Subspaces alignment and graph convolutional networks performance

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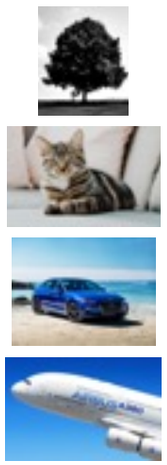
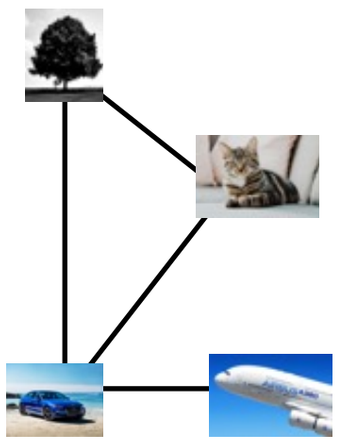
Outline



- Many types of artificial neural networks architecture: Multi-Layer Perceptrons, Recurrent Neural Networks, Autoencoders, Convolutional Neural Networks, Graph Convolutional Neural Networks.

- They are extremely good at image and speech recognition and classification in general with the increase of computational power and the availability of large dataset (data is the new oil, « Big Data », Alpha XX, etc …).

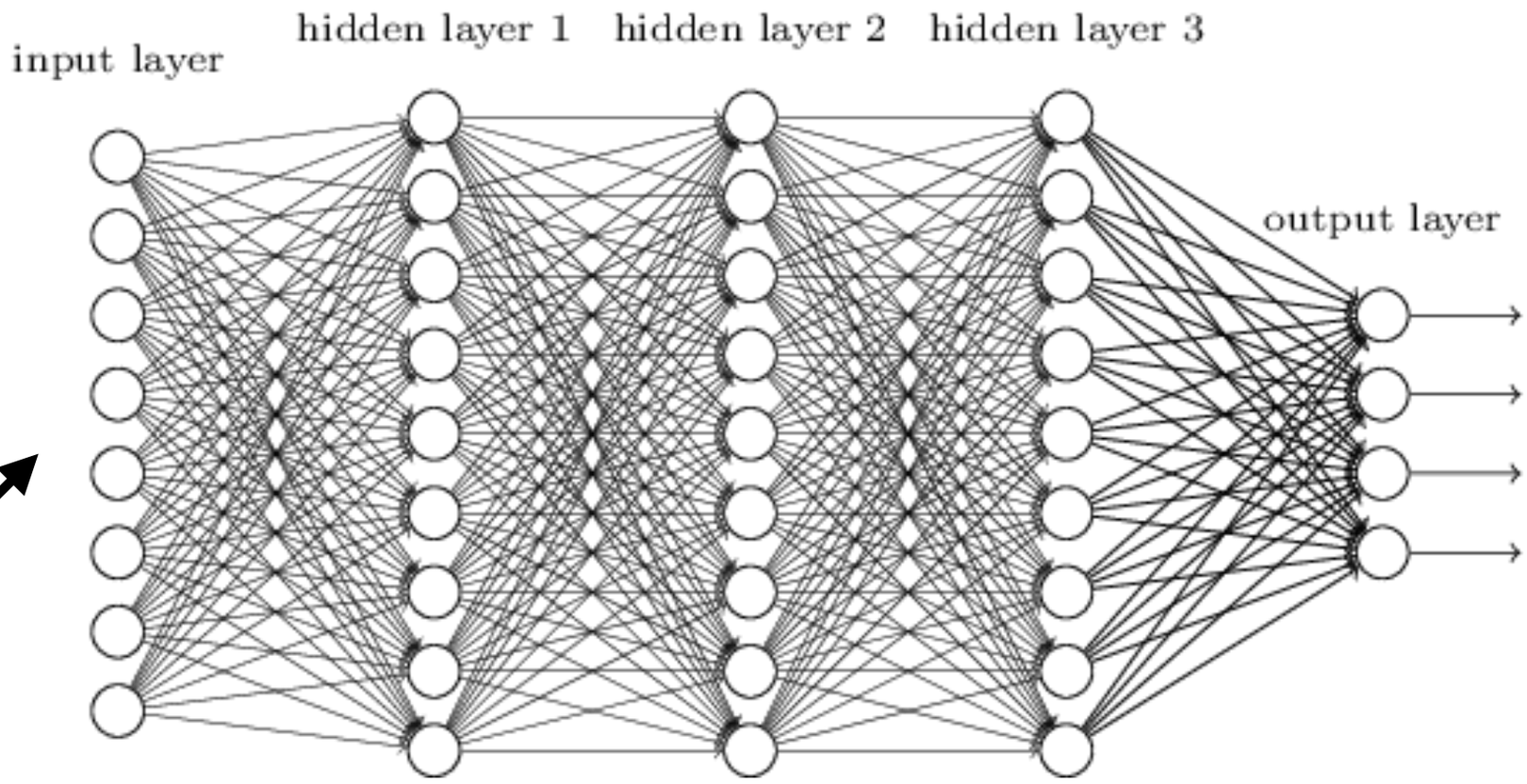


- Is using relational information between objects to be classified always advantageous?
  And can we predict whether is advantageous?

Prototypical goal: classification

Deep neural network

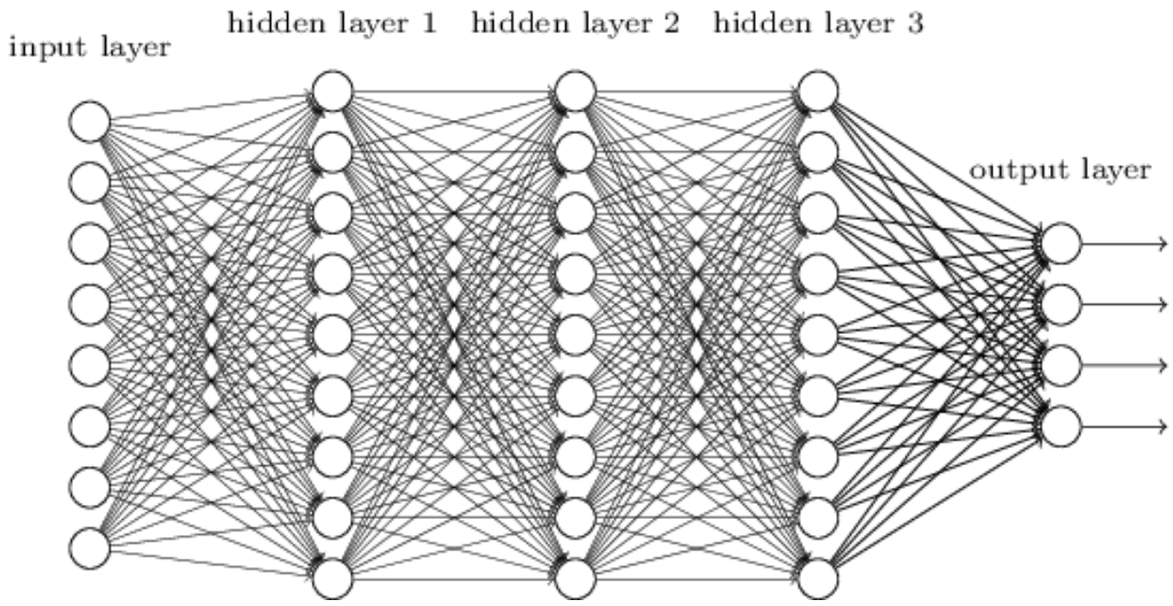
Features



It's a tree!

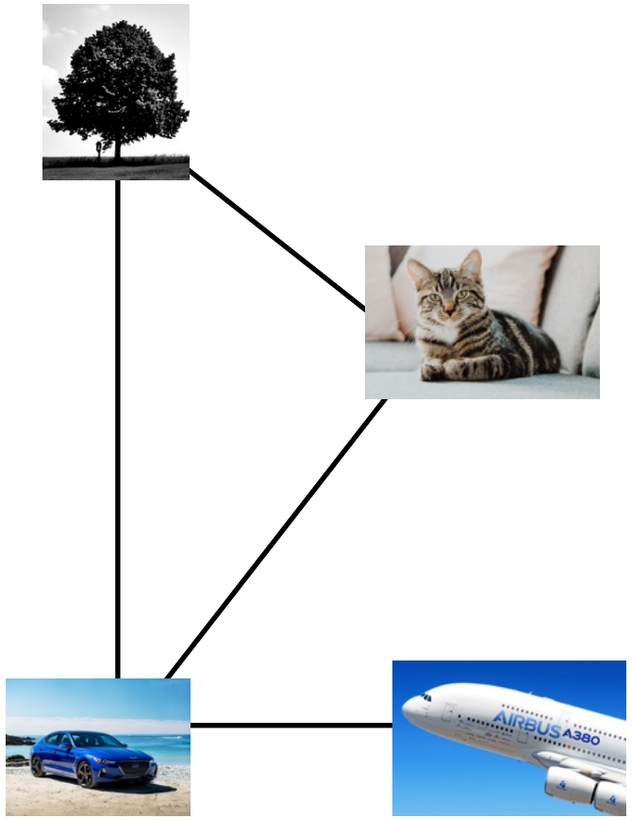
http://playground.tensorflow.org/

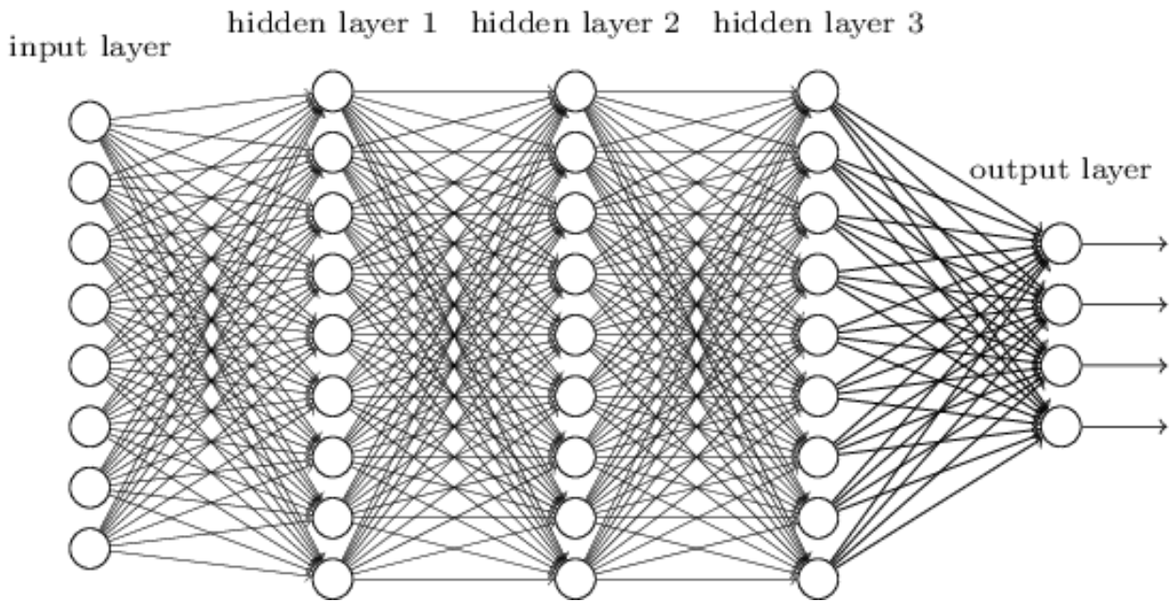
Independent versus interdependent data



Tree
Cat
Car
Plane

Independent versus <u>interdependent</u> data





Tree
Cat
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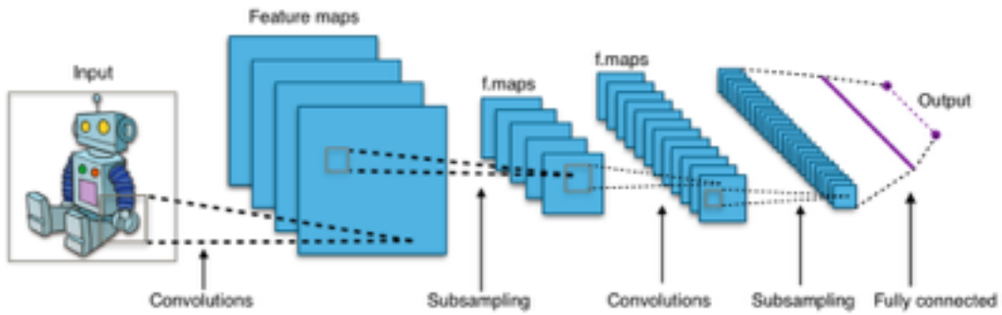
Plane

(Very) Short intro about Convolutional Neural Networks

Slide filters across an image.



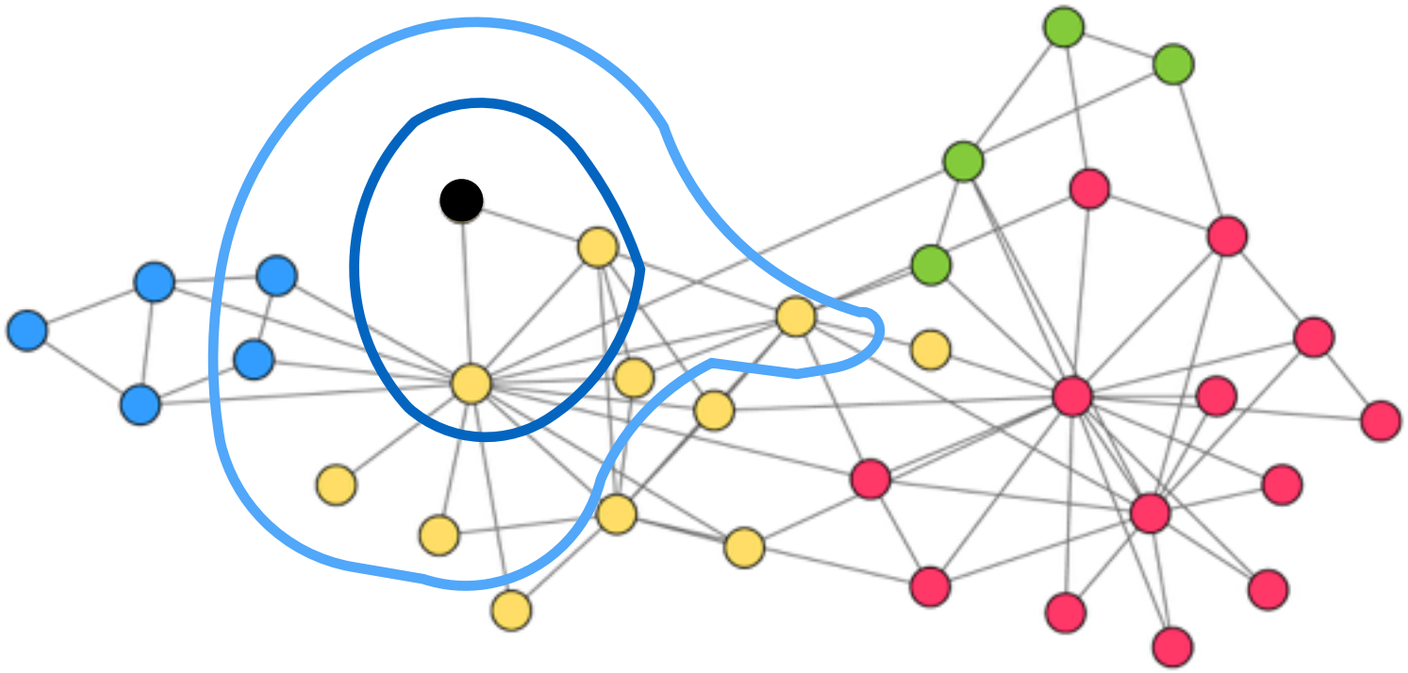
Good for « Euclidean » data, but how to generalise to « non-Euclidean » i.e. graph structured data?

Y. LeCun, Y. Bengio, and G. Hinton, Nature 521, 436 (2015).

https://ujjwalkarn.me/2016/08/11/intuitive-explanation-convnets/

(Very) Short intro about Graph Convolutional Networks

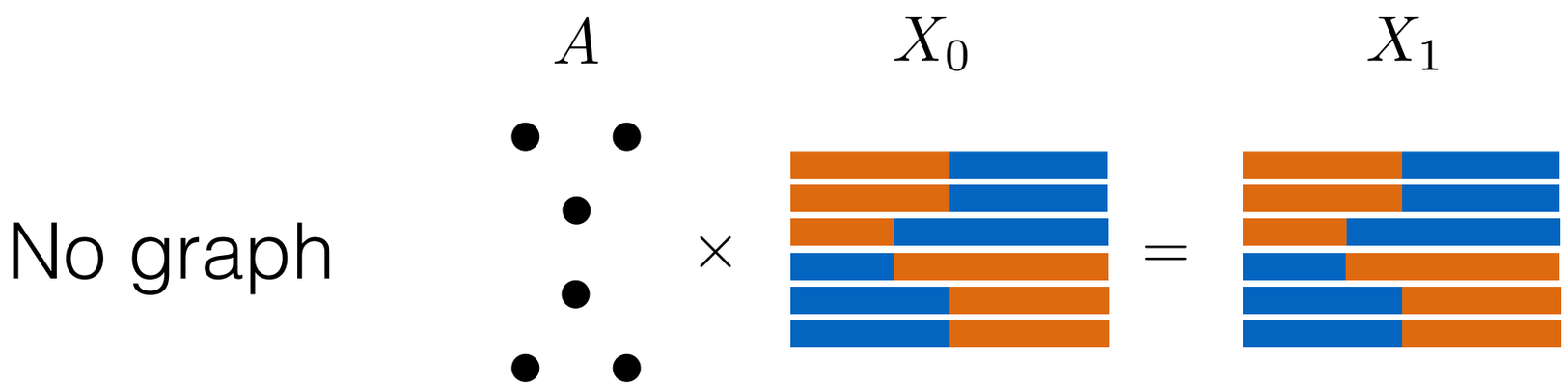
How to average information/find similar nodes in a principled way in a relational graph?



Define a convolution operation in the spectral domain of the graph.

D. I. Shuman *et al.*, *IEEE Sig Proc Mag,* 2013
Bronstein *et al.,* Geometric deep learning: going beyond Euclidean data, *IEEE Sig Proc Mag, 2017*
Wu *et al.*, A Comprehensive Survey on Graph Neural Networks, *arxiv 2019*

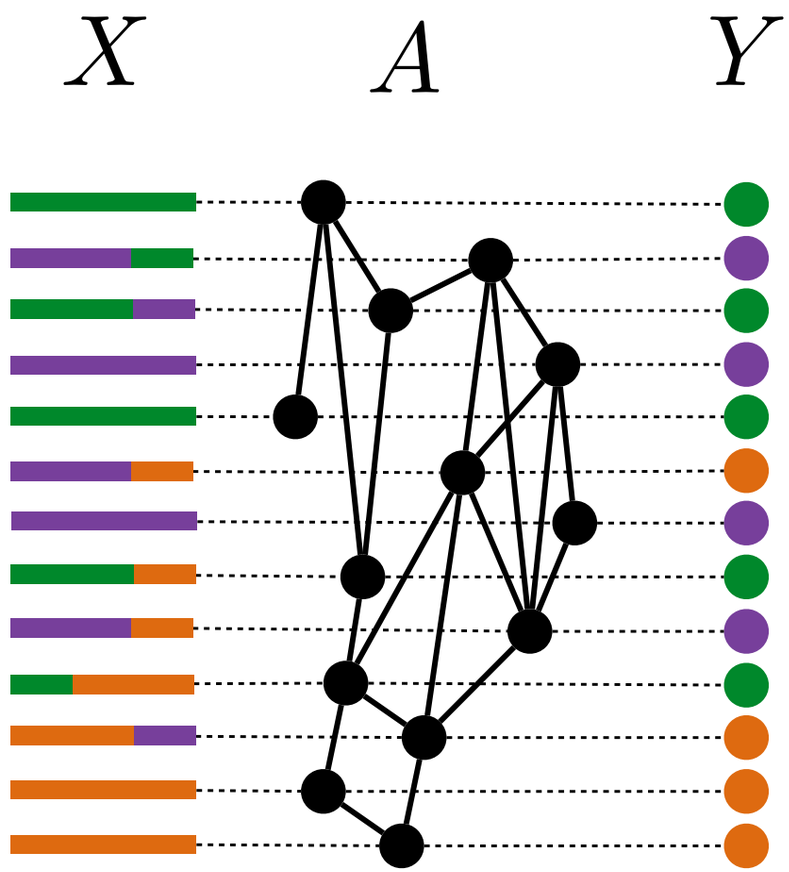
What happens in a « graph convolution »?



Each node is an object with its associated features

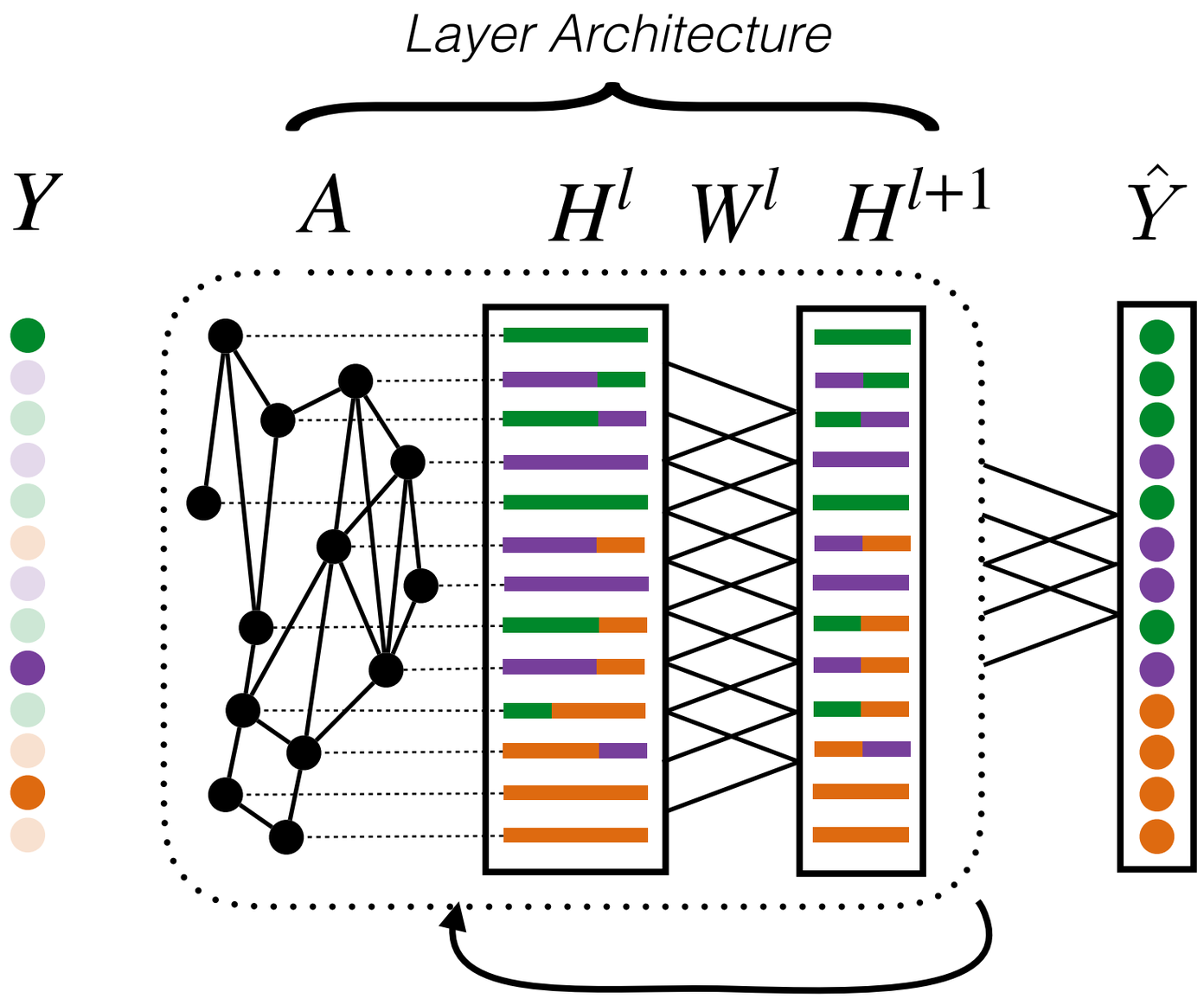
Graph Convolutional Neural Networks

Task: node classification



X: features associated to the nodes, *F*
A: relational graph between nodes, *N*
Y: ground truth, *C*

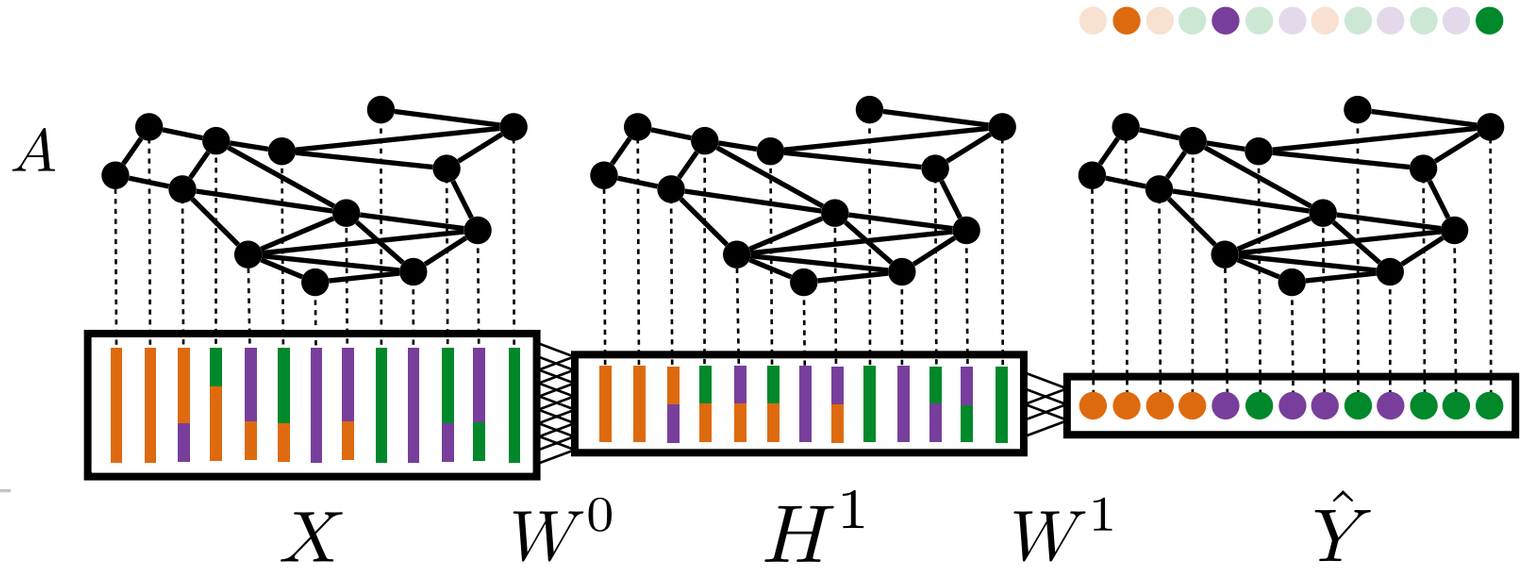
Typical GCN architecture

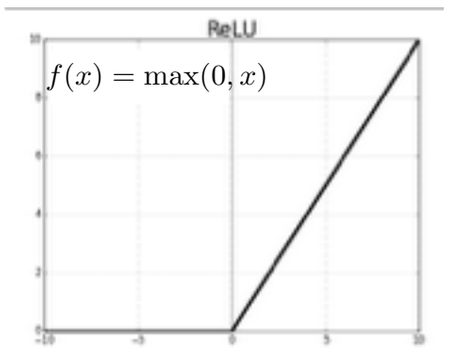


Transductive semi-supervised learning

Kipf & Welling, « Semi-supervised classification with graph convolutional networks » *ICLR 2017*

Simplest model





ReLU

softmax

$$\text{softmax}(x_i) = \frac{\exp(x_i)}{\sum_{j=1}^{C} \exp(x_j)}$$

$$\begin{aligned}\hat{Y} &= f(X, A) \\ &= \text{softmax}(\hat{A} H^1 W^1) \\ &= \text{softmax}(\hat{A}\ \text{ReLU}(\hat{A} X W^0)\ W^1)\end{aligned}$$

Convolution

Kipf & Welling, « Semi-supervised classification with graph convolutional networks » *ICLR 2017*

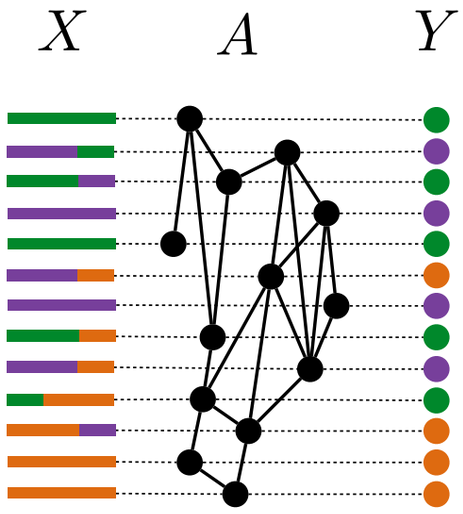
Seems awesome !!

Method	**Citeseer**	**Cora**	**Pubmed**	**NELL**
ManiReg [3]	60.1	59.5	70.7	21.8
SemiEmb [28]	59.6	59.0	71.1	26.7
LP [32]	45.3	68.0	63.0	26.5
DeepWalk [22]	43.2	67.2	65.3	58.1
ICA [18]	69.1	75.1	73.9	23.1
Planetoid* [29]	64.7 (26s)	75.7 (13s)	77.2 (25s)	61.9 (185s)
GCN (this paper)	**70.3** (7s)	**81.5** (4s)	**79.0** (38s)	**66.0** (48s)
GCN (rand. splits)	67.9 ± 0.5	80.1 ± 0.5	78.9 ± 0.7	58.4 ± 1.7

Accuracy: number of correct predictions out of all predictions

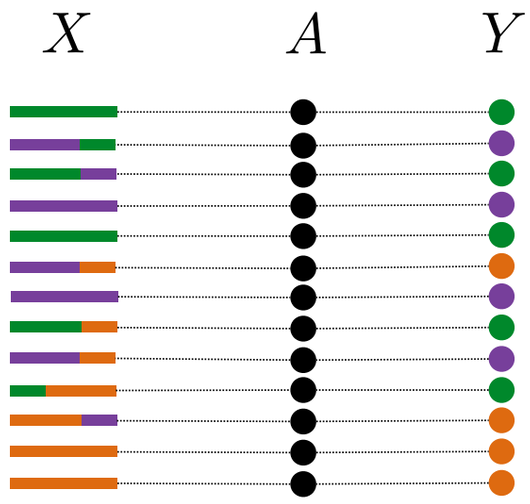
Kipf & Welling, « Semi-supervised classification with graph convolutional networks » *ICLR 2017*

But is it really?



GCN

VS



MLP

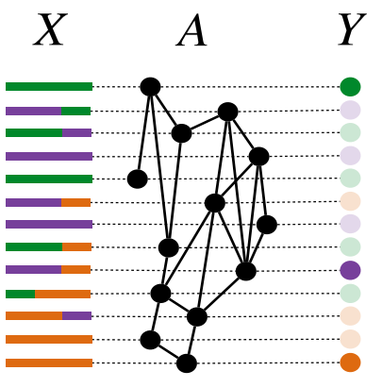
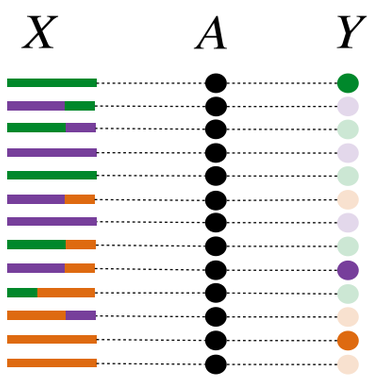
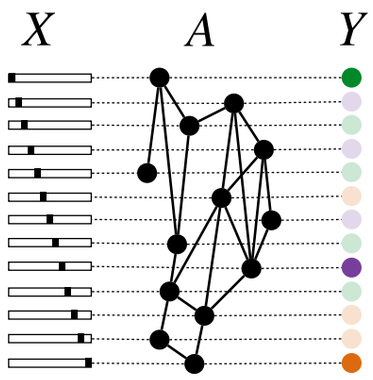
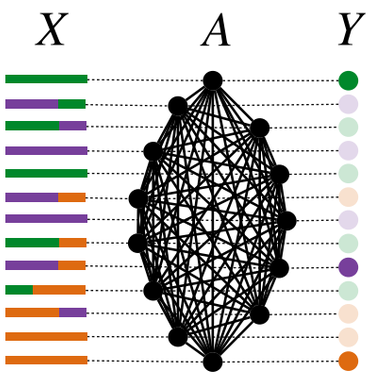
Data sets	GCN	MLP
Constructive example	**0.932** ± **0.006**	0.416 ± 0.010
CORA	**0.811** ± **0.005**	0.548 ± 0.014
AMiner	**0.748** ± **0.005**	0.547 ± 0.013
Wikipedia	0.392 ± 0.010	**0.450** ± **0.007**

Datasets

- Toy model with planted communities (SBM)
- CORA: benchmark citation network, from time immemorial
- Aminer: computer science citation network
- Wikipedia: home made, 12 classes

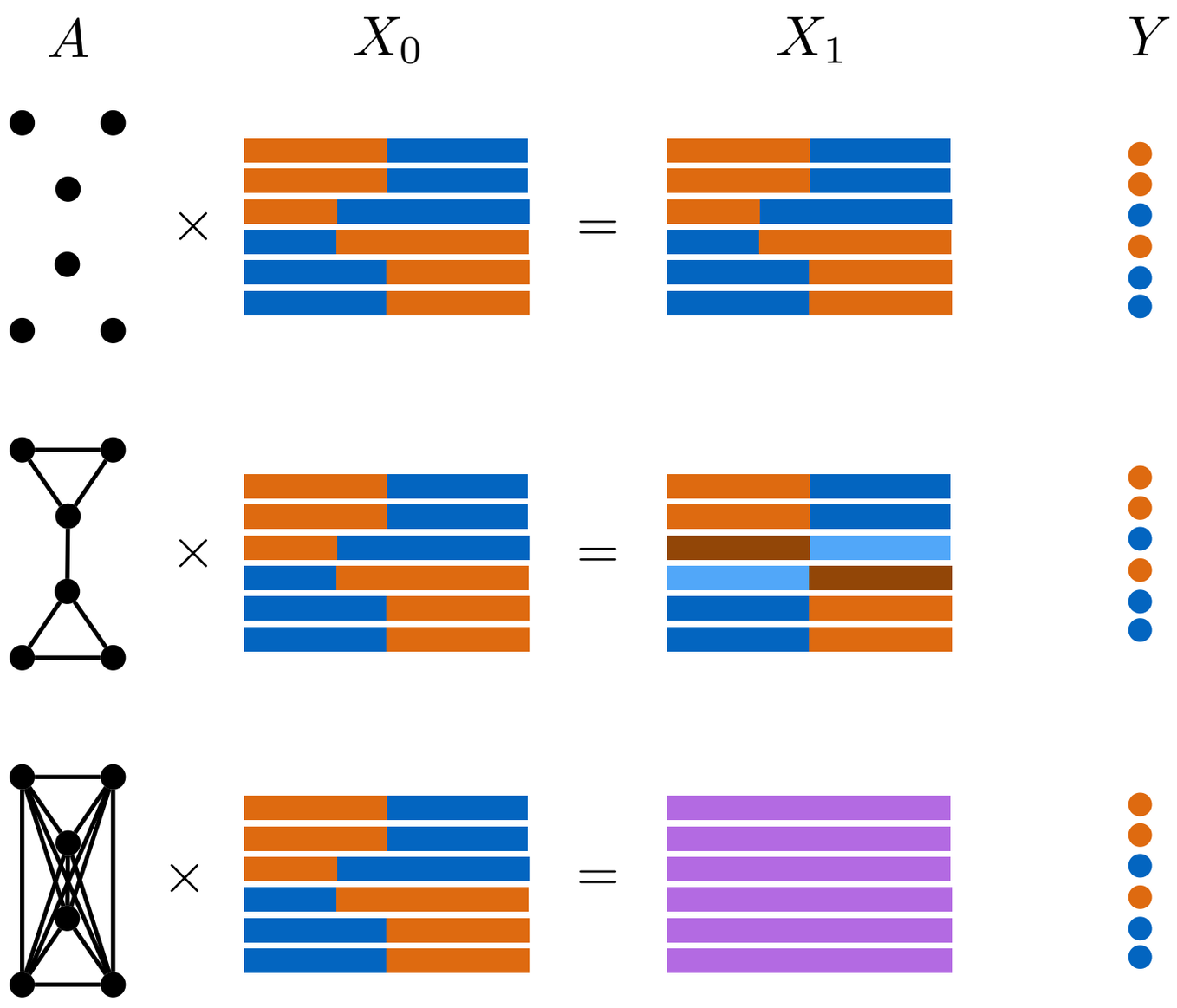
Data sets	Nodes	Edges	Features	Classes
Constructive example	$1,000$	$6,541$	500	10
CORA	$2,485$	$5,069$	$1,433$	7
AMiner	$2,072$	$4,299$	500	7
Wikipedia	$20,525$	$215,056$	100	12
Wikipedia I	$2,414$	$8,163$	100	5
Wikipedia II	$1,858$	$8,444$	100	5

MLP is just one limit case

	GCN	Limit cases		
		MLP (no graph)	No features	Complete graph
				
Data sets				
Constructive example	**0.932 ± 0.006**	0.416 ± 0.010	0.764 ± 0.009	0.100 ± 0.003
CORA	**0.811 ± 0.005**	0.548 ± 0.014	0.691 ± 0.006	0.121 ± 0.066
AMiner	**0.748 ± 0.005**	0.547 ± 0.013	0.591 ± 0.006	0.123 ± 0.045
Wikipedia	0.392 ± 0.010	**0.450 ± 0.007**	0.254 ± 0.037	O.O.M.
Wikipedia I	**0.861 ± 0.006**	0.796 ± 0.005	0.824 ± 0.003	0.163 ± 0.135
Wikipedia II	0.566 ± 0.021	**0.659 ± 0.011**	0.347 ± 0.012	0.155 ± 0.176

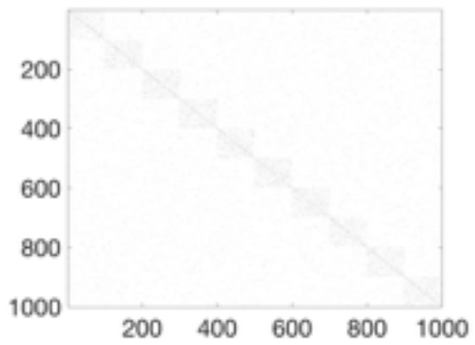
Could the performance be related to the congruence of information in the ingredients?

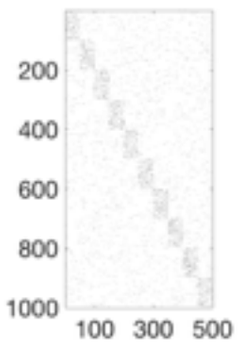
It gets more convoluted with the ground truth.

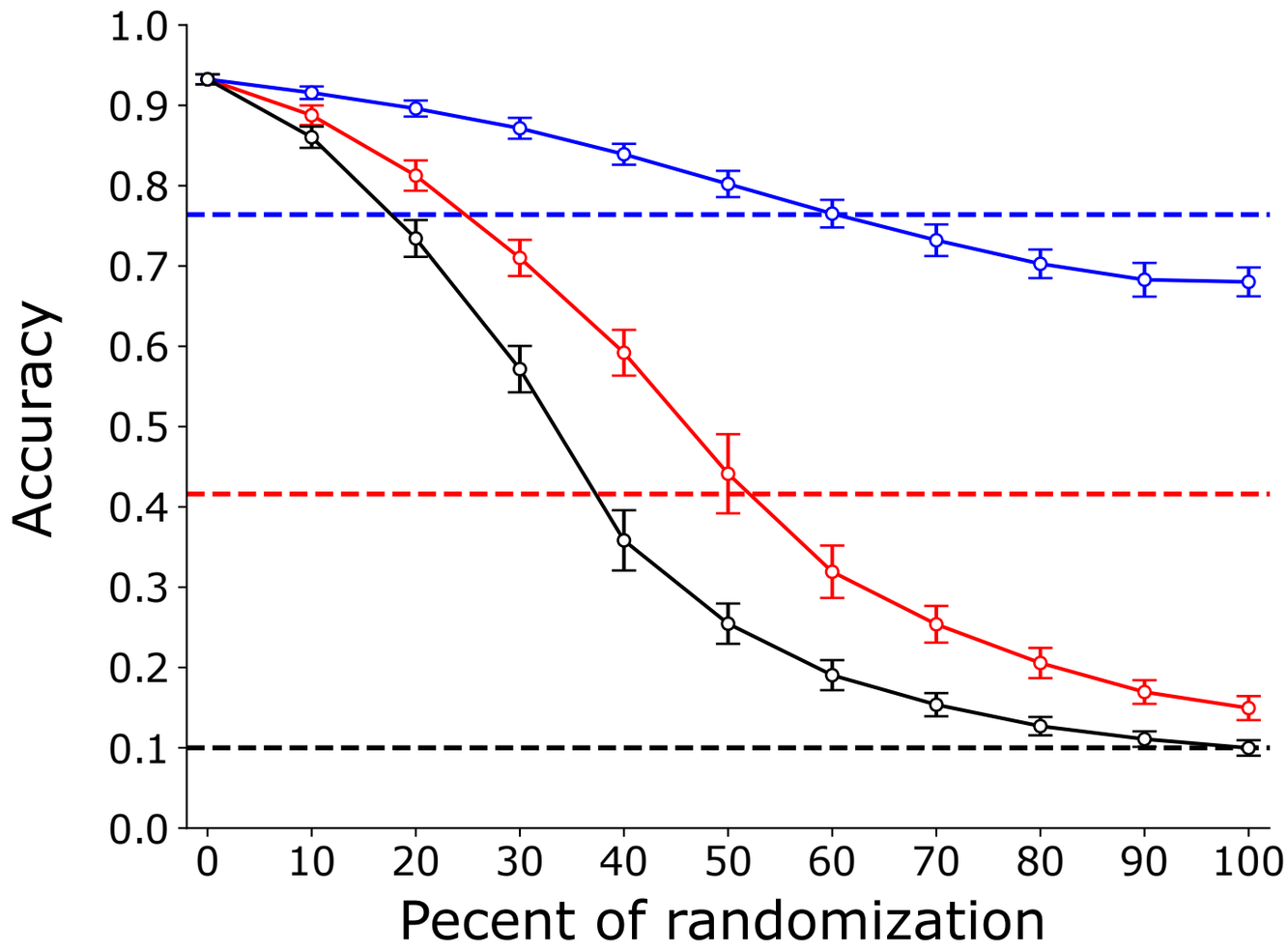


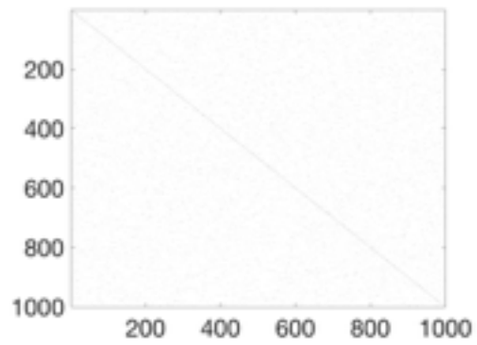
How aligned are *A*, *X* and *Y*?

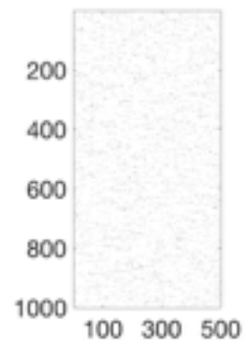
Misalignment by randomisation
Toy model





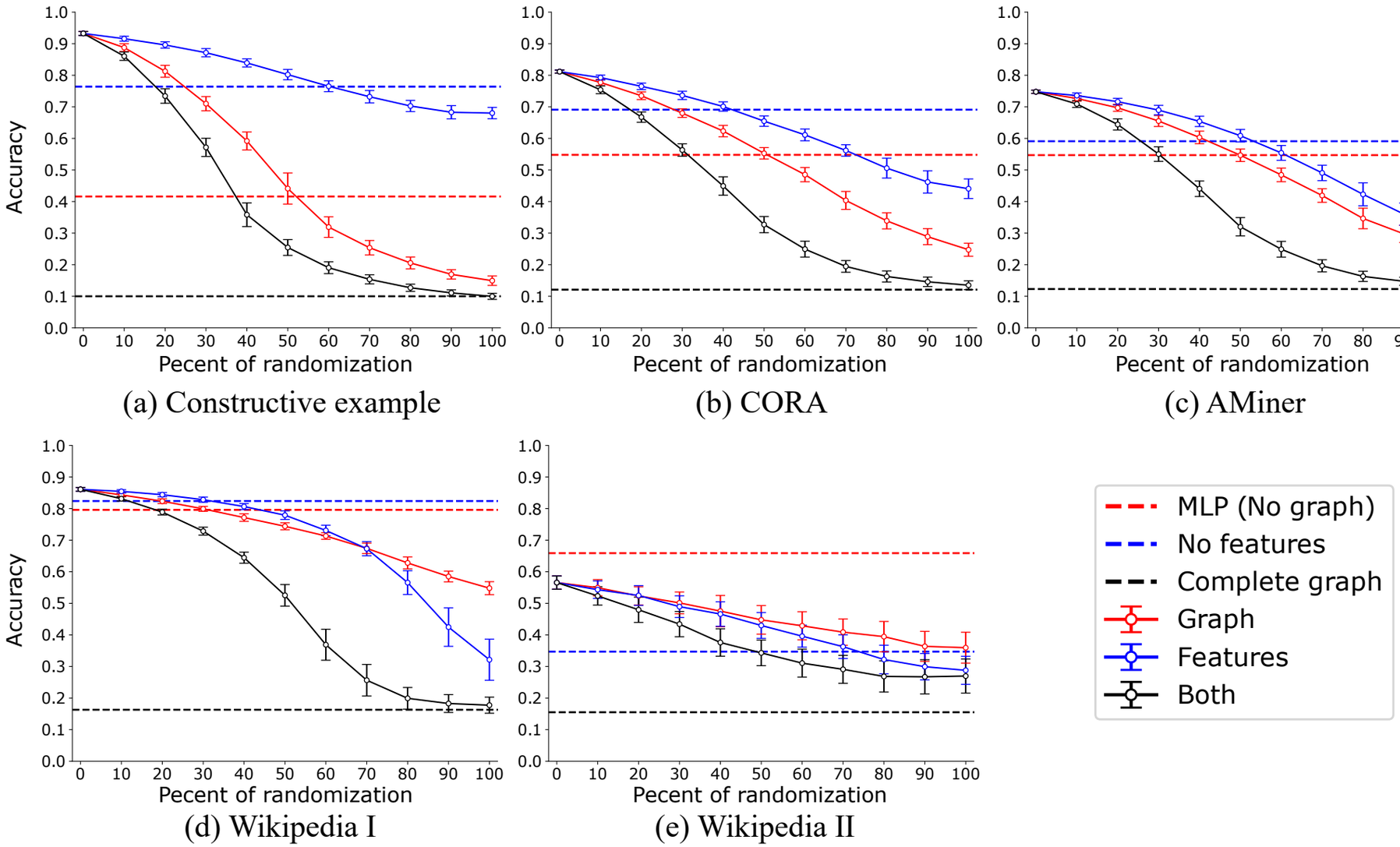






Features: label switching
Graph: configuration model

Randomisation - all datasets



As randomisation increases, information/alignment is lost and performance decreases.

Q: How to measure the alignment of subspaces?

A: Principal angles between $\mathcal{A}, \mathcal{B} \in \mathcal{R}^N$

$$\dim(\mathcal{A}) = \ell \leq \dim(\mathcal{B}) = p \leq N$$

Ye and Lim, « Schubert varieties and distances between subspaces of different dimensions », SIAM J. on Matrix Anal. and Appl., 2016

Q: How to measure alignment?

A: Principal angles between $\mathcal{A}, \mathcal{B} \in \mathcal{R}^N$

$$\dim(\mathcal{A}) = \ell \leq \dim(\mathcal{B}) = p \leq N$$

$$\theta_1 = \min_{a_1 \in \mathcal{A}, b_1 \in \mathcal{B}} \arccos\left(\frac{|a_1^T b_1|}{\|a_1\| \|b_1\|}\right),$$

$$\theta_j = \min_{\substack{a_j \in \mathcal{A}, b_j \in \mathcal{B} \\ a_j \perp a_1, \ldots, a_{j-1} \\ b_j \perp b_1, \ldots, b_{j-1}}} \arccos\left(\frac{|a_j^T b_j|}{\|a_j\| \|b_j\|}\right), \quad j = 2, \ldots, \ell.$$

By how much does $\mathcal{A}$ need to be rotated to « maximally overlap » with $\mathcal{B}$.

Björck and Golub, « Numerical methods for computing angles between linear subspaces », Mathematics of Computation, 1973.

Chordal distance

Any distance between subspaces has to be a function of the principal angles.

$$d(\mathcal{A}, \mathcal{B}) = \sqrt{\sum_{j=1}^{\ell} \sin^2 \theta_j}$$

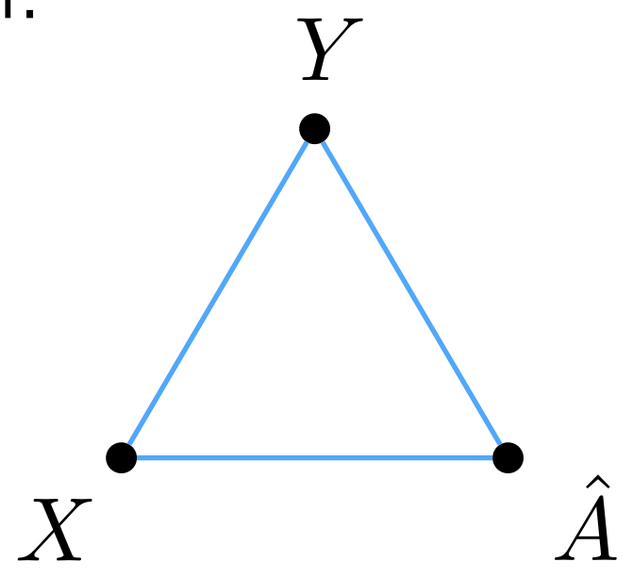
Ye and Lim, « Schubert varieties and distances between subspaces of different dimensions », SIAM J. on Matrix Anal. and Appl., 2016

Pairwise distances

$$D = \begin{bmatrix} 0 & d(X,\hat{A}) & d(X,Y) \\ d(X,\hat{A}) & 0 & d(\hat{A},Y) \\ d(X,Y) & d(\hat{A},Y) & 0 \end{bmatrix}$$

That we summarise with:

$$\|D\|_F = \sqrt{\sum_{i=1}^{3}\sum_{j=1}^{3} D_{ij}^2}$$



The need for dimensionality reduction

For the distance to be non trivial, the dimensions of the subspaces need to be strictly smaller than *N*.

$$\dim(\mathcal{A}) = \ell \leq \dim(\mathcal{B}) = p \boxed{<} N$$

We have:

$$\dim(X) = F < N$$

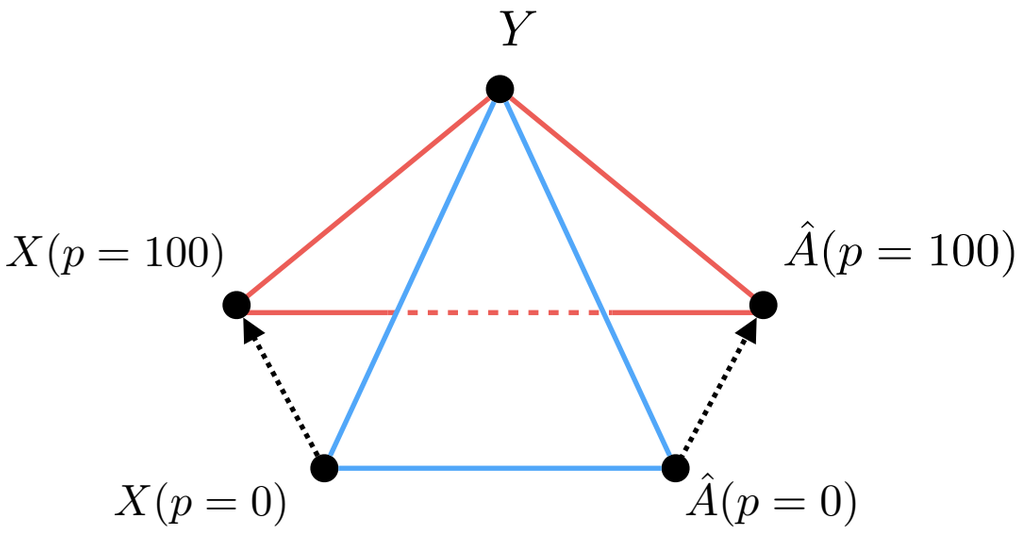
$$\dim(Y) = C < N$$

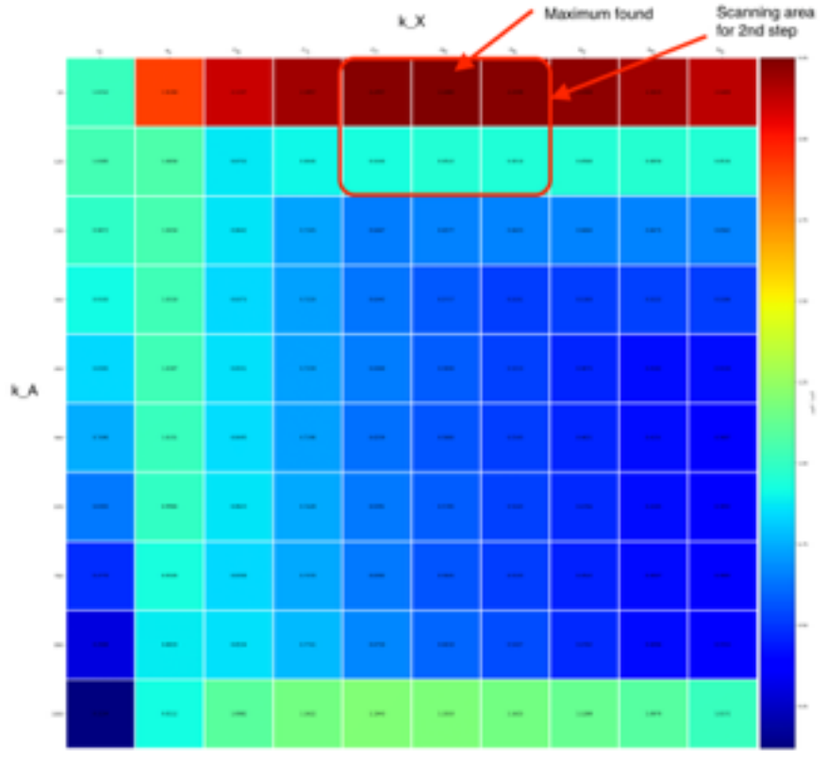
$$\underline{\dim(\hat{A}) = N}$$

How much information can we destroy?

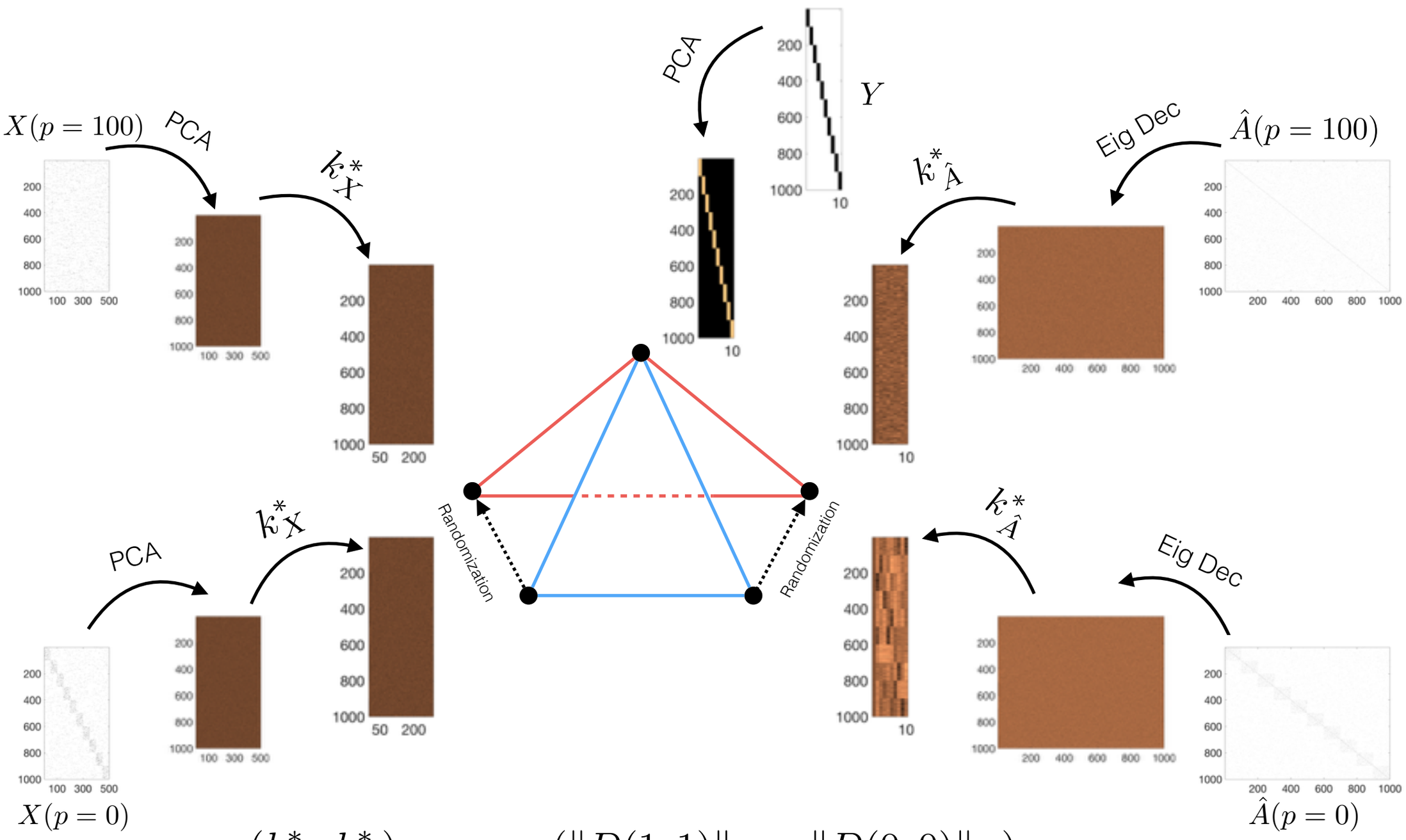
Maximum alignment loss between original and fully randomised data:

$$(k_X^*, k_{\hat{A}}^*) = \max_{k_X, k_{\hat{A}}} \left(\|D(1,1)\|_F - \|D(0,0)\|_F \right)$$



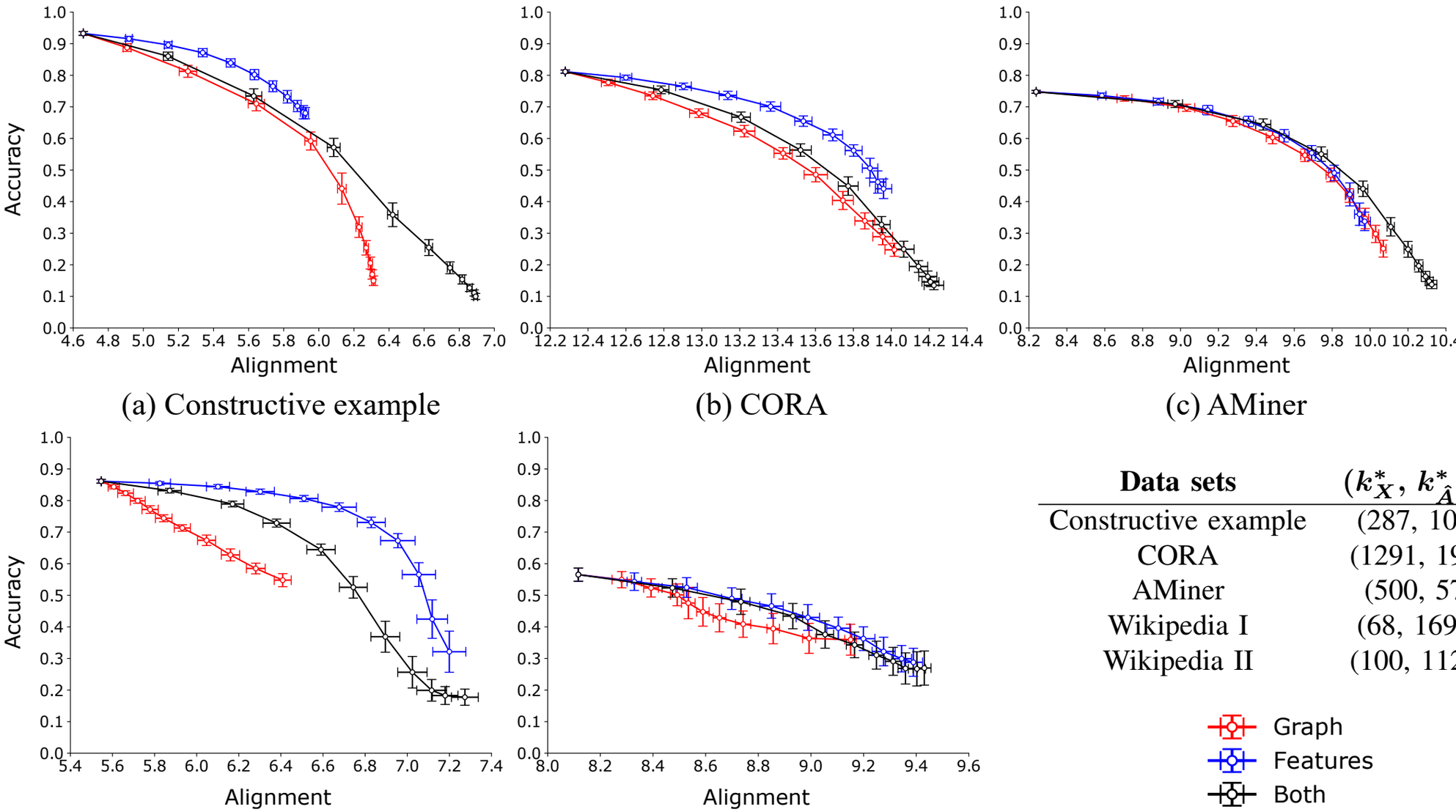


Summary of the pipeline



$$(k^*_X, k^*_{\hat{A}}) = \max_{k_X, k_{\hat{A}}} \left(\|D(1,1)\|_F - \|D(0,0)\|_F \right)$$

Performance versus alignment



(a) Constructive example (b) CORA (c) AMiner

(d) Wikipedia I (e) Wikipedia II

Data sets	$(k^*_X, k^*_{\hat{A}}, k^*_Y)$
Constructive example	(287, 10, 10)
CORA	(1291, 190, 7)
AMiner	(500, 57, 7)
Wikipedia I	(68, 1699, 5)
Wikipedia II	(100, 1125, 5)

Graph
Features
Both

Take home messages

- A degree of alignment (and modular structure) is needed for GCN to perform well.
- Principled way to reduce the dimensionality of the subspaces to have a meaningful notion of distance/alignment.
- General applicability to data alignment measurement.

Preprint: https://arxiv.org/abs/1905.12921

Code: https://github.com/haczqyf/gcn-data-alignment

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Pietro Panzarasa, QMUL

Thank you for listening, questions?

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