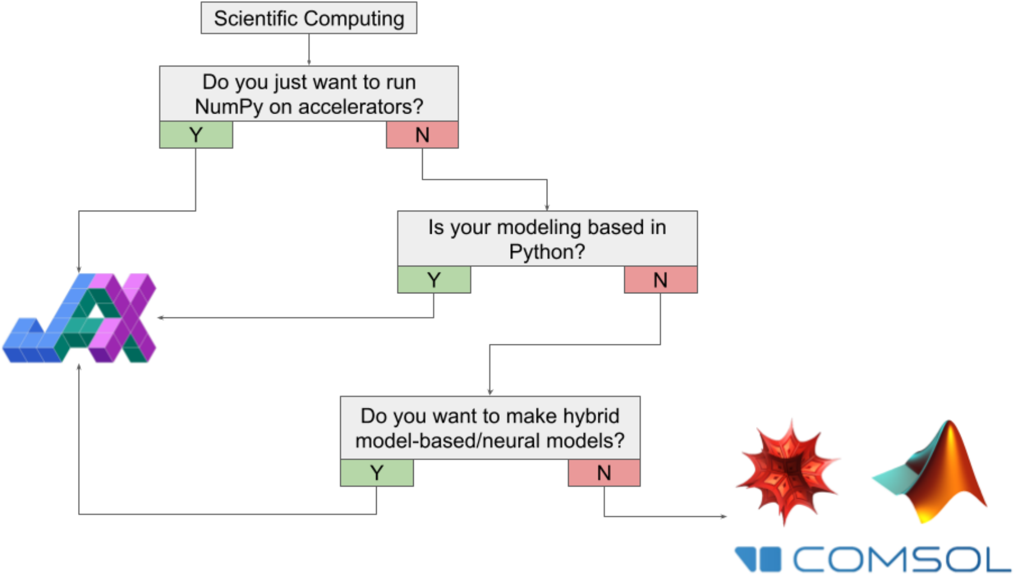
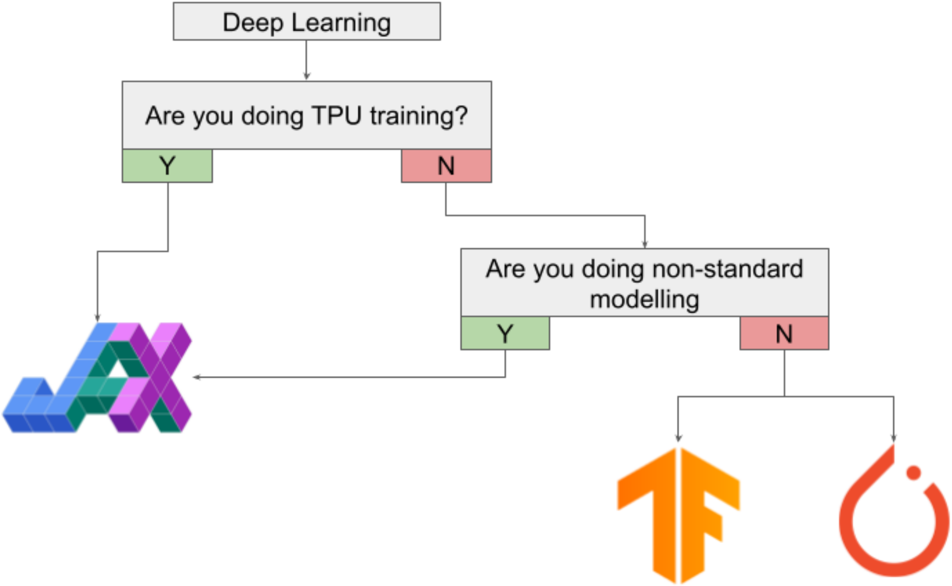
$$\rho(\mathsf{FGNN}) \not\subset \rho(2 - \mathsf{WL}) = \rho(\mathsf{MGNN})$$

JAX intro

just autograd and XLA



https://www.assemblyai.com/blog/why-you-should-or-shouldnt-be-using-jax-in-2023/



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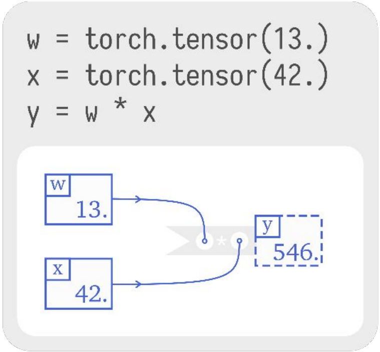
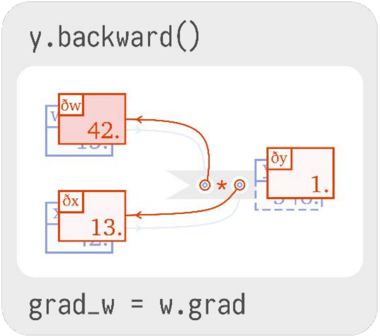
Tape-based autograd, e.g. PyTorch:

Executing code produces graph/tape



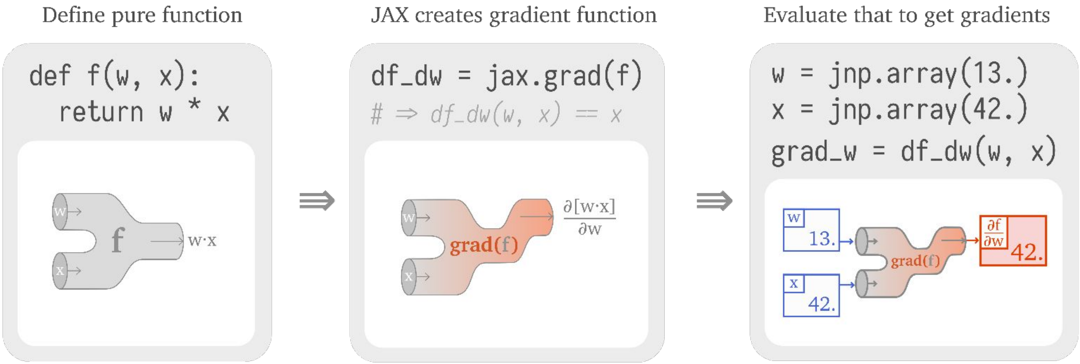
$\Rrightarrow$

Backprop/reverse-mode autodiff
by following the graph/tape



https://sjmielke.com/jax-purify.htm

Pure transformation-based autograd: JAX



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Two introductory colabs

https://github.com/deepmind/dm-haiku/blob/main/docs/notebooks/basics.ipynb

https://github.com/deepmind/dm-haiku/blob/main/docs/notebooks/parameter_sharing.ipynb

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