SUSAN: The Structural Similarity Random Walk Kernel

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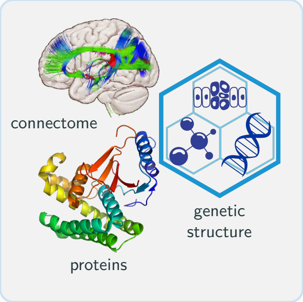
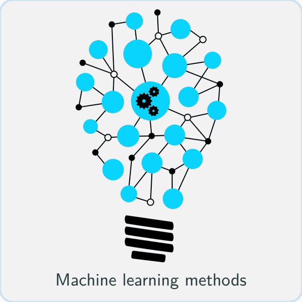
Comparing graphs

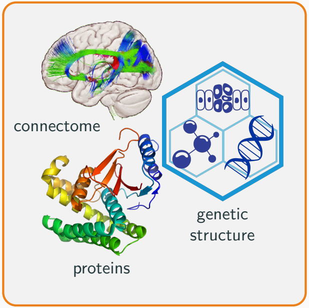


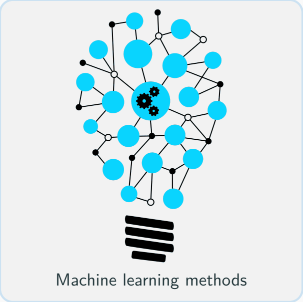


Applications

Standard Tools

Comparing graphs





Applications

Classification, Regression, Clustering, Dim. Reduction

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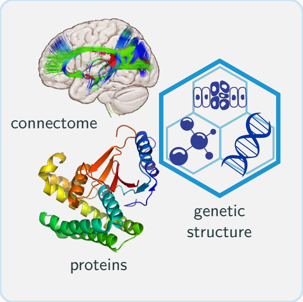

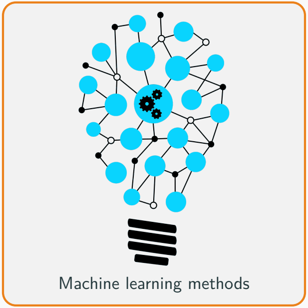

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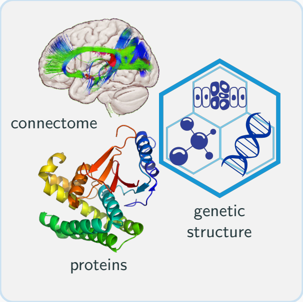

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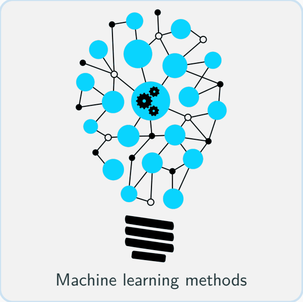

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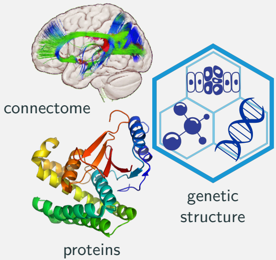

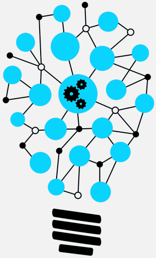

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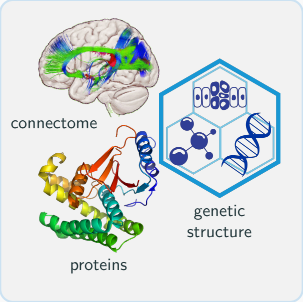

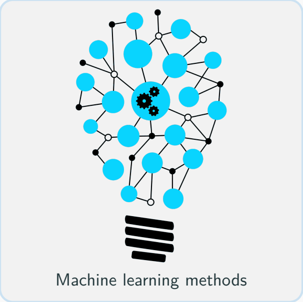

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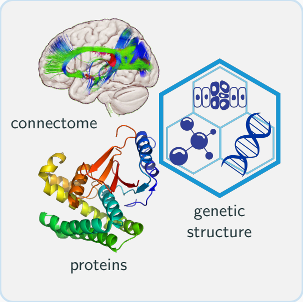

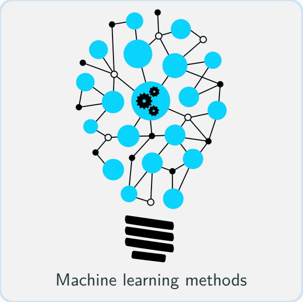

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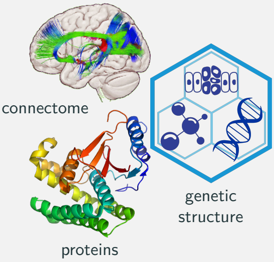

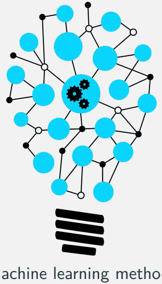

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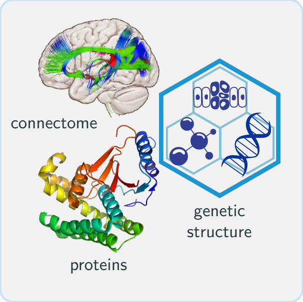

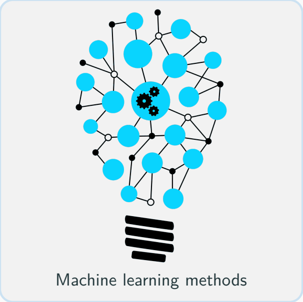

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Can we apply standard tools on graphs?

$\Longrightarrow$ Use a kernel on graphs

How do kernels compare graphs?

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Goal: Can we define something like $\langle G_1, G_2 \rangle$?

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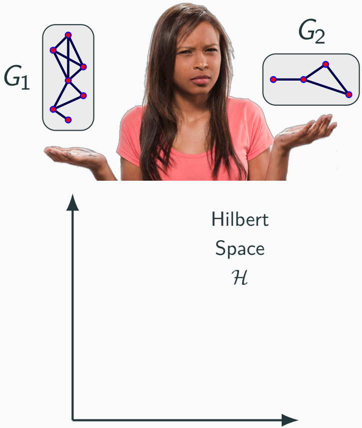

Kernels define a space $\mathcal{H}$
with $\langle \cdot, \cdot \rangle$ and mapping function ϕ

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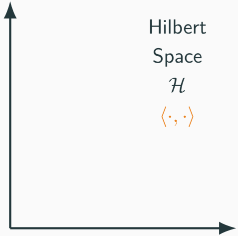

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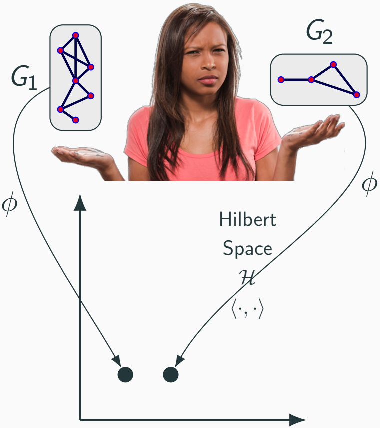

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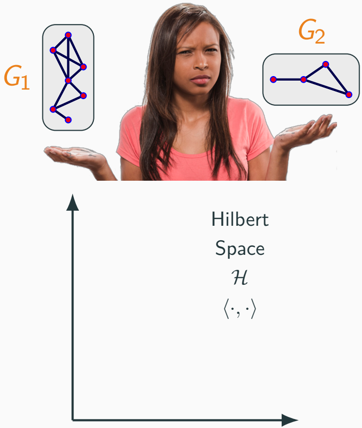

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$\Longrightarrow$ Use as graph similarity

G_1 , G_2

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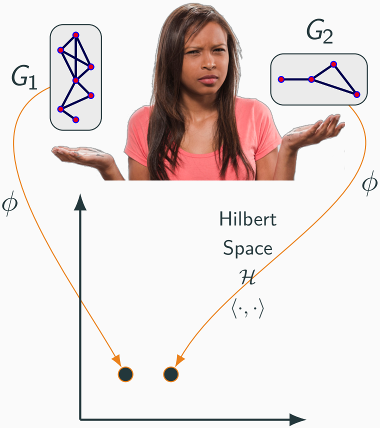

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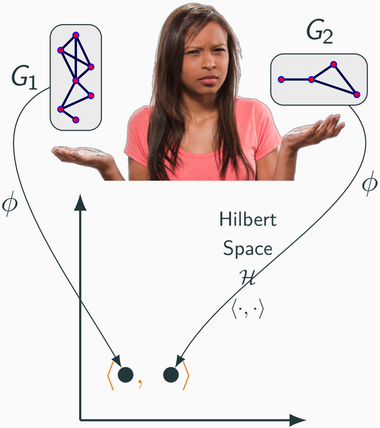

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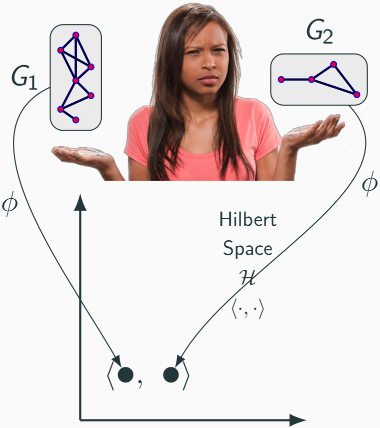

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$\Longrightarrow$ Use as graph similarity
$k(G_1, G_2) := \langle \phi(G_1), \phi(G_2) \rangle_{\mathcal{H}}$

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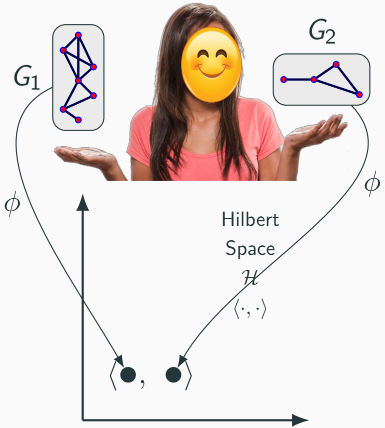

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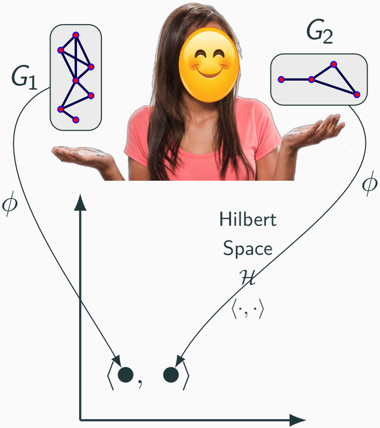

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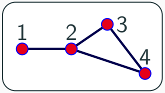
We focus on Random Walk kernels

Random Walk (Reproducing) Kernels [Gärtner et al., 2003]

G_1



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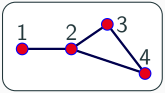

ex: 3-step walk: $(1, 2, 3, 4)$

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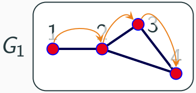

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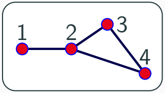

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1-step walks from 1, 3?

$$\underbrace{\begin{bmatrix}0\\2\\0\\1\end{bmatrix}}_{x_1} = \underbrace{\begin{bmatrix}0&1&0&0\\1&0&1&1\\0&1&0&1\\0&1&1&0\end{bmatrix}}_{A}\underbrace{\begin{bmatrix}1\\0\\1\\0\end{bmatrix}}_{x_0}$$

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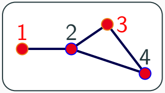

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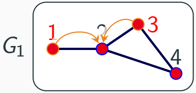

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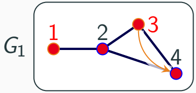

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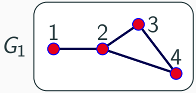

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#k-step walks from x_0?

$$x_k = A^k x_0$$

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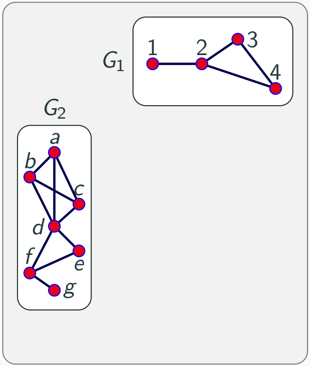

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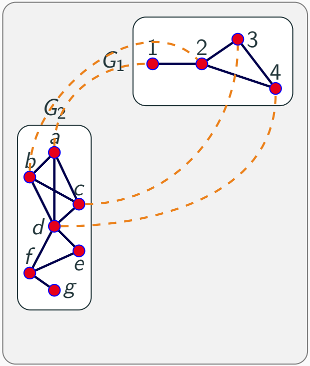
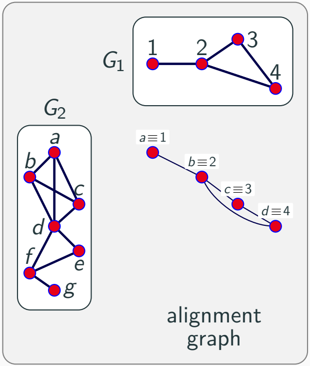


Goal: Count common walks

But: in 2 graphs?

- Assume vertex alignment
  e.g.: $a \equiv 1$, $b \equiv 2$, $c \equiv 3$, $d \equiv 4$



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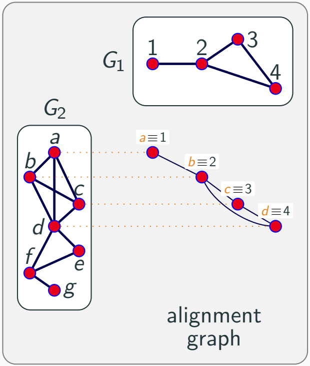

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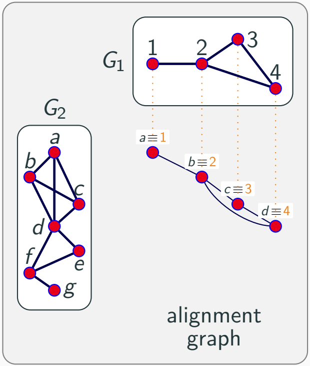

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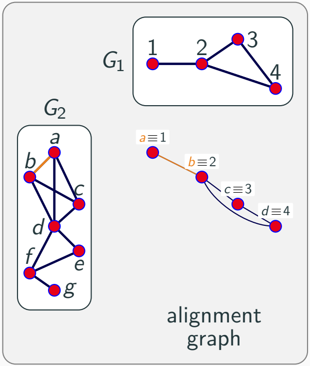

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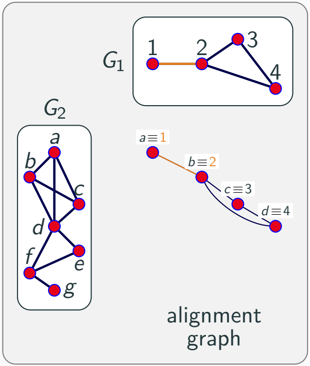

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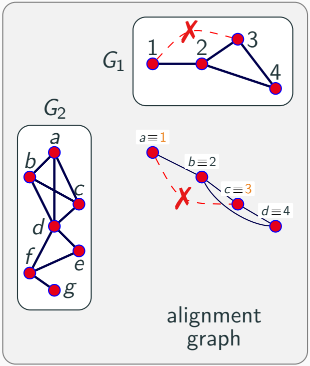

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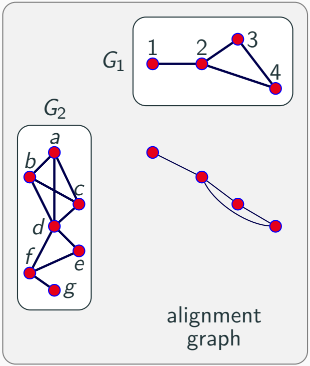

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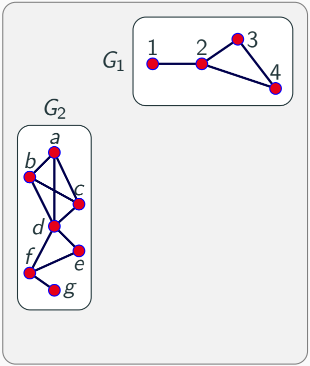

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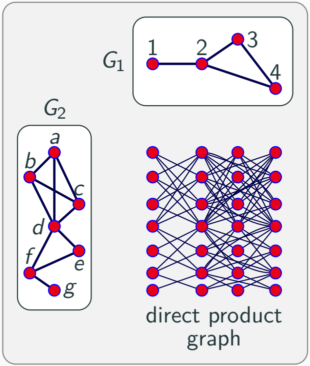

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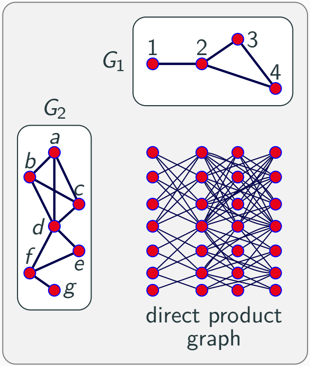
But: Alignments are rarely available

$\Longrightarrow$ Use all possible alignments



Direct product graph:

$$A_\times = A \otimes A'$$

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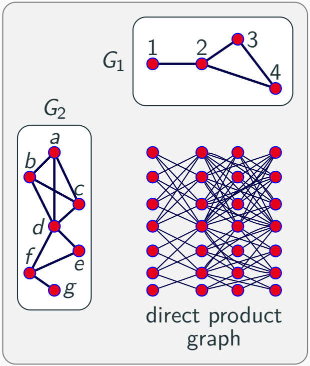

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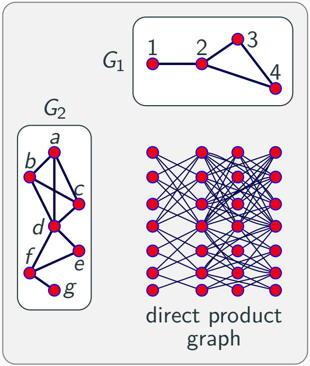

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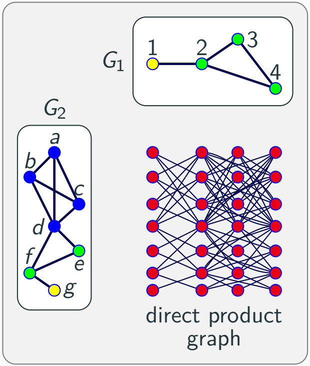

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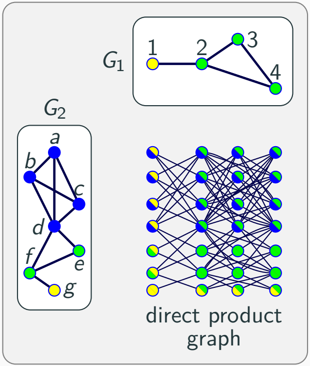

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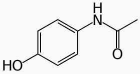

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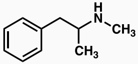

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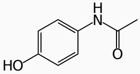

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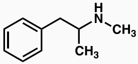

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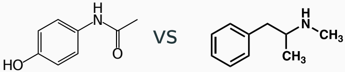

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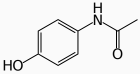

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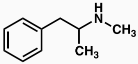

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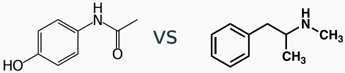

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We propose to use

$\Longrightarrow$ core decomposition

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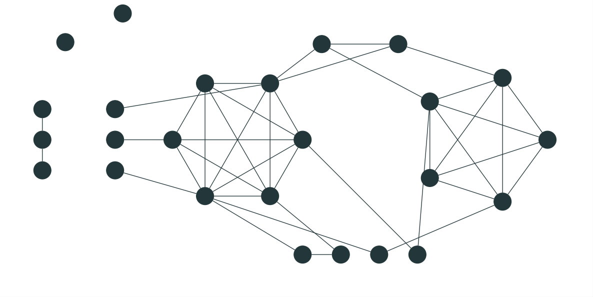

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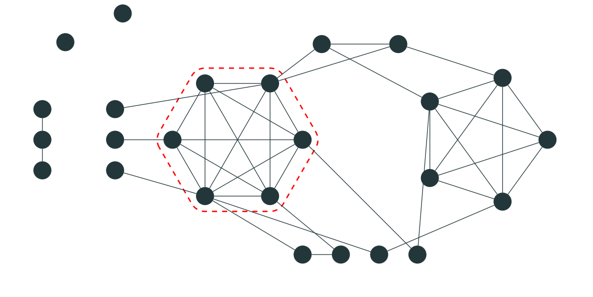

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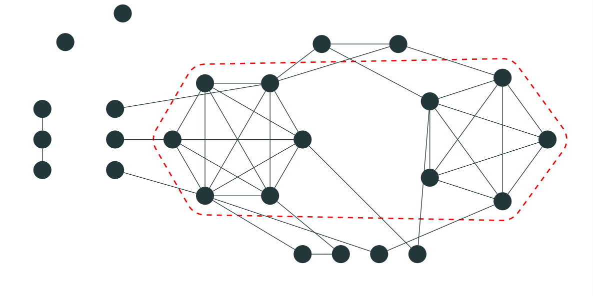

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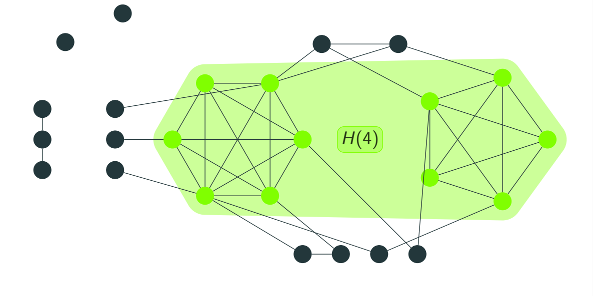

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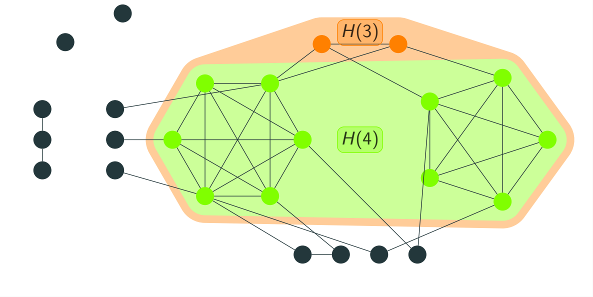

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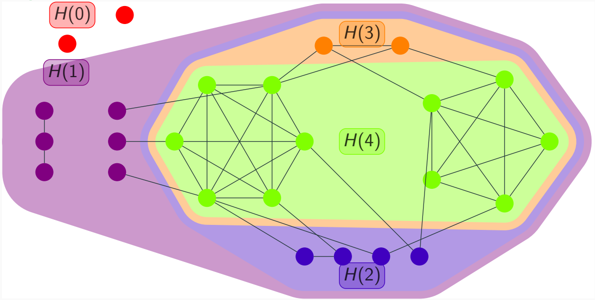

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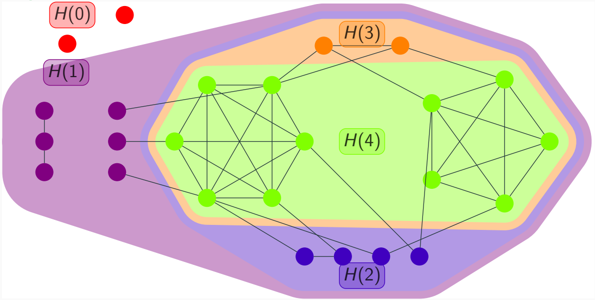

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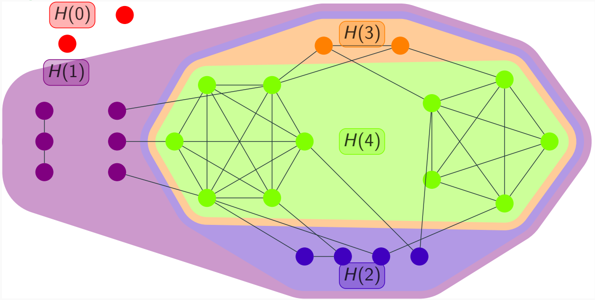

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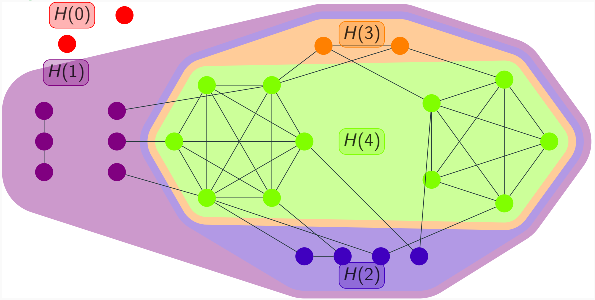

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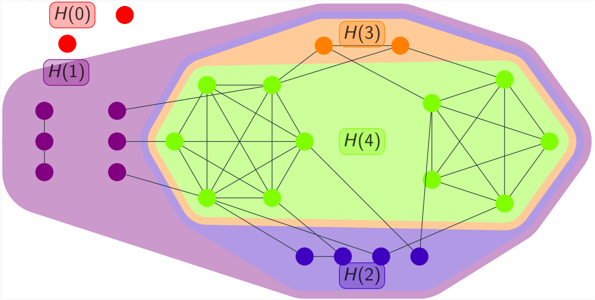

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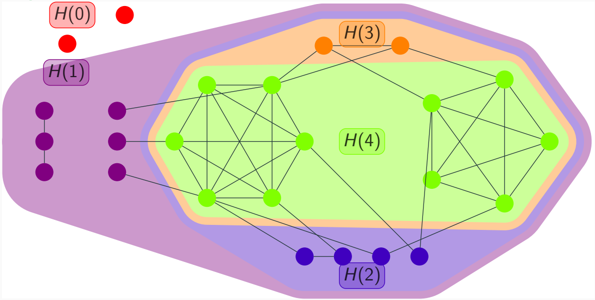

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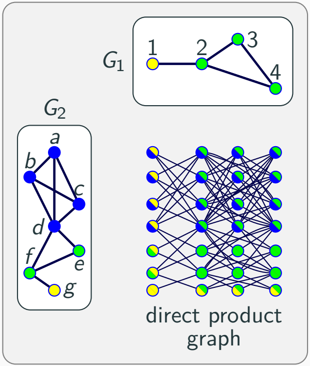

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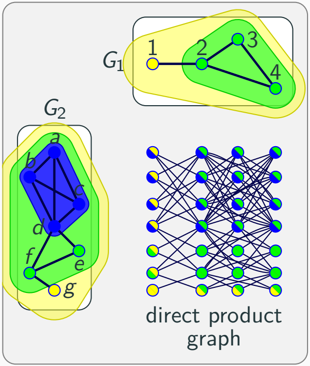

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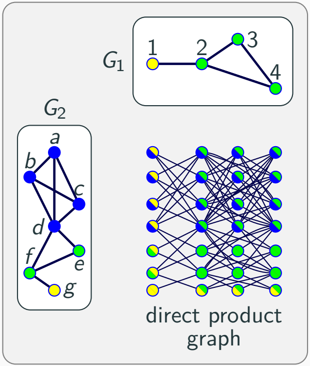

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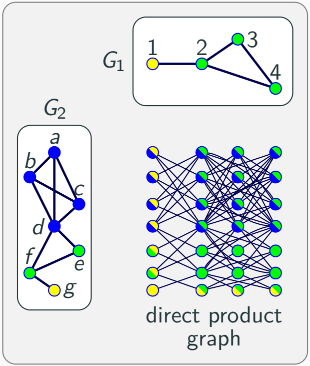

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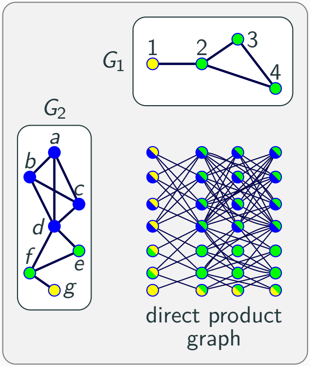

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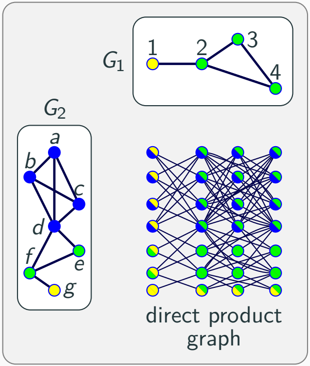

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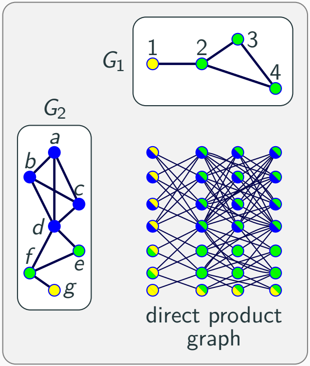

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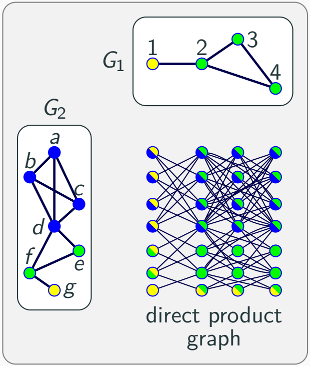

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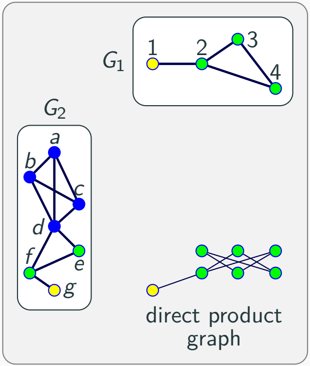

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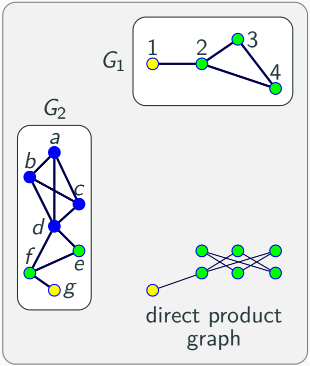

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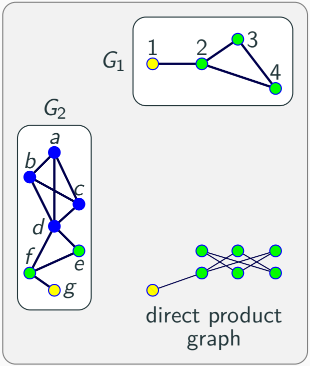

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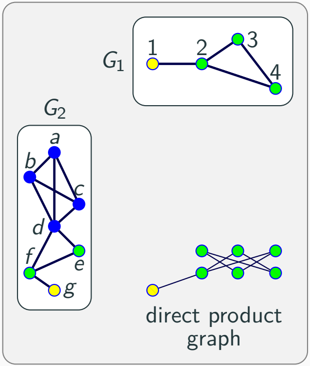

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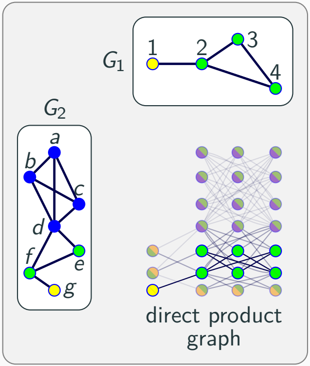

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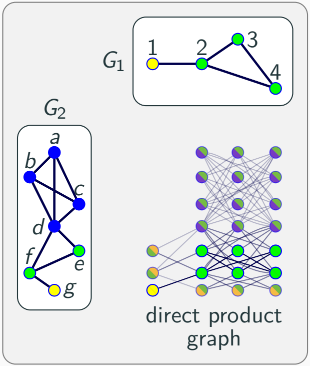

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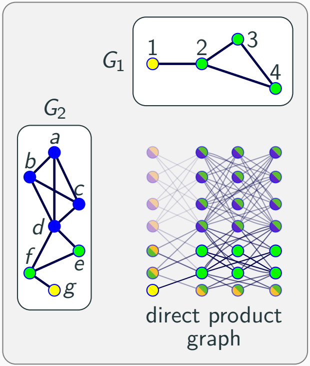

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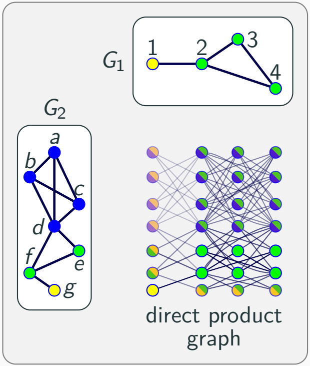

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Depending on δ:

- $\delta = \infty$ vanilla RW
  too loose
- $\delta = 0$ [Gärtner et al., 2003]
  too strict
- $\delta \in \mathbb{R}_+$ SUSAN
  adaptive! **e.g.:** 0,0.5,1,1.5,2

Computing the Kernel II

Finally: sum # common walks:

- of any # steps (with weight μ_n)
- from each vertex to every other

$$k(G_1, G_2) = \mathbf{e}^\top \underbrace{\sum_{n=0}^{\infty} \mu_n \mathbf{A}_\times^n \mathbf{e}}$$

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- Geometric: $\mathbf{B}_g = (I - \lambda \mathbf{A}_\times)^{-1}\mathbf{e}$
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Practical weights μ give:

- Geometric: $\mathbf{B}_g = (I - \lambda \mathbf{A}_\times)^{-1}\mathbf{e}$ — Conjugate Gradient
- Exponential: $\mathbf{B}_e = \exp(\mathbf{A}_\times)\mathbf{e}$ — [Al-Mohy and Higham, 2011]

$\Longrightarrow$ computable as matrix vector (MV) operations with $\mathbf{A}_\times$

But: How do we compute the MV operations efficiently?

Computing the kernel II: Efficiently

To compute SUSAN efficiently

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Lemma

The MV operator for SUSAN with bandwidth δ is computable as

$$\mathbf{A}_\times x = \mathbf{T} \odot (\mathbf{A}''(\mathbf{T} \odot \mathbf{X})\mathbf{A}'^\top)$$

for $\mathbf{T}$ *block banded with constant blocks and bandwidth δ, time*

$$O((\delta + 1)(n' + n'')b^2)$$

for b the largest core size and n', n'' the vertex numbers of G', G''.

To compute SUSAN efficiently

- we decompose the contribution of each graph

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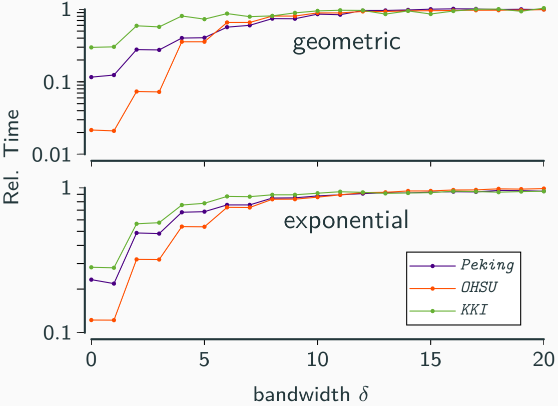
Results

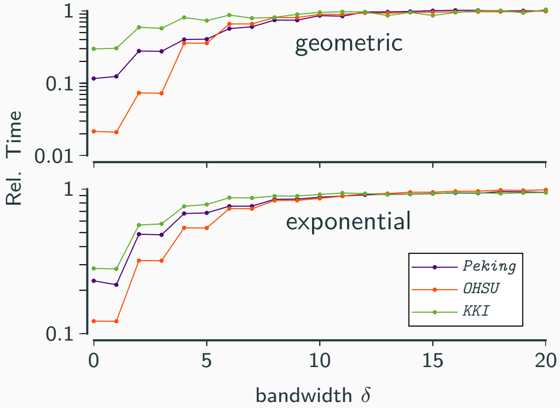
Time comparison



Relative wall-clock time

(SUSAN vs. naïve)

Time comparison



SUSAN

- outperforms naive computation, especially for small δ.

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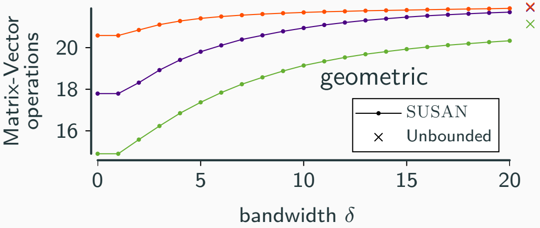

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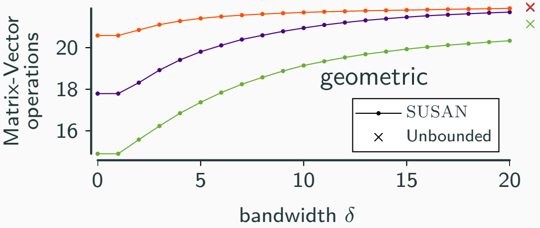


Number of iterations until convergence

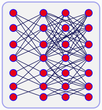
SUSAN

- outperforms naive computation, especially for small δ.
- (geometric) converges faster for smaller δ.

Conclusion

We study

- random walk graph kernels
- weighted vertex alignments



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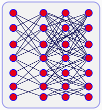

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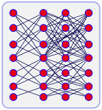

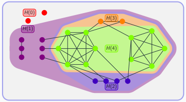

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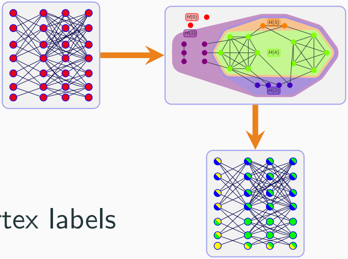

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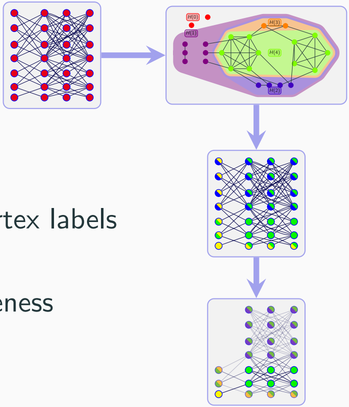

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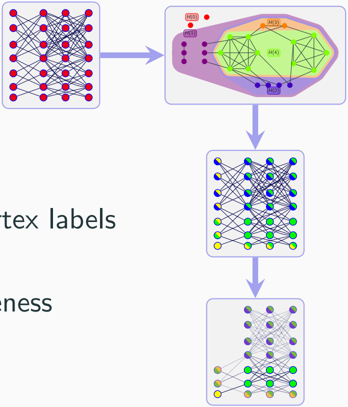

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With our work

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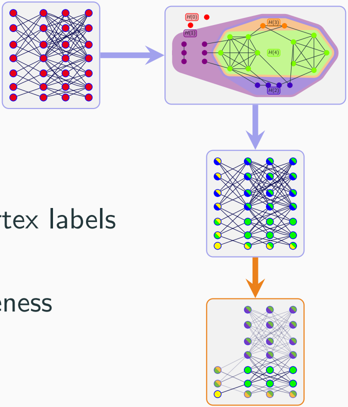

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- close the gap between loose and strict alignment constraints

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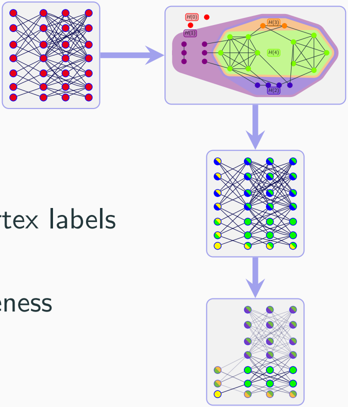

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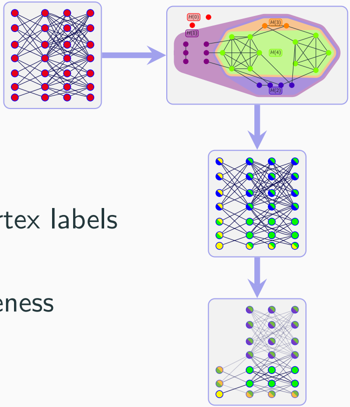

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Thank you!

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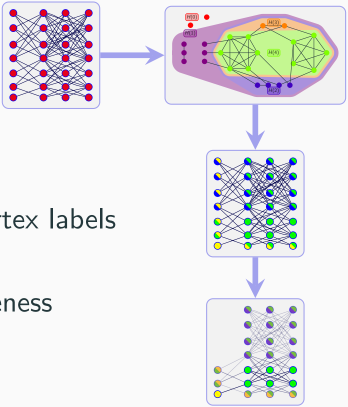

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