NeurIPS 2019
Graph Representation Learning Workshop

Approximation Power of Invariant Graph Networks

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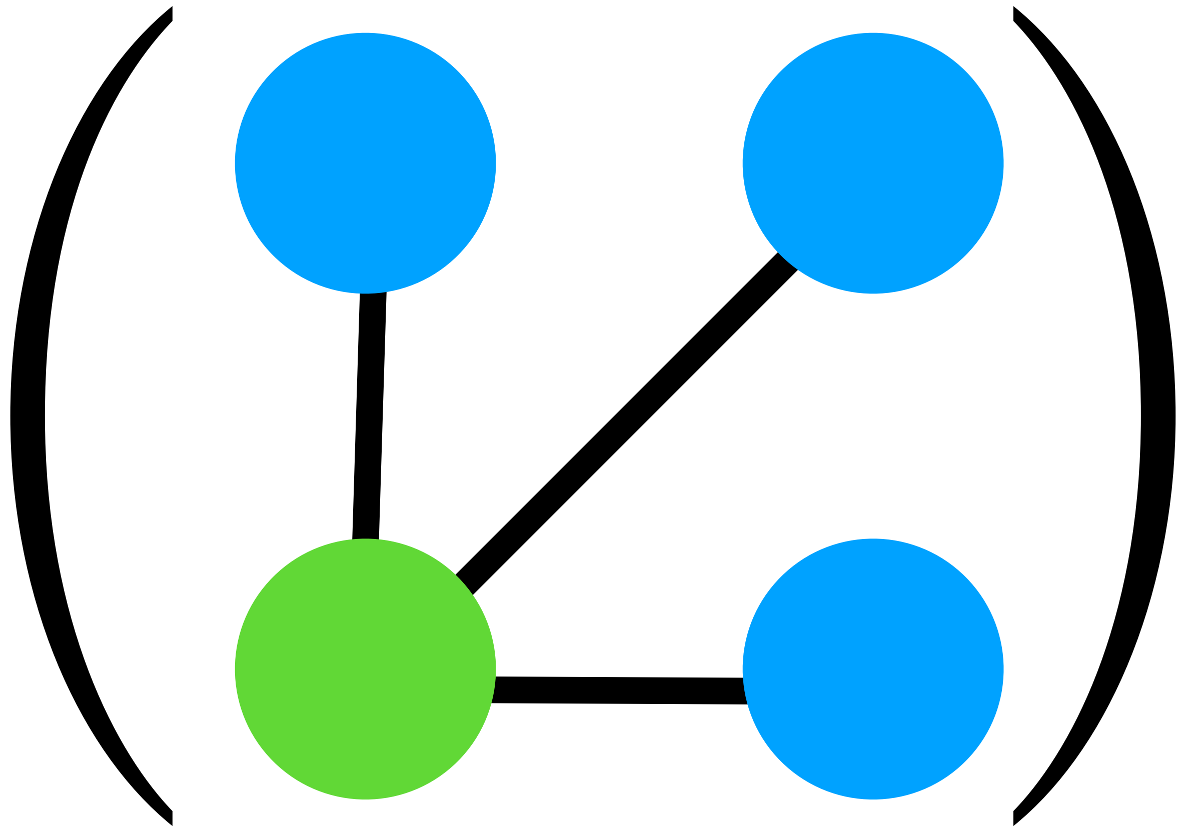
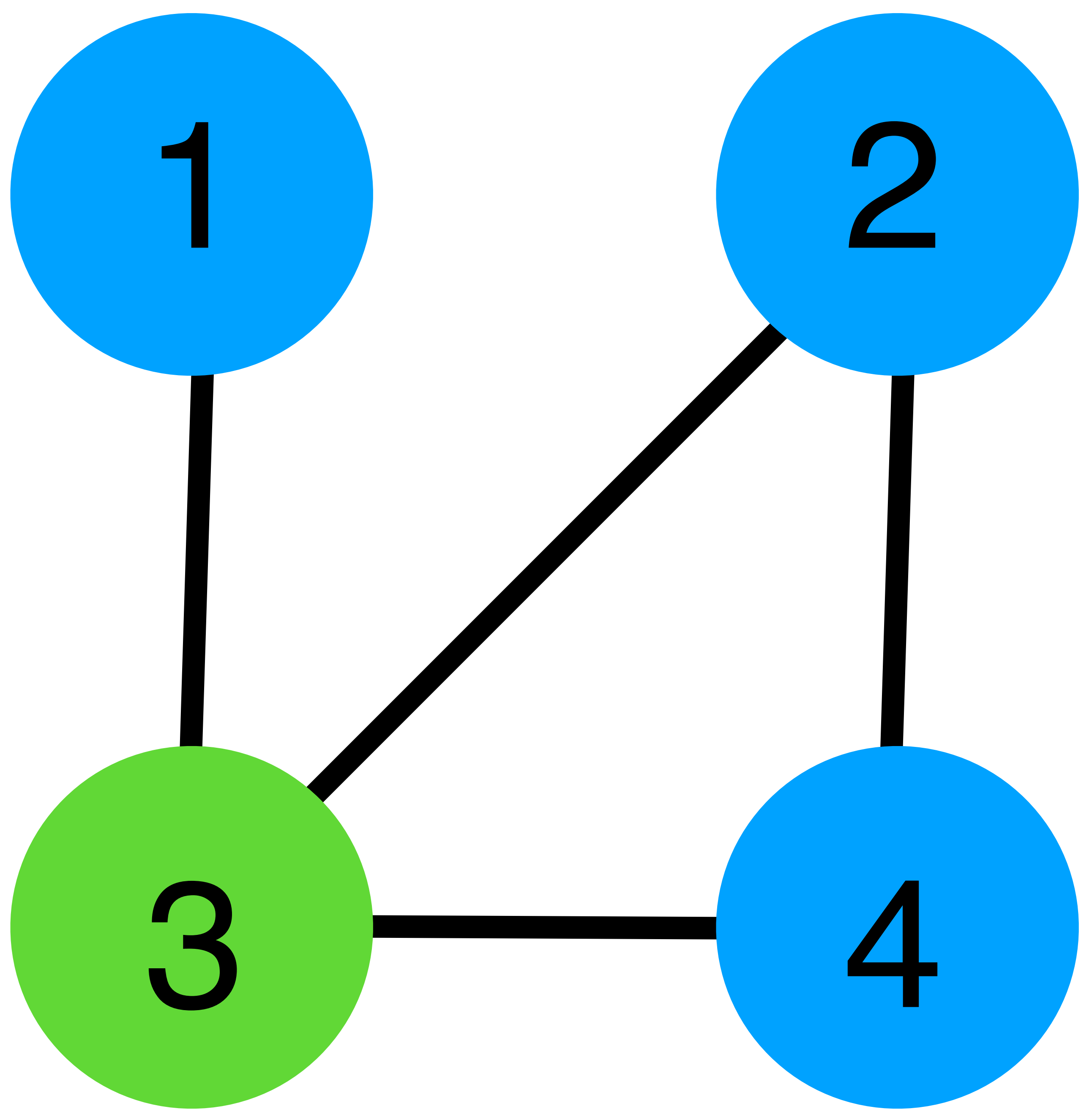
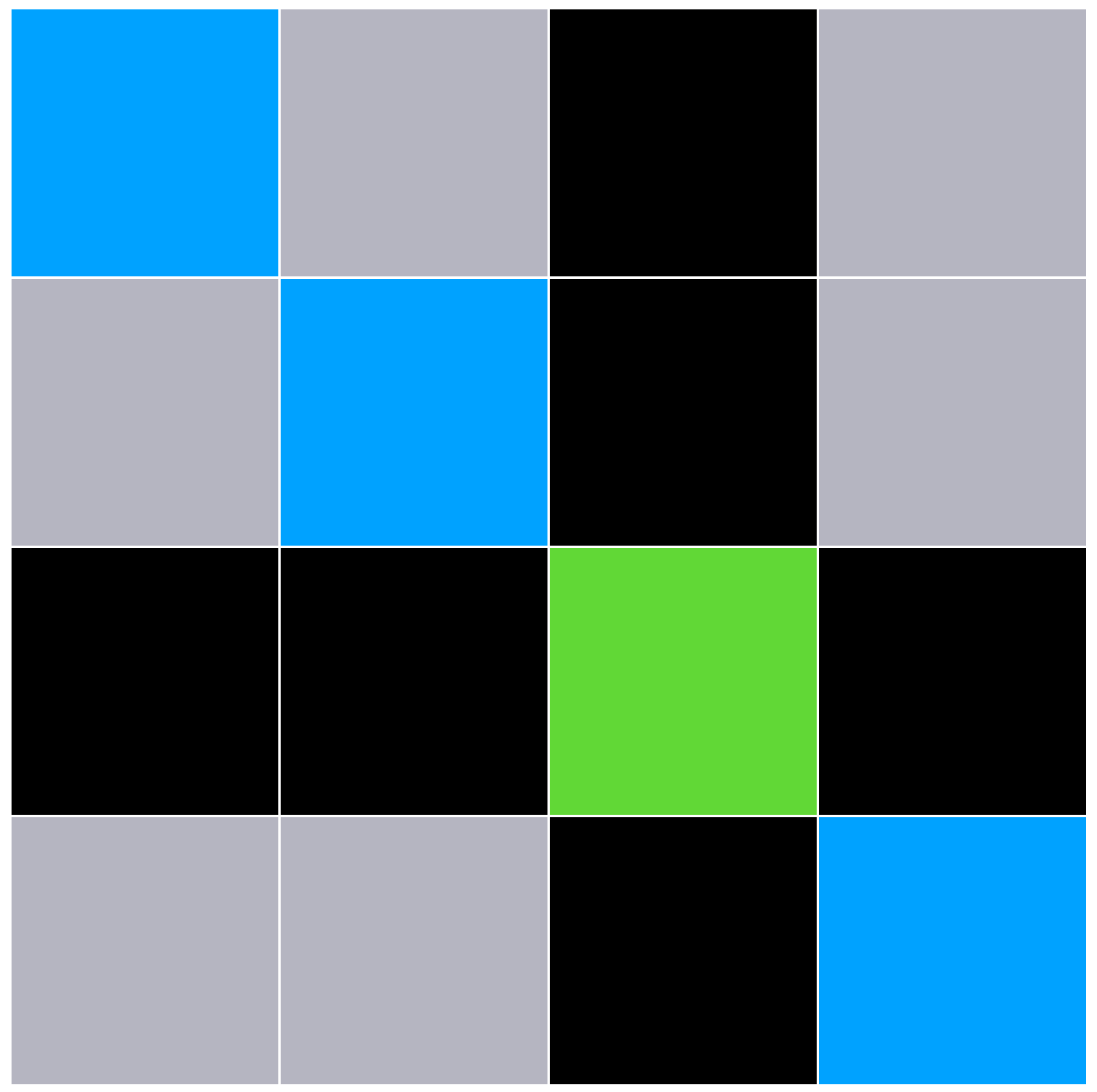
Supervised learning on graphs

f  = ‘label’

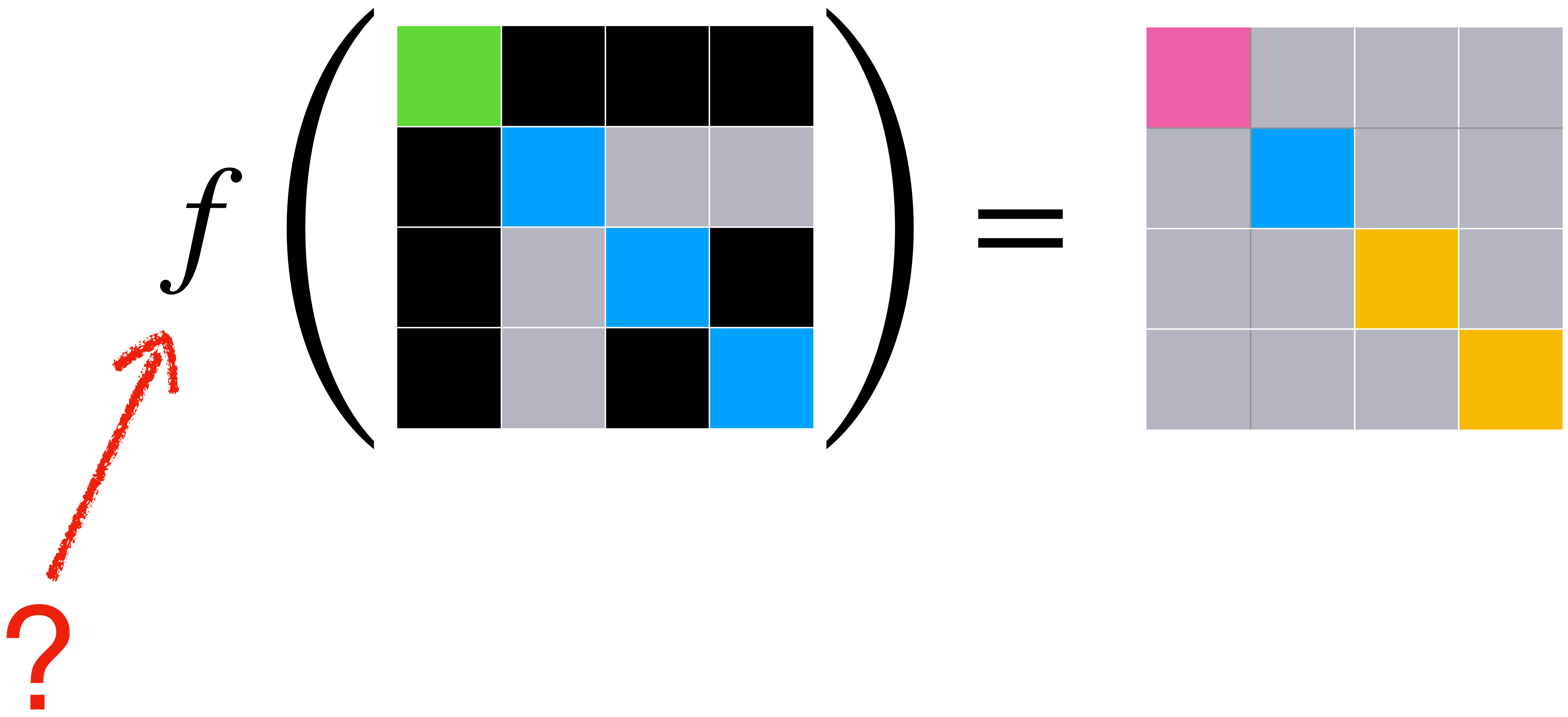
Graphs encoded as matrices



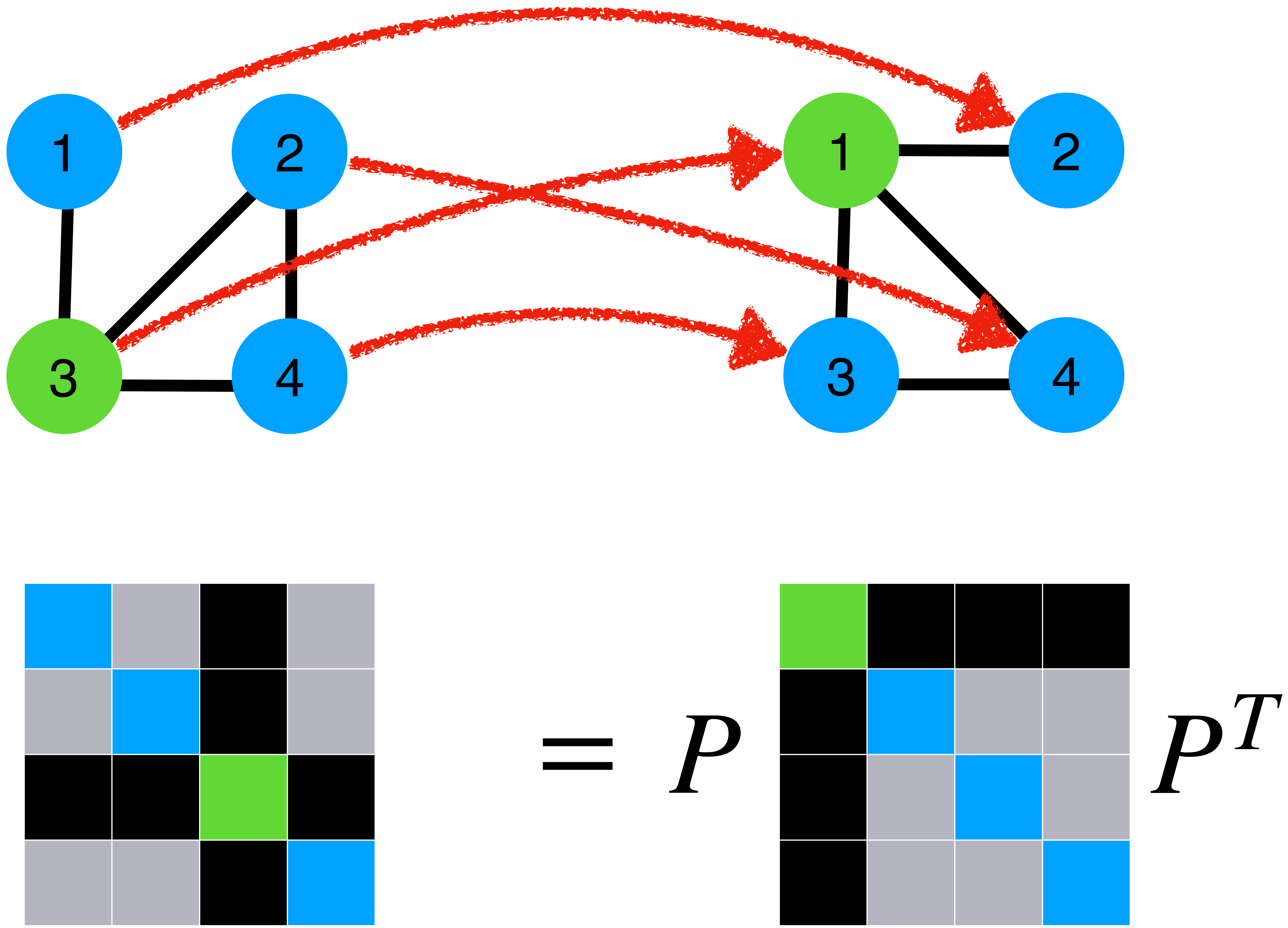


X

Graph learning

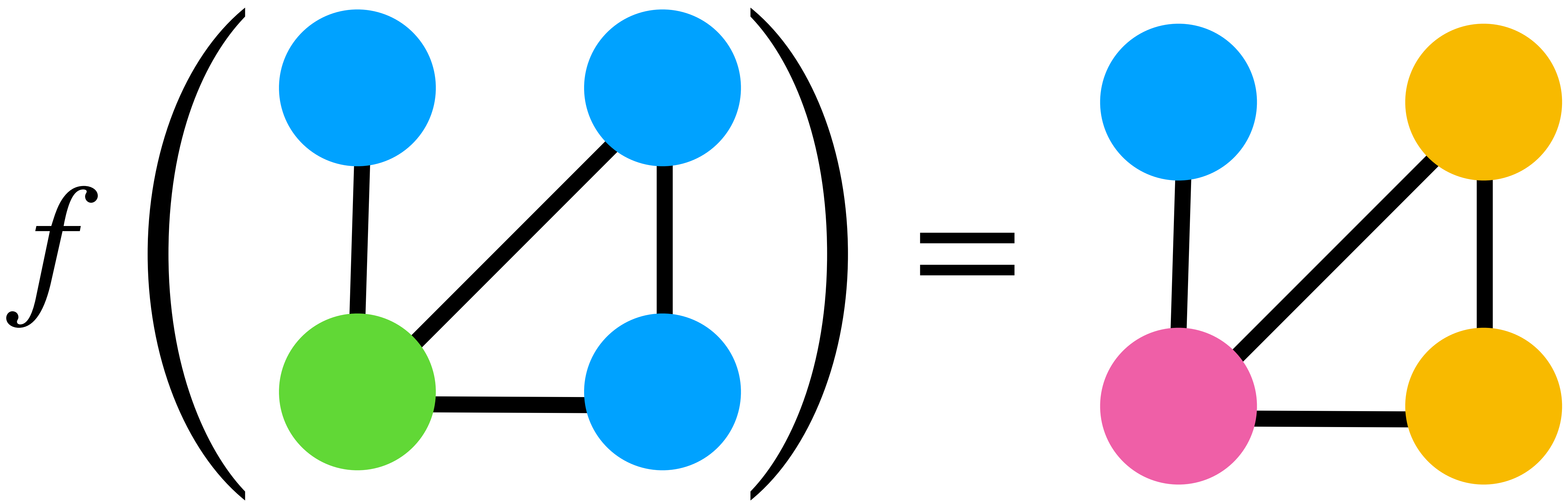


Graph isomorphism

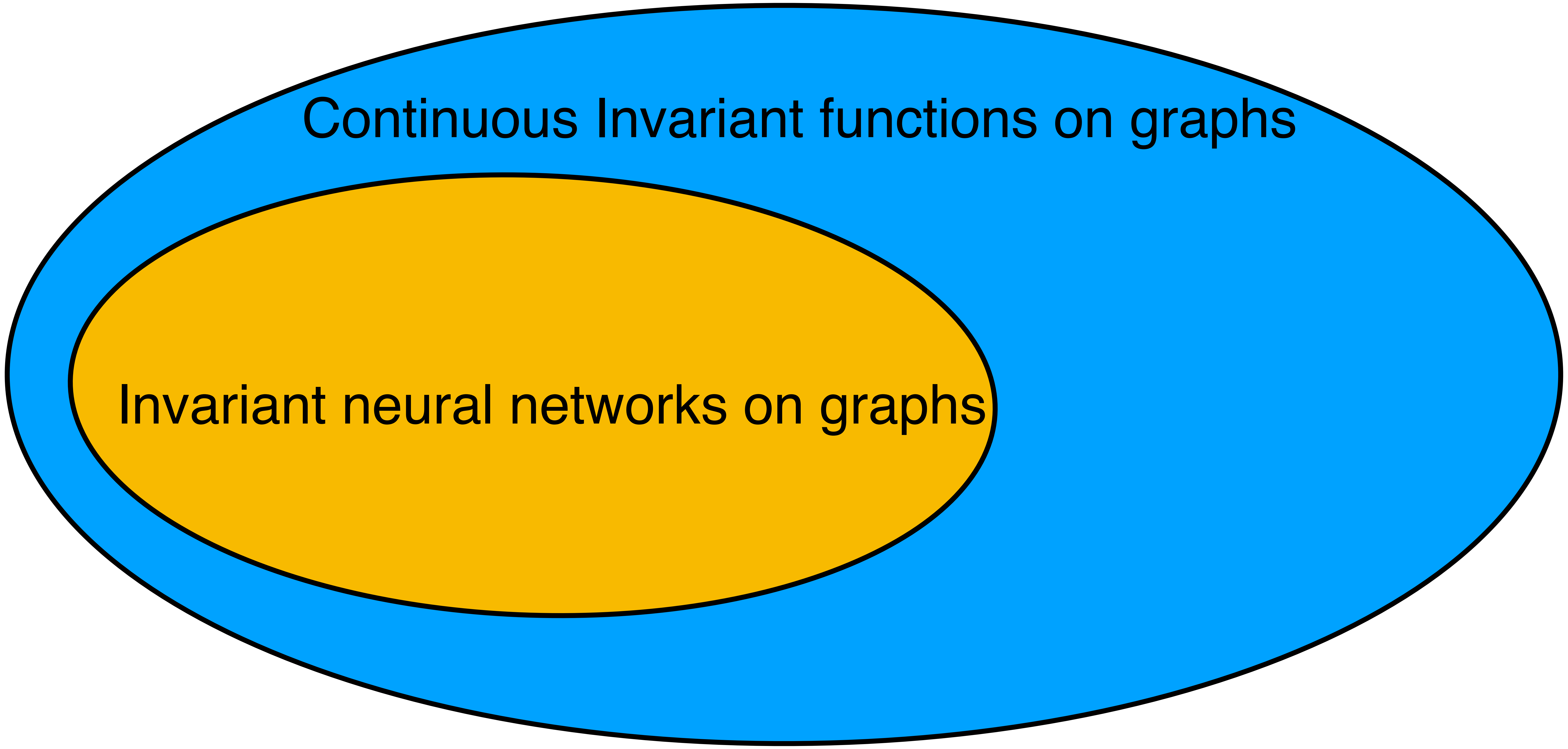


Basic requirement: equivariance

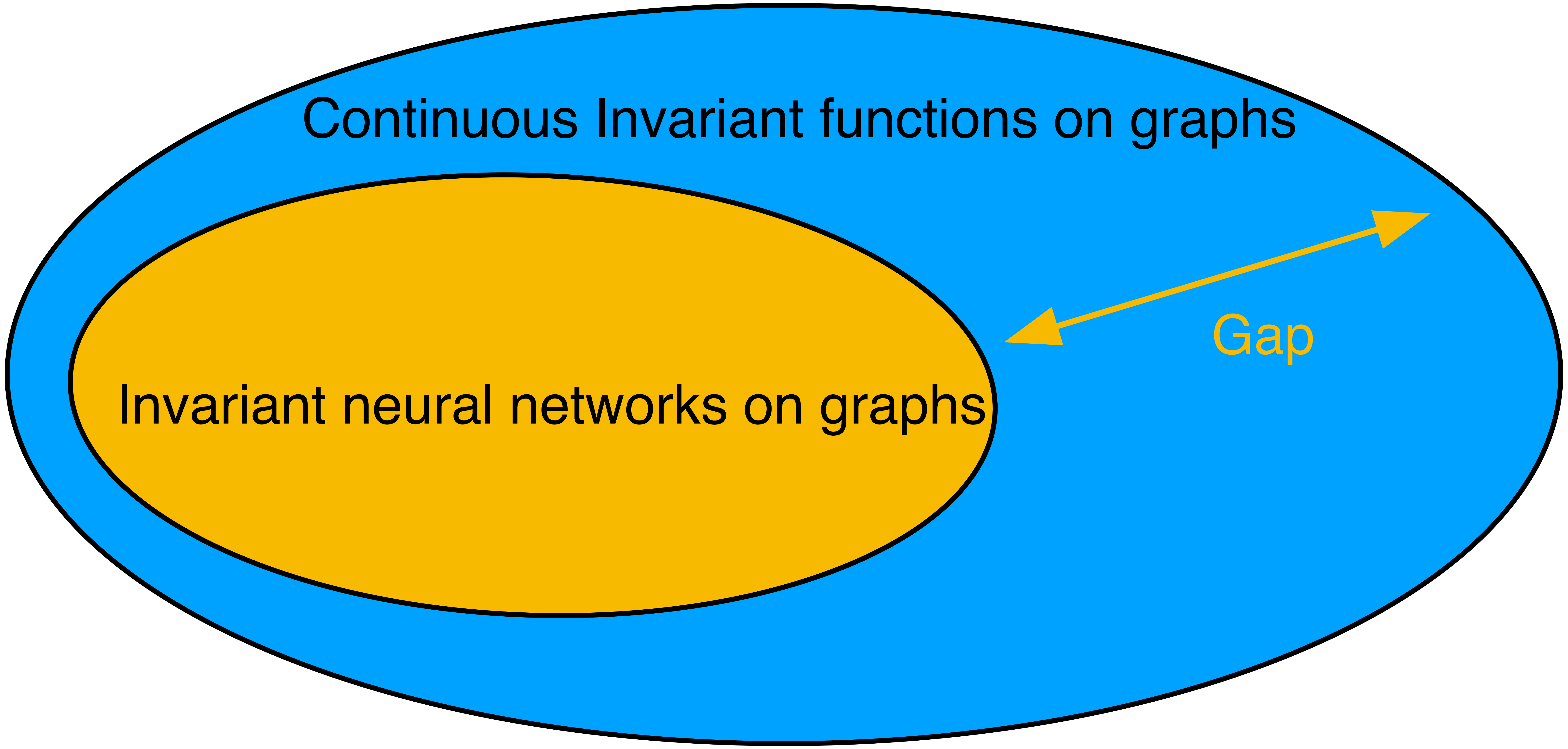
$$f(\, P\, X\, P^T\,) = P\, f(X)\, P^T$$



Restriction might cause loss of expressivity



Restriction might cause loss of expressivity



Main Goal

Find models that are:

Invariant

Expressive

Scalable

Framework: Invariant Graph Networks (IGNs)

$$F = M \circ H \circ L_d \circ \cdots \circ L_1$$

- $L_i : \mathbb{R}^{n^k} \to \mathbb{R}^{n^{k'}}$ are polynomial S_n-equivariant functions
- H polynomial S_n-invariant function
- M is a fully connected network

Framework: Invariant Graph Networks (IGNs)

$$F = M \circ H \circ L_d \circ \cdots \circ L_1$$

- $(k, l)-$IGN:
  - Tensors up to <u>order k</u>
  - Polynomials up to <u>degree l</u>

Framework: Invariant Graph Networks (IGNs)

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  - Tensors up to <u>order k</u>
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- **Example**: $F(X) = X^2, \;\; X \in R^{n^2}$ is a $(2{,}2)$-layer

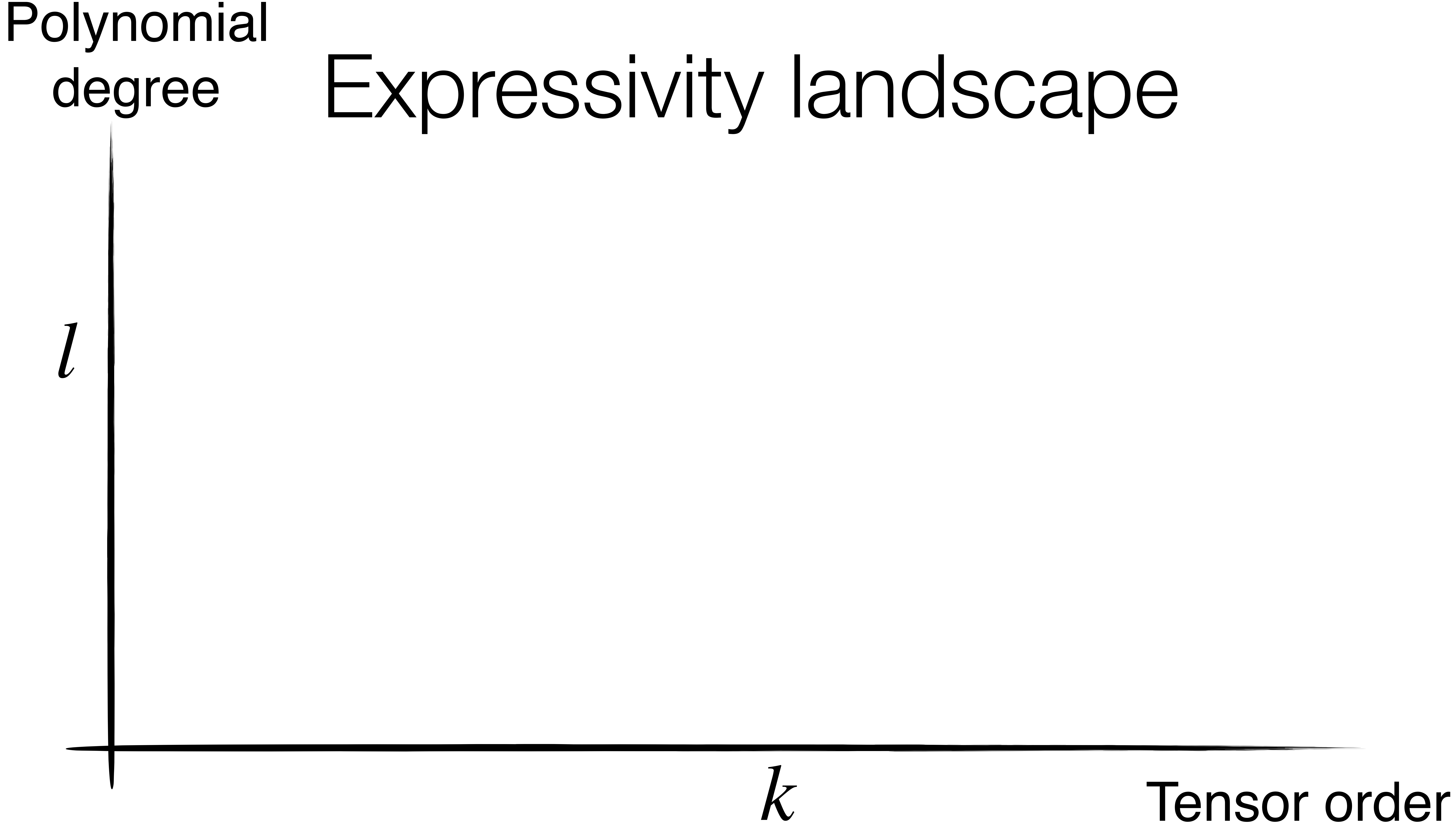
Expressivity landscape

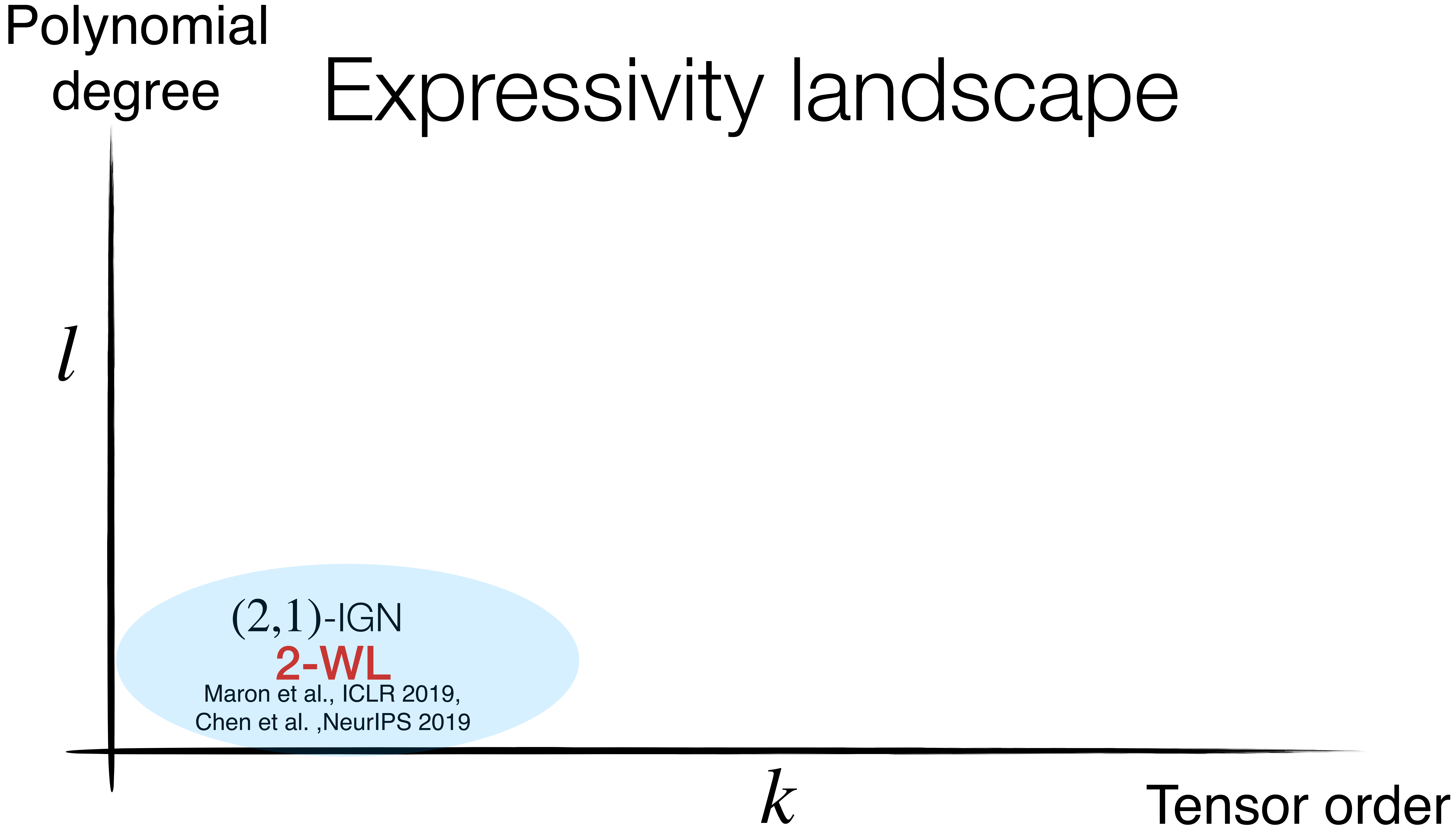
Polynomial degree

Expressivity landscape

l

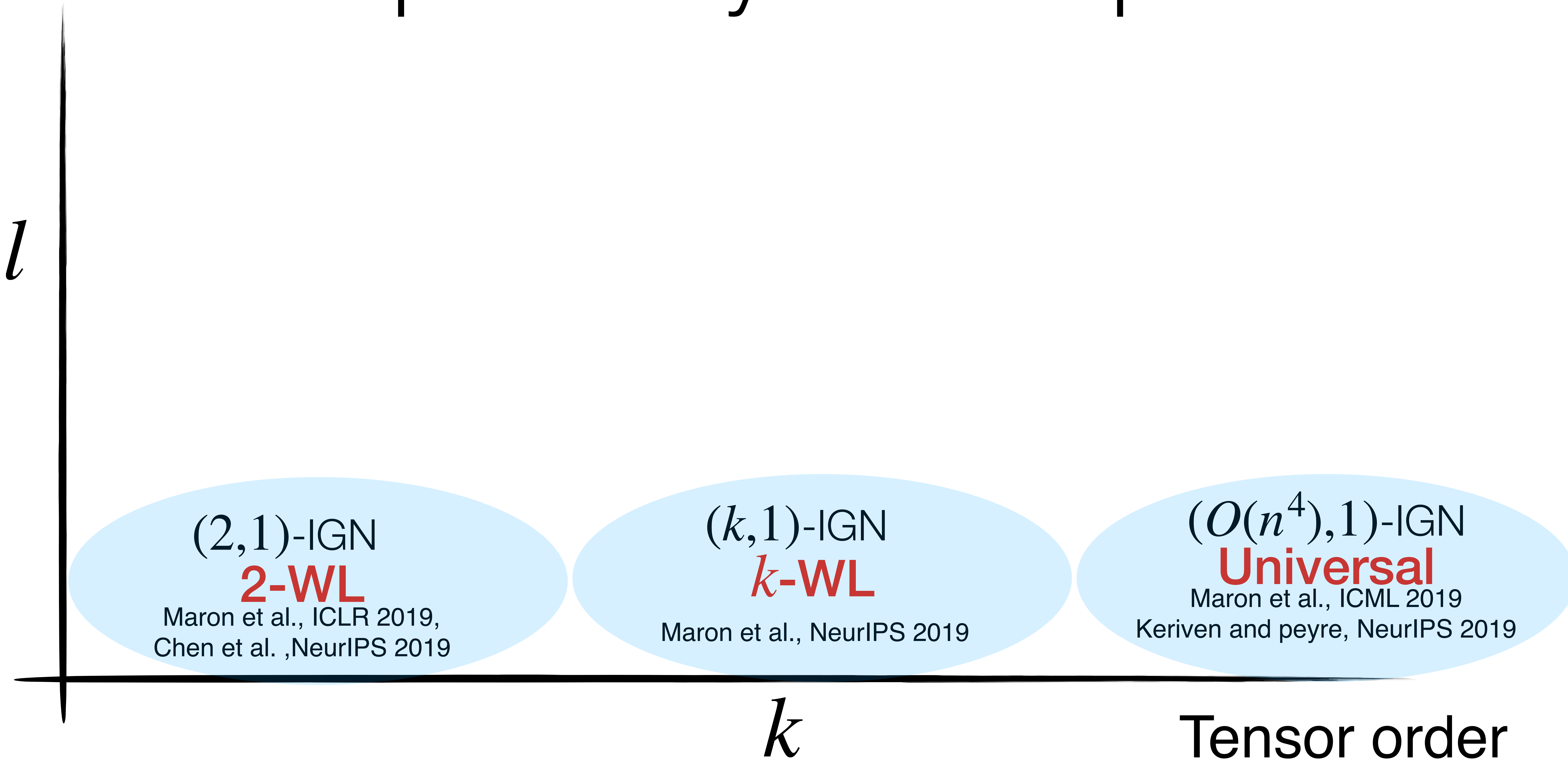
Expressivity landscape




Polynomial degree
Expressivity landscape
l
(2,1)-IGN
2-WL
Maron et al., ICLR 2019,
Chen et al. ,NeurIPS 2019
k
Tensor order

Expressivity landscape

Expressivity landscape



Expressivity landscape

Expressivity landscape


Polynomial degree
Expressivity landscape
l
$(2, poly(n))$-IGN
Universal
Yarotsky, ICML workshops 2018
$(2,2)$-IGN
3-WL
Maron et al., NeuriIPS 2019
?
$(2,1)$-IGN
2-WL
Maron et al., ICLR 2019,
Chen et al. ,NeurIPS 2019
$(k,1)$-IGN
k-WL
Maron et al., NeurIPS 2019
$(O(n^4),1)$-IGN
Universal
Maron et al., ICML 2019
Keriven and peyre, NeurIPS 2019
k
Tensor order

Expressivity landscape

Blog:

irregulardeep.org

Paper:

Approximation Power of Invariant Graph Networks

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