

Graph Convolutional Neural Networks

Liad Magen

BrickHouse Security
980 Ave of the Americas
3rd Floor
New York, NY 10018
800-654-7008

Sales Receipt

SHIP TO
Elizabeth McFarland 5062178924

8165059042

MO

te: 7/18/2008

19346
\$29.50 - 2nd Day Air - USA ONLY
r ID: 34835

ed via: \$29.50 - 2nd Day Air - USA ONLY Payment Method: Mastercard Last 4 digits: 9 56

SKU	DESCRIPTION	ORDERED	SHIPPED	UNIT PRICE	TOTAL
0	Mobile Alarm GPS Locator	1	1	\$499.95	\$499.95
IUB-UP-750	750 locates per month subscription UP	1	1	\$49.95	\$49.95
civation	Service activation for the PT8200	1	1	\$69.95	\$69.95
Subtotal				\$619.85	
Shipping				\$29.50	
Discounts				\$0.00	
Sales Tax				\$0.00	
Total				\$649.35	

Subtotal \$619.85
Shipping \$29.50
Discounts \$0.00
Sales Tax \$0.00
Total \$649.35

for purchasing the P-Trac. In order to get you started quickly so that you will be better acquainted with some of the great features we

name is the first initial and last name of the person the unit was shipped to.
ult password is: sbodsfy (Change this in your profile after you login)
ts |Beacon ID: 00006585951

(a) Purchase receipt

3200162350 江苏增值税专用发票 No 18330712

¥160.19 (小写) ¥165.00

¥4.81

Tax Amount

¥160.19 (小写) ¥165.00

913209023239760758

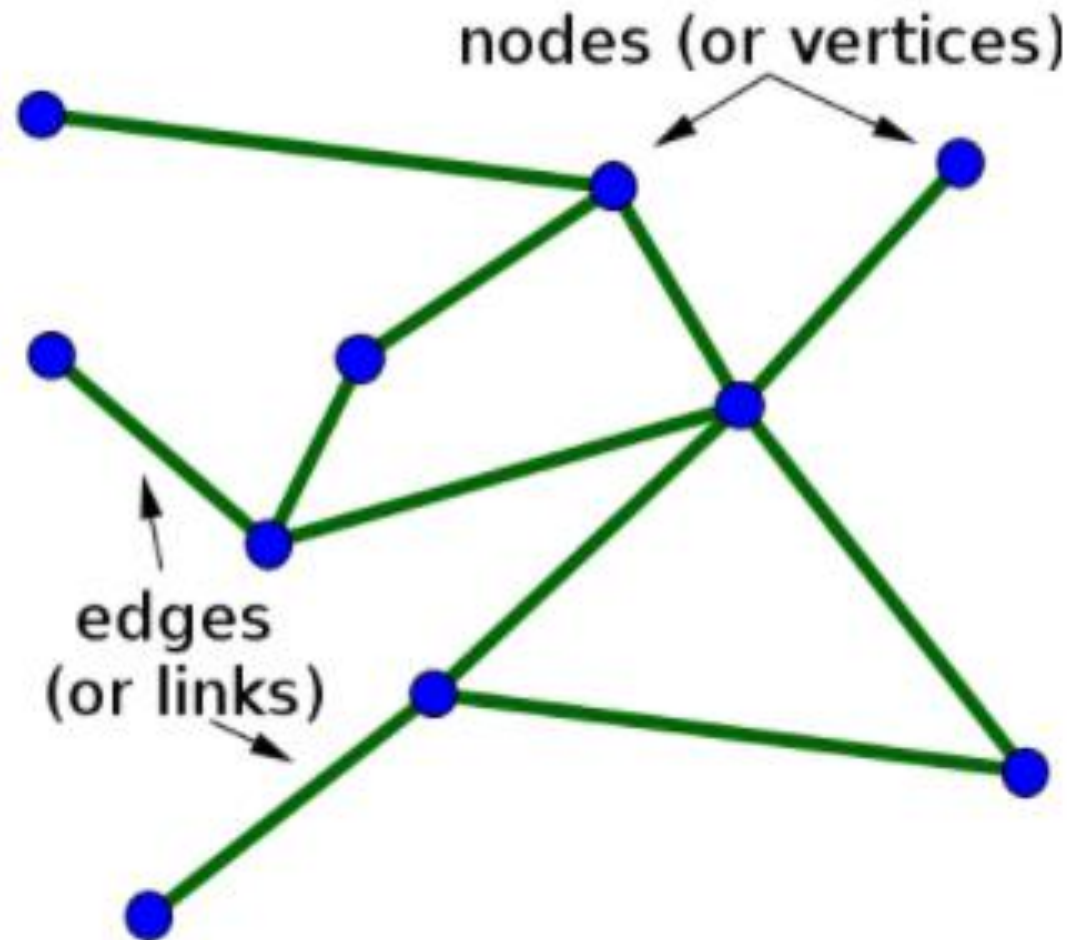
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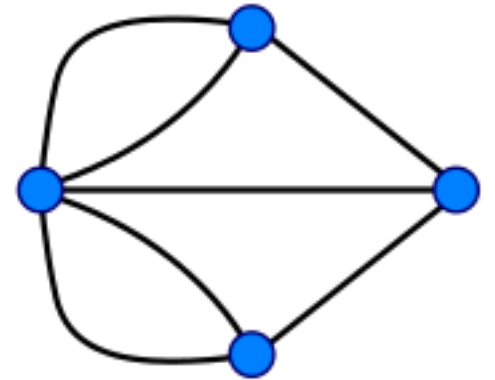
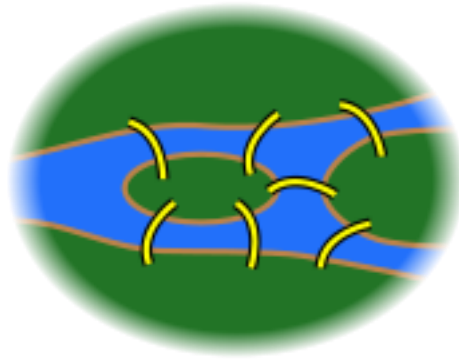
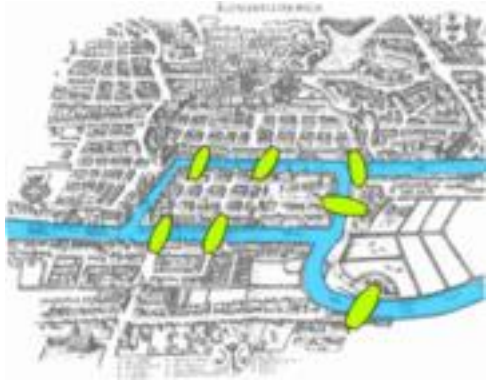
(b) Value-added tax invoice

Is it NLP or
Computer
Vision?

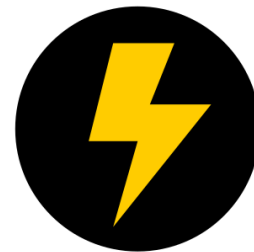
NER for visually rich
documents

What are
graphs?

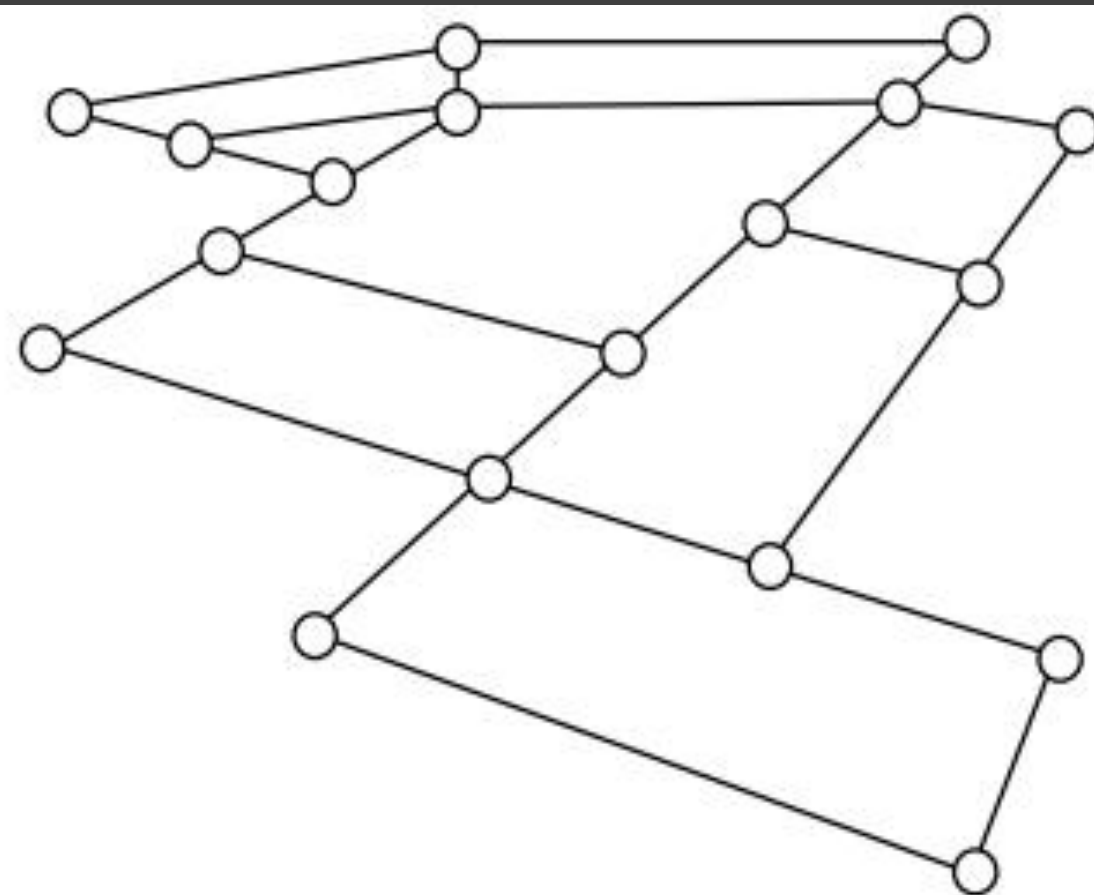




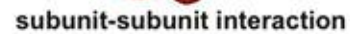
Seven Bridges of Königsberg



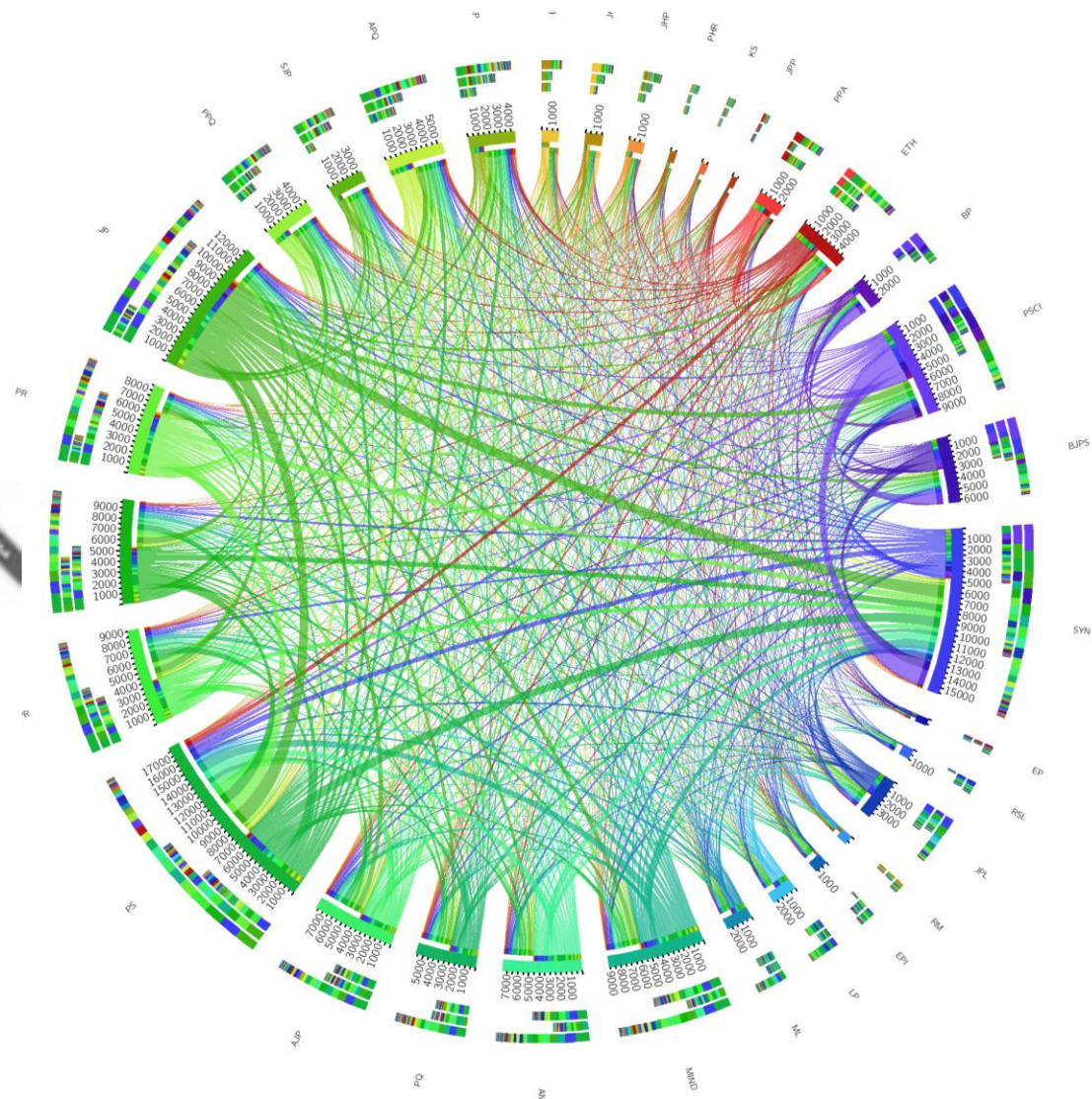
Can you
connect the
facilities to
all 3 houses?



Location & Street
representation



Paper citations as a graph





Company Name

INVOICE

[Street Address]
[City], [State], [ZIP Code]
[Phone]
[Email Address]
[Company Website]

Date: 2019-04-10
Invoice #: 00198847
Due Date: 2019-05-10

BILL TO:

[Recipient Name]
[Company Name]
[Street Address]
[City], [State], [ZIP Code]
[Phone]

SHIP TO:

[Recipient Name]
[Company Name]
[Street Address]
[City], [State], [ZIP Code]
[Phone]

Description	Qty	Unit Price	Amount
Product 1	1	\$100.00	\$100.00
Product 2	10	\$200.00	\$2,000.00
Product 3	100	\$10.00	\$1,000.00

TERMS:

- Payment due in 30 days.
- Please note the invoice number in your payment method.

Banking and wire transfer information may also be included here.

Total
Subtotal
Discount
Taxes
Total

\$1,100.00
\$1,100.00
\$0.00
\$0.00
\$1,100.00

Thank you for
your business!

MONOSI


ORDERS

LOOKBOOKS

0 items in your cart

ALL PRODUCTS / NEWS / BAGS

Search ...



Duffle Bag by Drife




S M L XL

Currently available on stock 22

€78.00

BUY THIS

€100.00 Recommended retail price
includes VAT and shipping



ZOOM

Show more photos

DUFFLE BAG

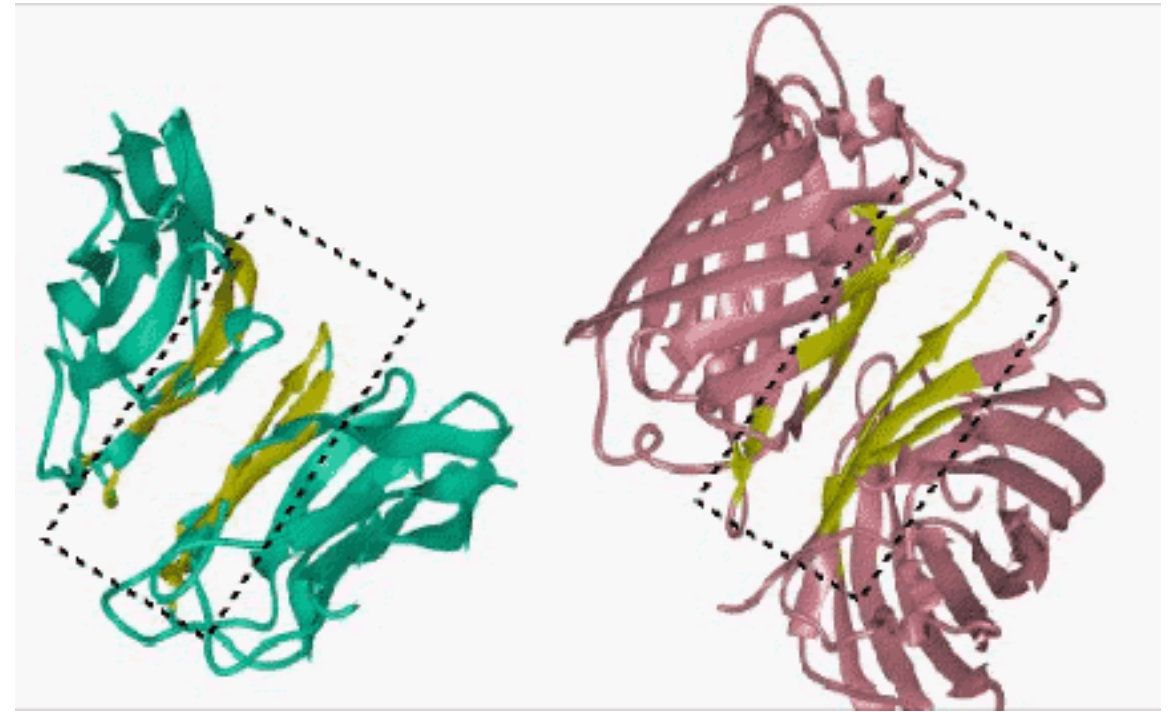
The practical and elegant Duffle Bag by South Korean label Drife was designed in collaboration with the up-and-coming collective Bontis & Partners. Aesthetically punctuated with thoughtful combinations of sturdy canvas, vegetable-tanned leather, and lovingly designed details.

SHIPPING INFORMATION

SKU MG0000021015_09

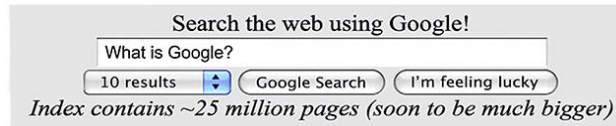
Visually
Rich Data

Process other (non-Euclidean) formats of data

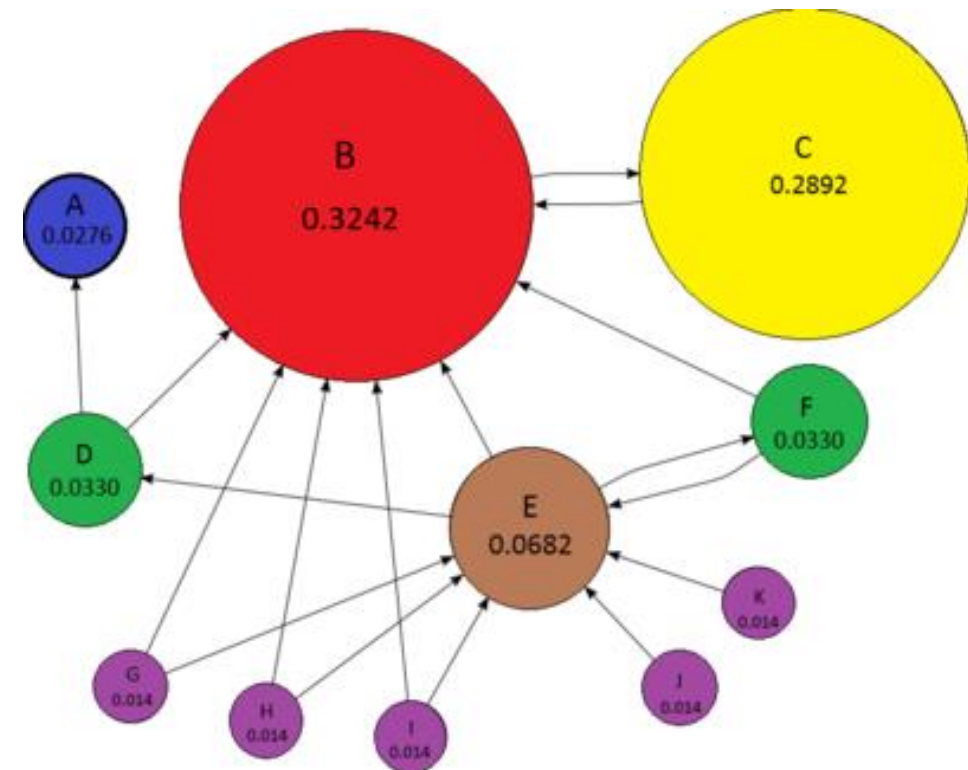
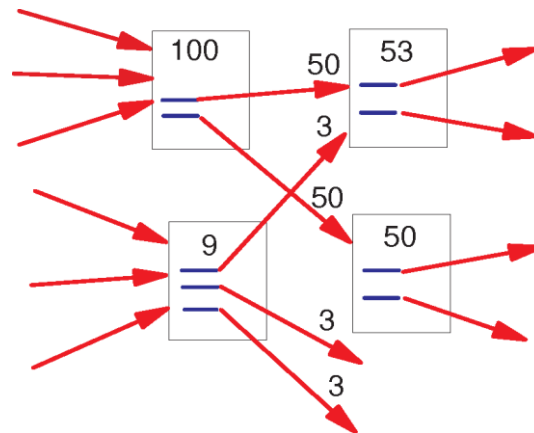


Google PageRank

Google!



$$PR_i = \frac{1-d}{n} + d \sum_{j=1}^n \frac{PR_j}{c_j}$$



How PageRank Works (A Simplified View)

PageRank is divided equally between the total number of links on a page.



Source: <https://ahrefs.com/blog/google-pagerank/>

ahrefs

PageRank



PLoS One. 2015; 10(8): e0134794.
Published online 2015 Aug 19. doi:

OPEN ACCESS Freely available online

Google Goes Cancer: Improving Outcome Prediction for Cancer Patients by Network-Based Ranking of Marker Genes

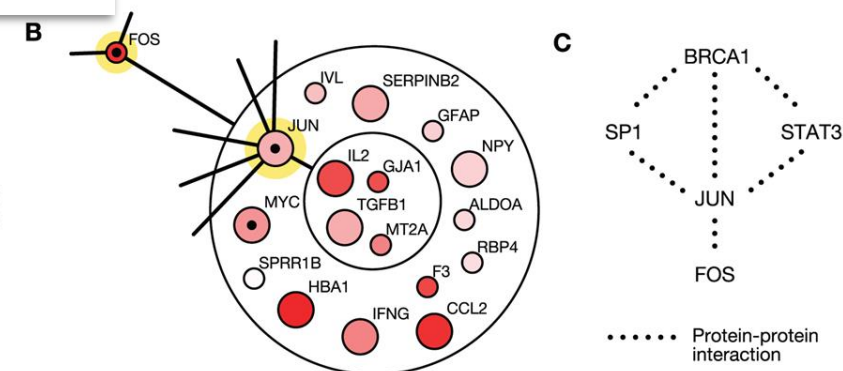
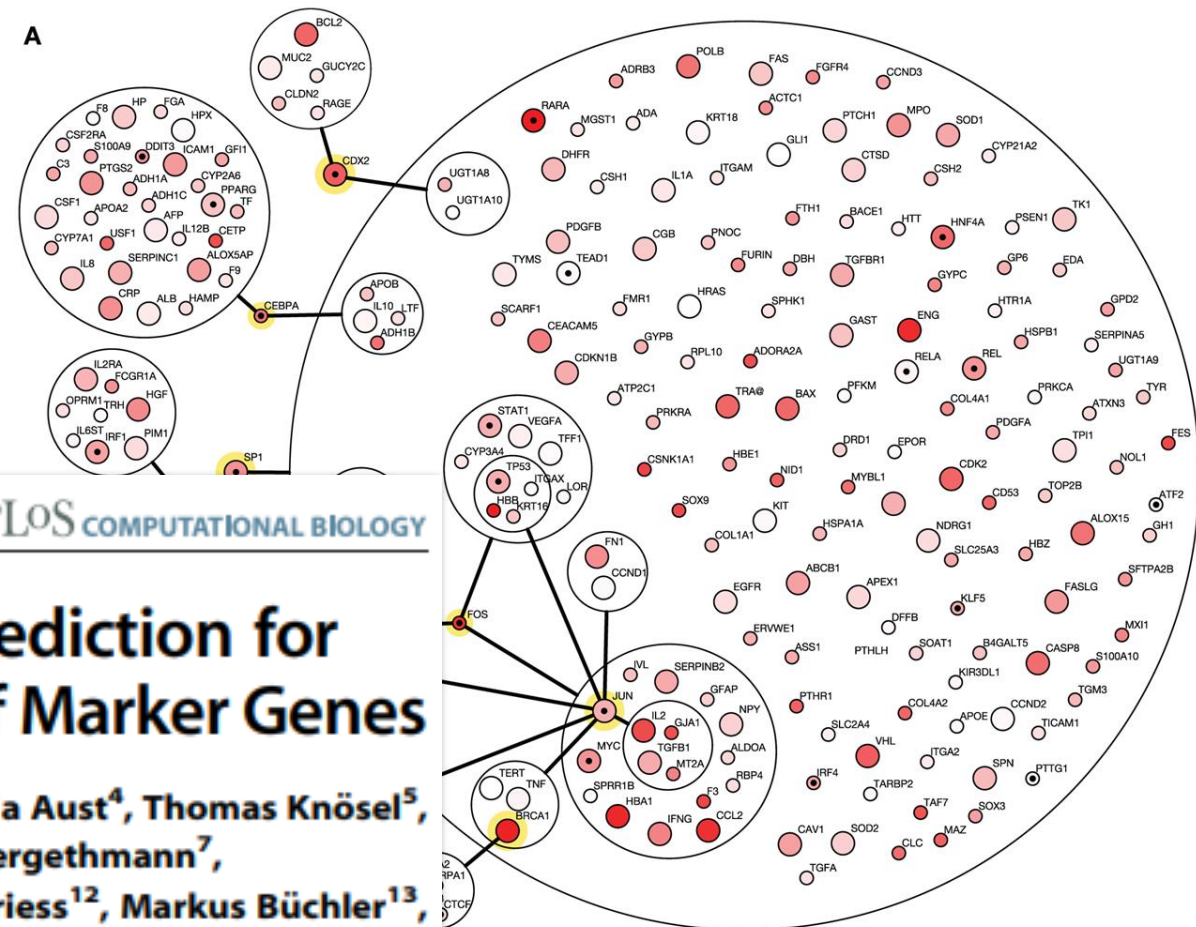
Christof Winter^{1*}, Glen Kristiansen^{2,3}, Stephan Kersting^{3,9}, Janine Roy¹, Daniela Aust⁴, Thomas Knösel⁵, Petra Rümmele⁶, Beatrix Jahnke³, Vera Hentrich³, Felix Rückert³, Marco Niedergethmann⁷, Wilko Weichert⁸, Marcus Bahra⁹, Hans J. Schlitt¹⁰, Utz Settmacher¹¹, Helmut Friess¹², Markus Büchler¹³, Hans-Detlev Saeger³, Michael Schroeder¹¹, Christian Pilarsky^{3,1}, Robert Grützmann^{3,1}

Page

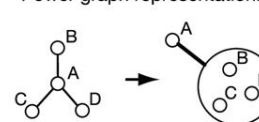
PR
Ying Ding¹, Erjia Yan, Arthur

Inspired

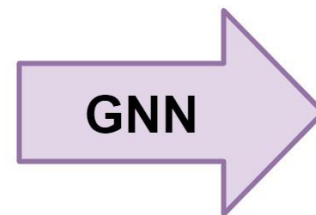
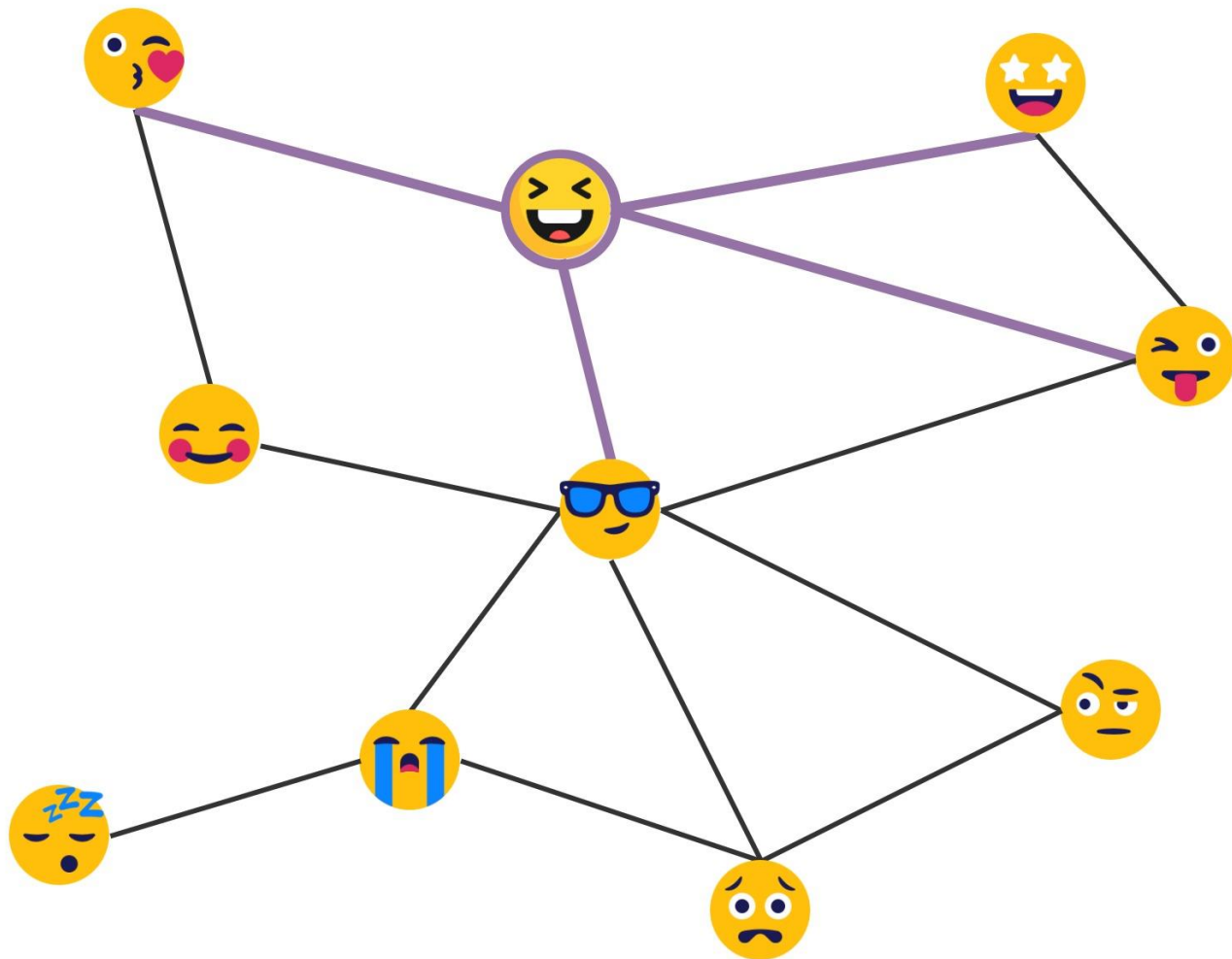
Gene is transcription factor yes no Gene is related to pancreas cancer survival in literature yes no Signature gene Absolute correlation of gene expression with survival in our data 0 0.6



Power graph representation:



A is connected to B, C, and D



Most influential? 🧐

Least influential? 😴

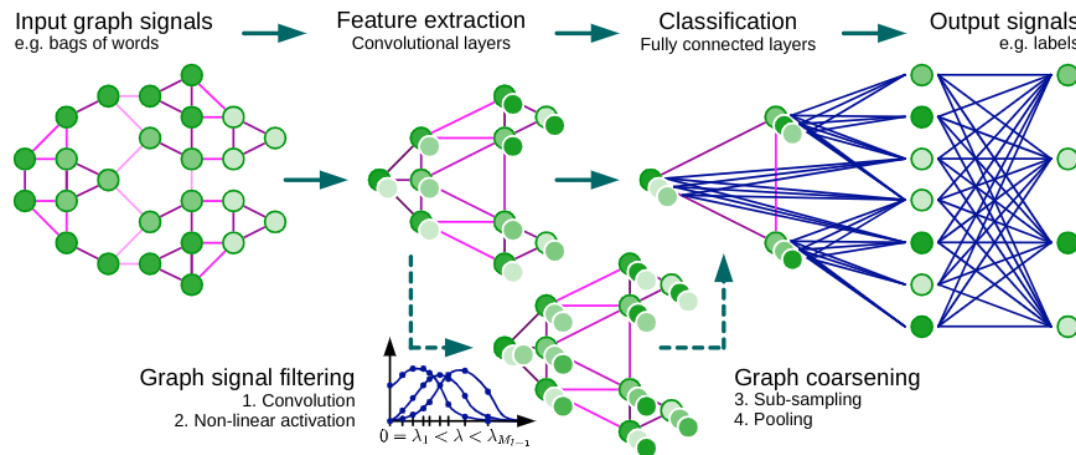
Possible connection? 😊

Unrelated? 😴 😊

Most similar? 😄 😜 😊

GCN

2016



Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering

Michaël Defferrard

Xavier Bresson

Pierre Vandergheynst

EPFL, Lausanne, Switzerland

{michael.defferrard,xavier.bresson,pierre.vandergheynst}@epfl.ch

SEMI-SUPERVISED CLASSIFICATION WITH GRAPH CONVOLUTIONAL NETWORKS

Thomas N. Kipf

University of Amsterdam

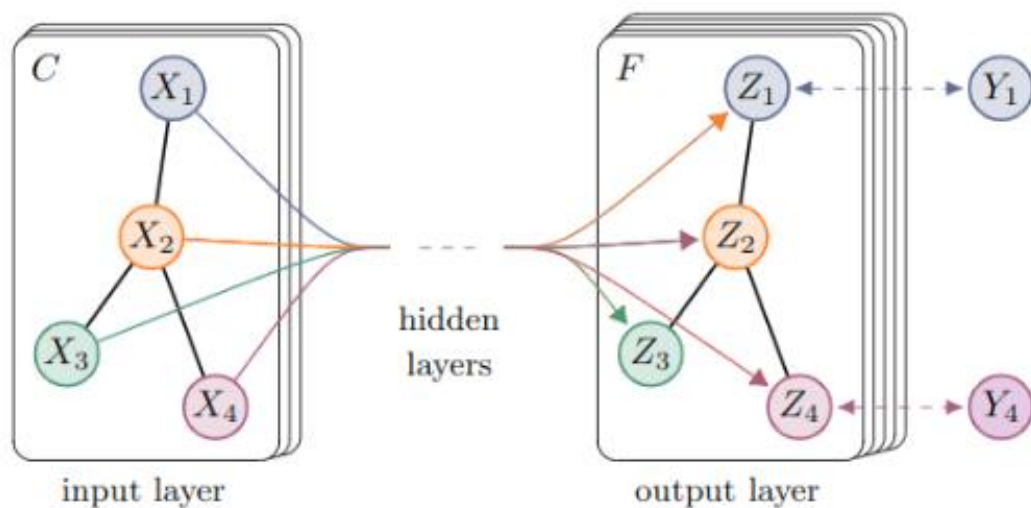
T.N.Kipf@uva.nl

Max Welling

University of Amsterdam

Canadian Institute for Advanced Research (CIFAR)

M.Welling@uva.nl

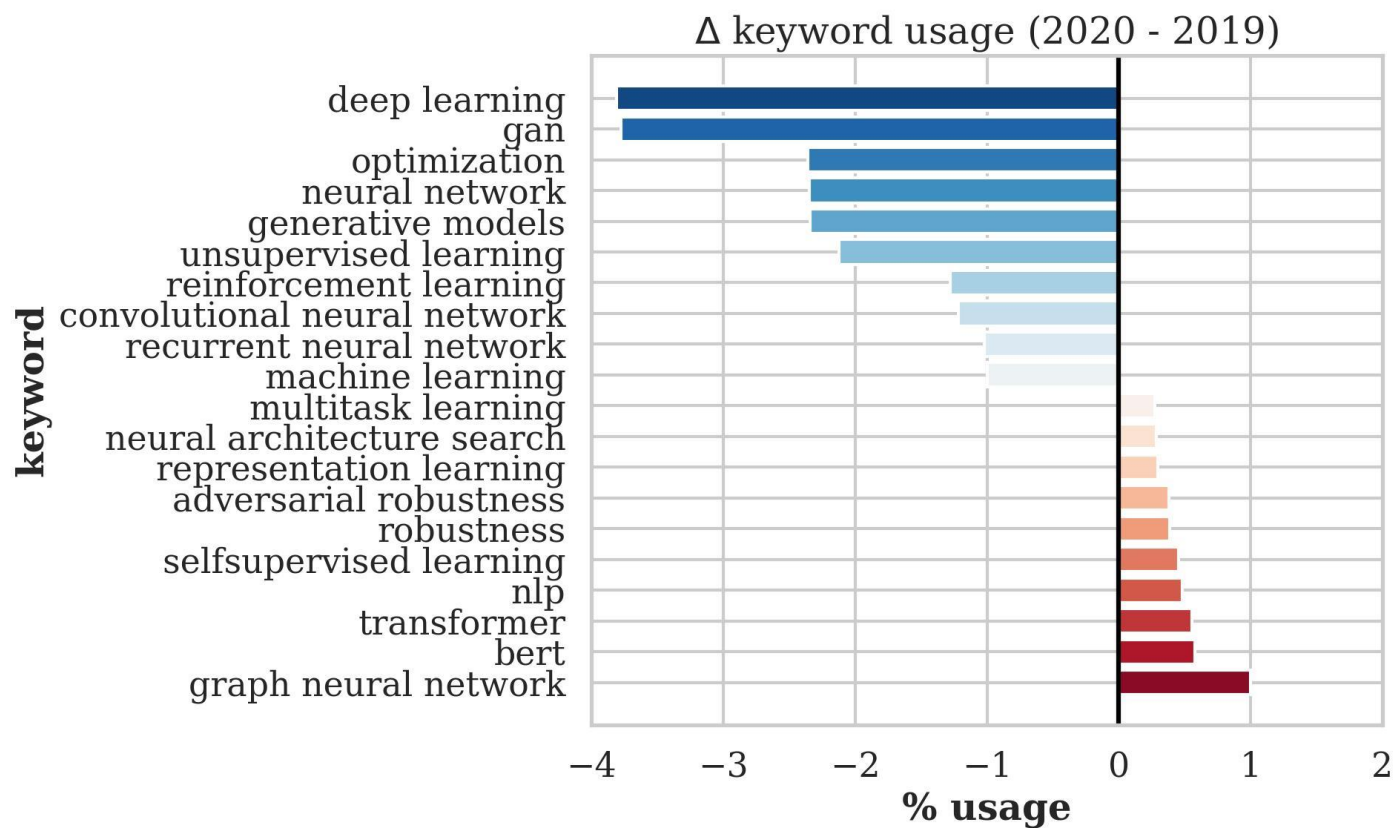


(a) Graph Convolutional Network



(b) Hidden layer activations

Figure 1: *Left*: Schematic depiction of multi-layer Graph Convolutional Network (GCN) for semi-



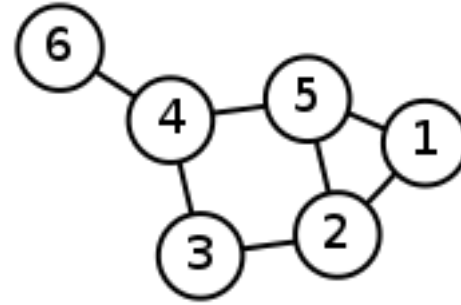
Graph Neural Networks

ICLR Submissions

Source:
Twitter - @prlz77

Graphs, Mathematically

- $G = (\mathbf{V}etrices, \mathbf{E}dges)$
- $V = \{v_1 \dots v_n\}$
- $E = \{(v_i, v_j), \dots\}$

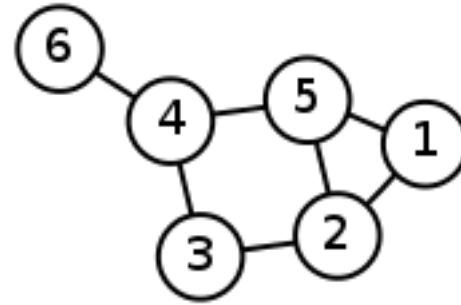


Graphs, Mathematically

$G = (\mathbf{V} \text{etices}, \mathbf{E} \text{dges})$

Adjacency matrix

$A_{ij} = \begin{cases} 1 & \text{if } \{v_i, v_j\} \in \mathbf{E} \text{ \& \& } i \neq j \\ 0 & \text{Otherwise} \end{cases}$



$$\begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

Graph - algebraic representation

$$G = (\mathbf{V}_{\text{etices}}, \mathbf{E}_{\text{dges}})$$

Laplacian matrix *

$$\mathbf{L} = \mathbf{D} - \mathbf{A}$$

$$\begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Degree

=

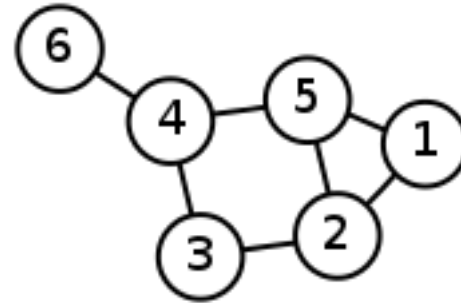
$$\begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

Adjacency

=

$$\begin{pmatrix} 2 & -1 & 0 & 0 & -1 & 0 \\ -1 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & -1 & 0 & -1 & 3 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}$$

Laplacian



* For undirected graphs


```
for object to mirror_mod.mirror_object
operation == "MIRROR_X":
    mirror_mod.use_x = True
    mirror_mod.use_y = False
    mirror_mod.use_z = False
operation == "MIRROR_Y":
    mirror_mod.use_x = False
    mirror_mod.use_y = True
    mirror_mod.use_z = False
operation == "MIRROR_Z":
    mirror_mod.use_x = False
    mirror_mod.use_y = False
    mirror_mod.use_z = True

selection at the end -add
mirror_ob.select= 1
modifier_ob.select=1
context.scene.objects.active
("Selected" + str(modifier_ob.name))
mirror_ob.select = 0
= bpy.context.selected_objects
data.objects[one.name].select

print("please select exactly one object")

-- OPERATOR CLASSES --
```

GCN - Algorithm

```
types.Operator):
    X mirror to the selected
object.mirror_mirror_X"
mirror X"
```

GCN

GCN Layer:

$$Y = \text{ReLU}(A \cdot X \cdot W)$$

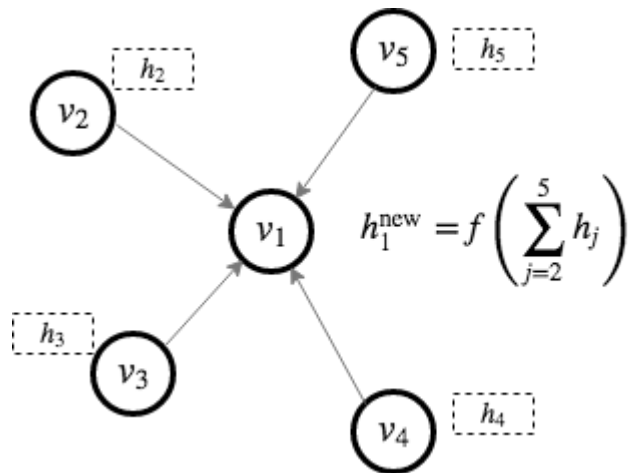
...but with message passing

$$H^{(l+1)} = \sigma(\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)})$$

Message Passing

For each node u

- Aggregate neighbor nodes h_v into an intermediate representation \hat{h}_u
- Transform the aggregated representation \hat{h}_u with a linear projection followed by a non-linearity (ReLU) $h_u = f(W_u \hat{h}_u)$



Mathematically:

$$H^{(l+1)} = \sigma(\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)})$$

$H \rightarrow$ Network Layer

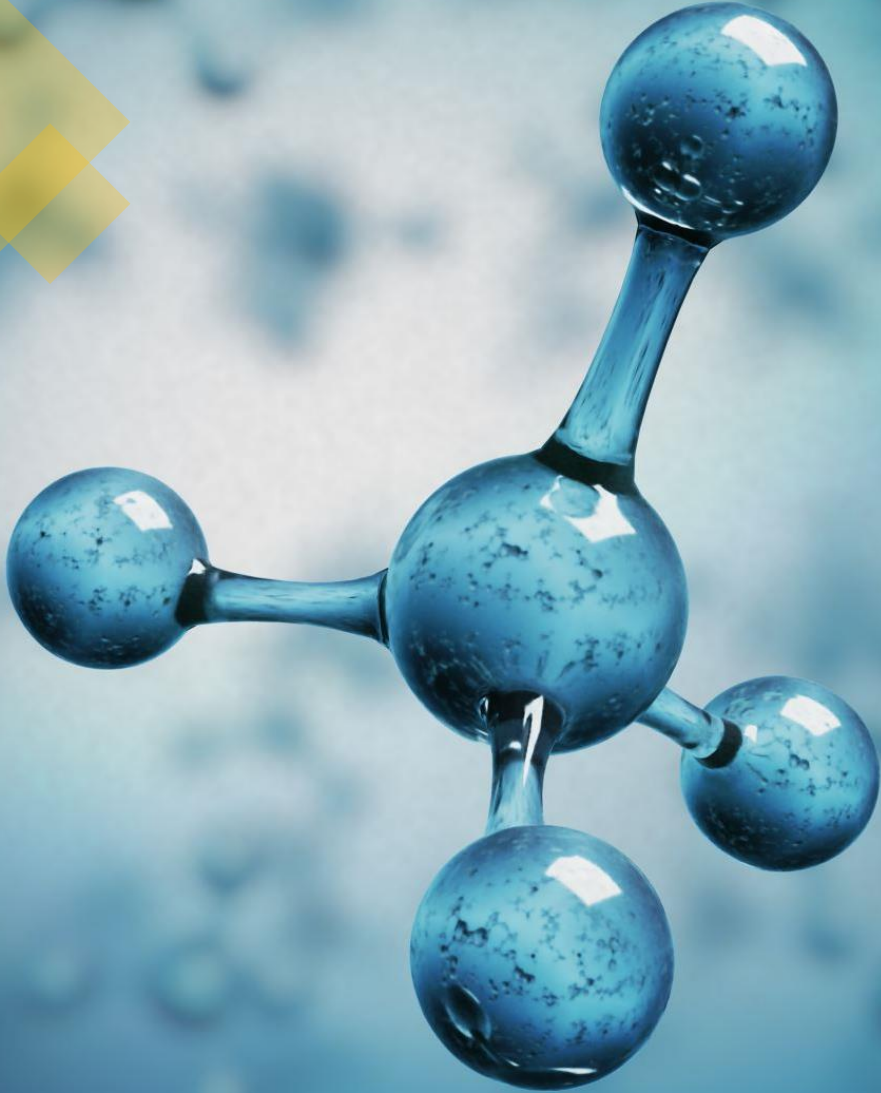
$W \rightarrow$ Network Weights

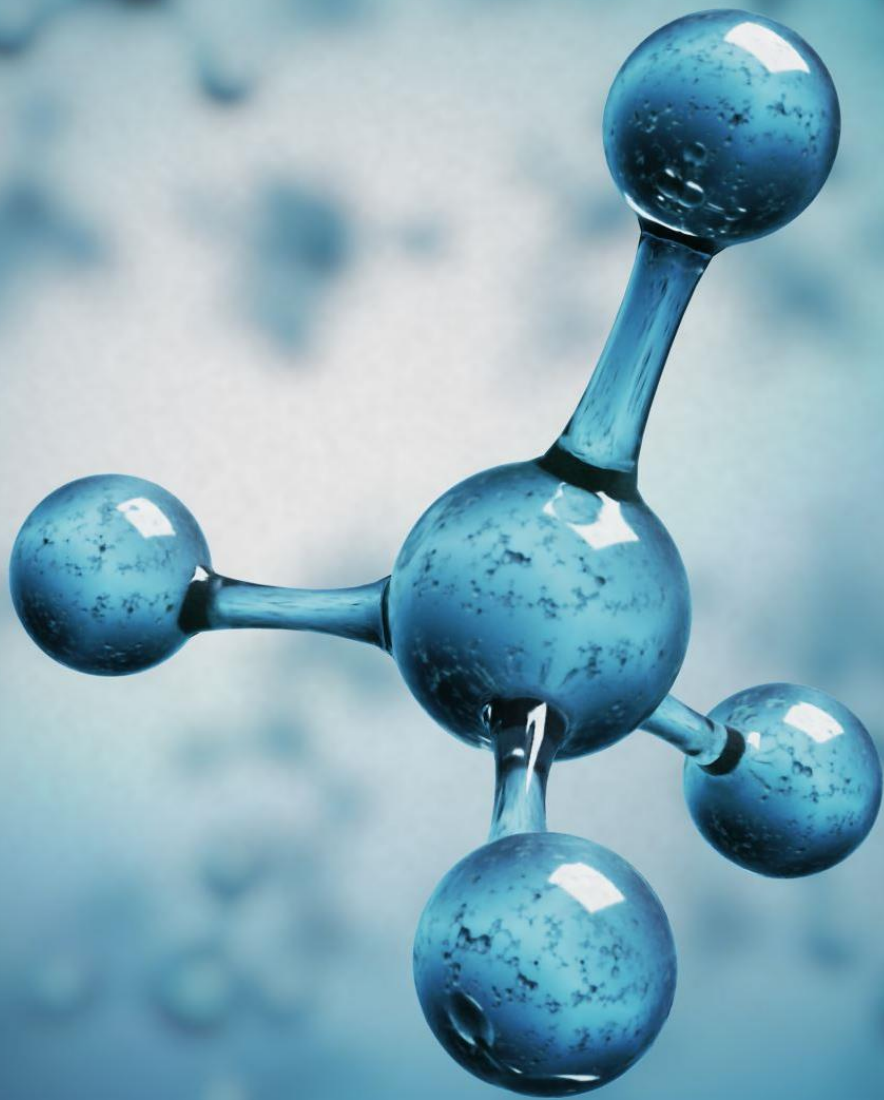
$A \rightarrow$ Adjacency Matrix

$D \rightarrow$ Degree Matrix

Model types

- Graph classification
 - Chemical properties of a molecule
 - Comparing user preferences / activities
- Node classification - node label prediction
 - Malicious users in a social network
 - Visually inferred Named Entity Recognition (NER)
 - Node clustering
- Edge prediction
 - Recommendation system
 - Protein-protein interaction
 - “Friend” suggestion





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civation	Service activation for the PT8200	1	1	\$69.95	\$69.95
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name is the first initial and last name of the person the unit was shipped to.
ult password is: sbdsefgy (Change this in your profile after you login)
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¥160.19 (小写) ¥165.00

¥4.81

Tax Amount

¥160.19 (小写) ¥165.00

开票人: 张

(b) Value-added tax invoice

NER for
visually rich
documents

Creating a graph out of a
visually rich document

Graph processing

- Document Graph --> Node Vectors
- Concatenate with Token Embedding
- Classify
 - FFNN
 - BiLSTM +CRF
 - BERT

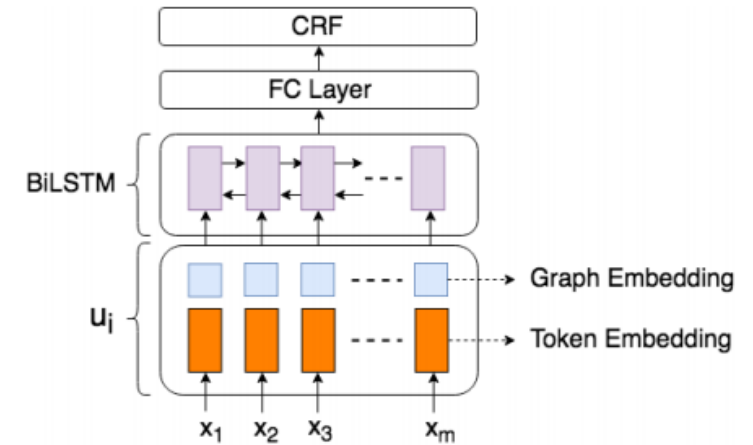
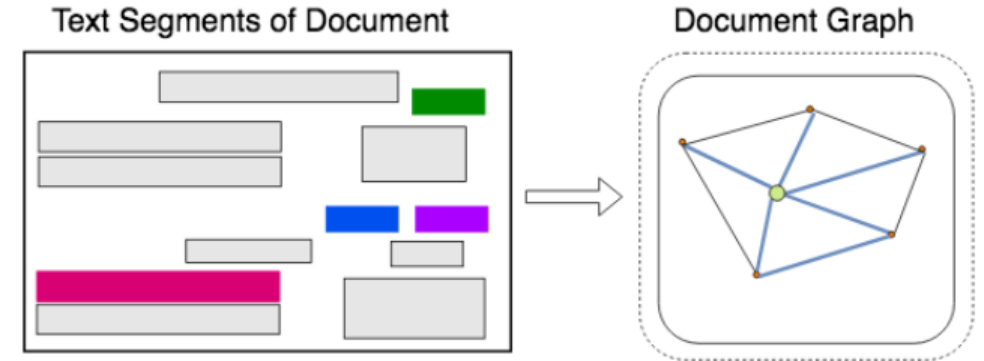


Figure 4: BiLSTM-CRF with graph embeddings.



NetworkX

Network Analysis in Python



Store and mutate Graphs

Graph algorithms:

- Shortest path – Dijkstra
- TreeWidth
- Clustering
- centrality

Network analysis

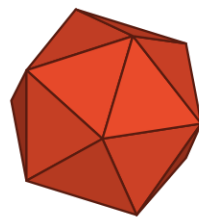
Node / edge data

Visualization tools

DGL

DeepGraphLibrary

- Building blocks
- Great tutorials
- Generative graphs
- Great for research and complicated tasks



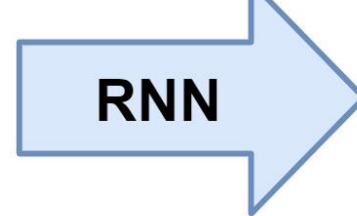
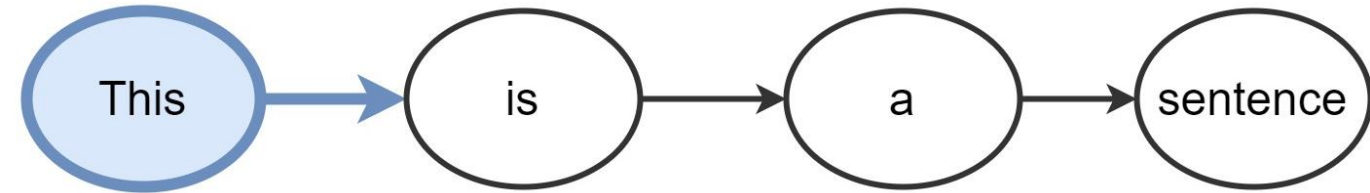
PyTorch geometric

- An extension library for pyTorch
- Officially part of the pyTorch ecosystem
- Easily extensible
- Papers are implemented directly in it
- Looooooooooooooooong list of ready-to-use methods and algorithms:
 - TransformerConf (2020)
 - GCN2Conv (2020)
 - DeeperGCN (2020)
 - Top-K Pooling
 - PairNorm
- Now is called PYG
- <https://pytorch-geometric.readthedocs.io/en/latest/>



Model types

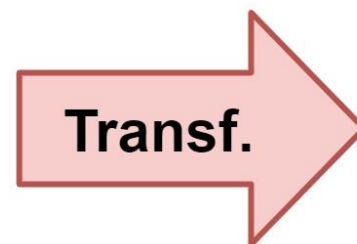
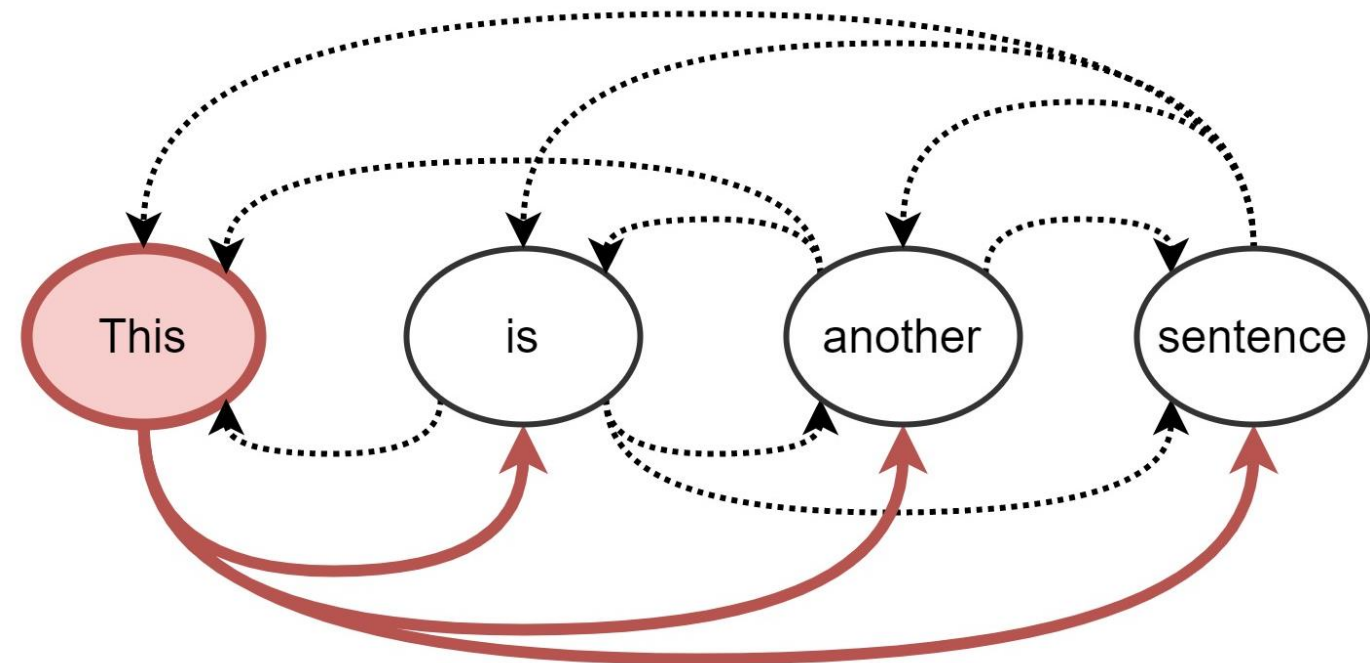
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Translation?

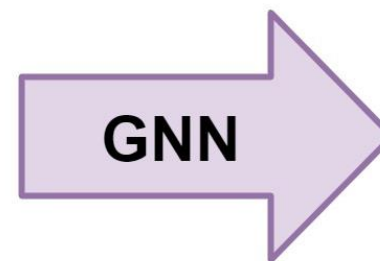
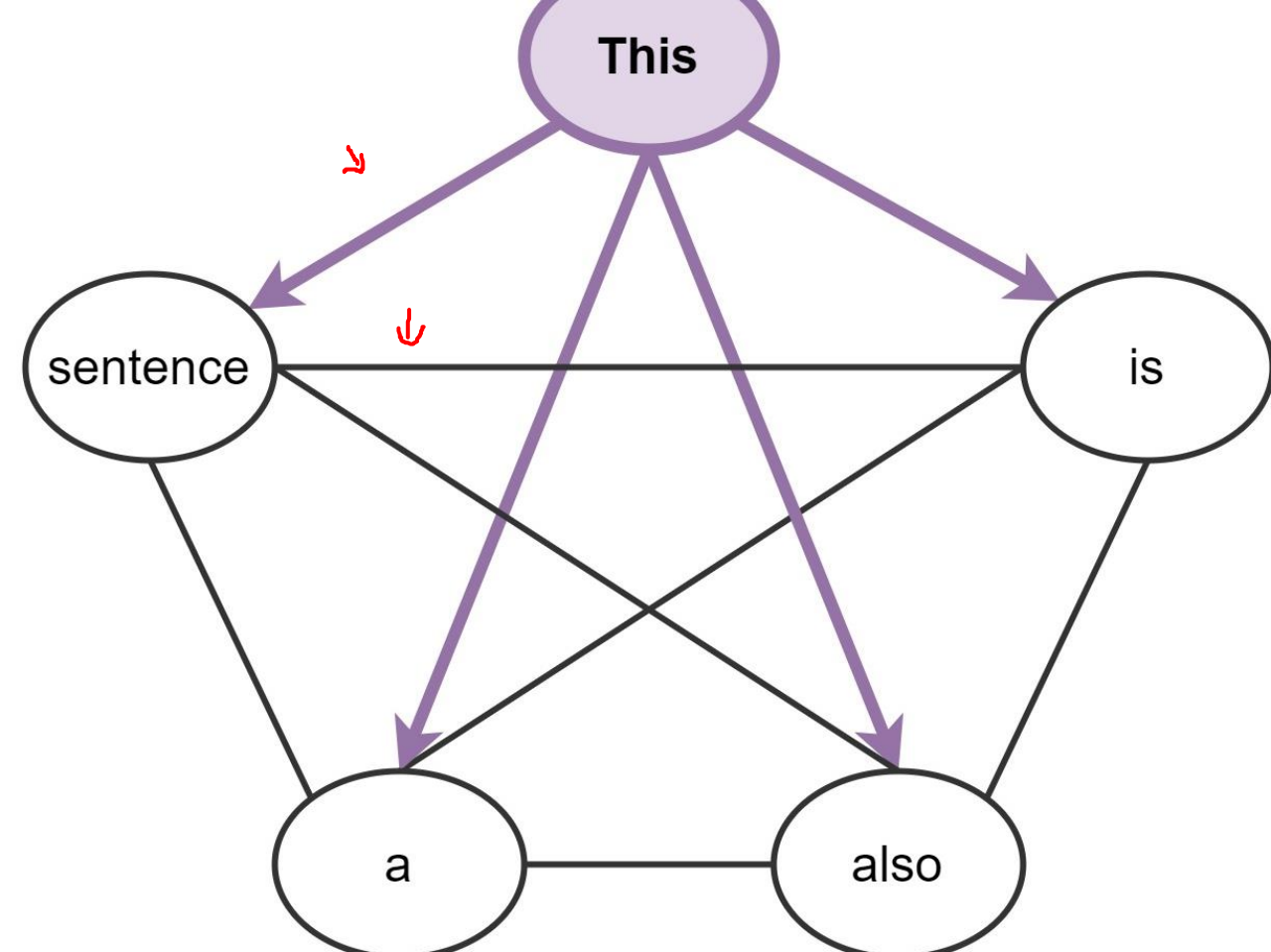
Sentiment?

Next word?



Part-of-speech tags?

Sentence as a graph |



Translation?

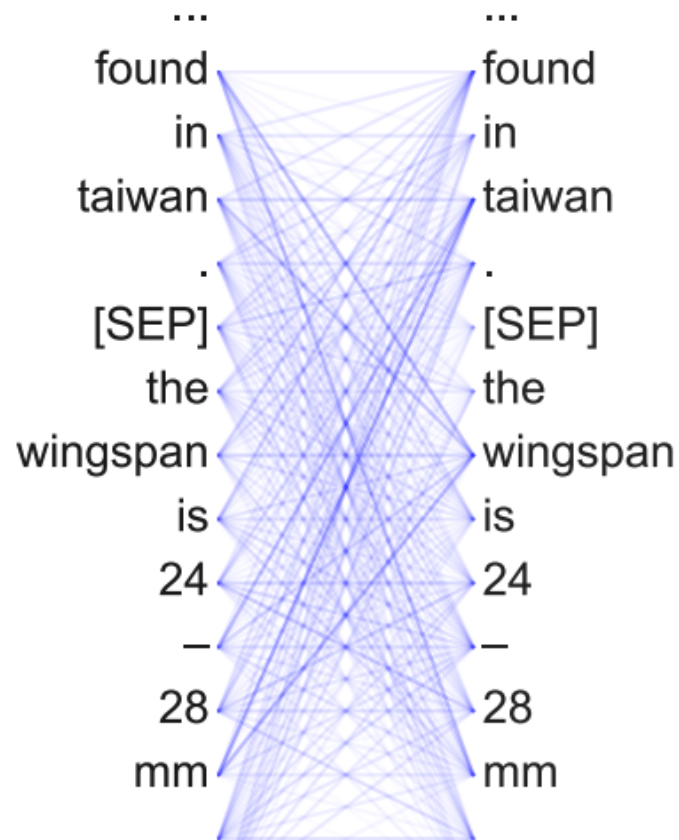
Sentiment?

Next word?

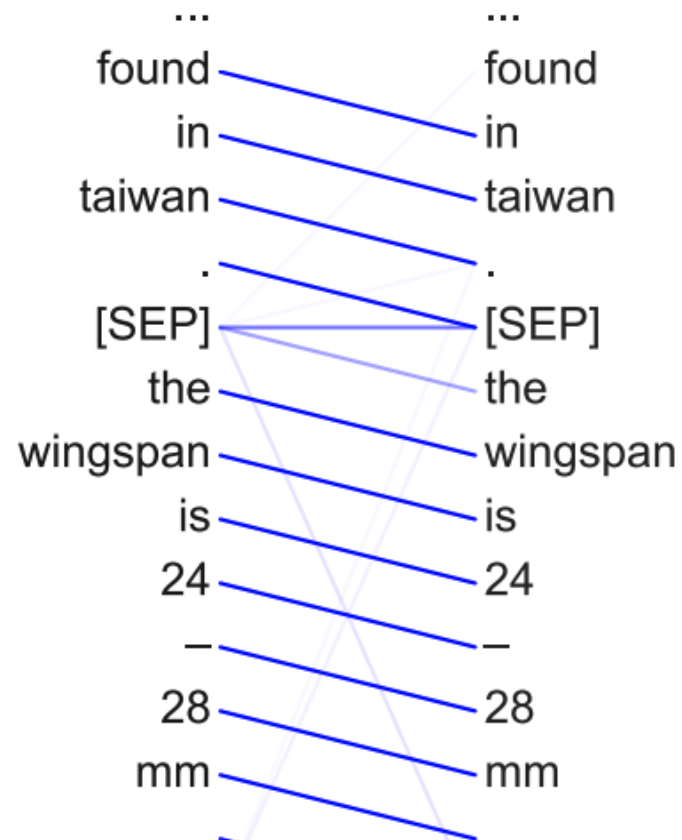
Part-of-speech tags?

Sentence as a graph |

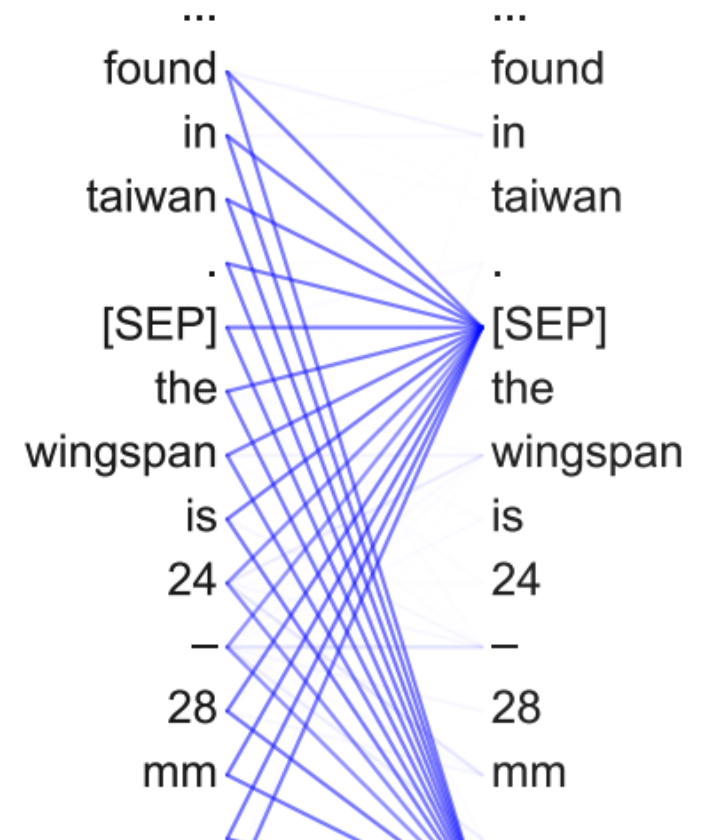
Head 1-1
Attends broadly



Head 3-1
Attends to next token



Head 8-7
Attends to [SEP]



BERT (Attention) is equivalent to deep GCN

<https://graphdeeplearning.github.io/post/transformers-are-gnns/>

Ongoing Topic

- LayoutLM v2
- HuggingFace
- Can use RoBERTa

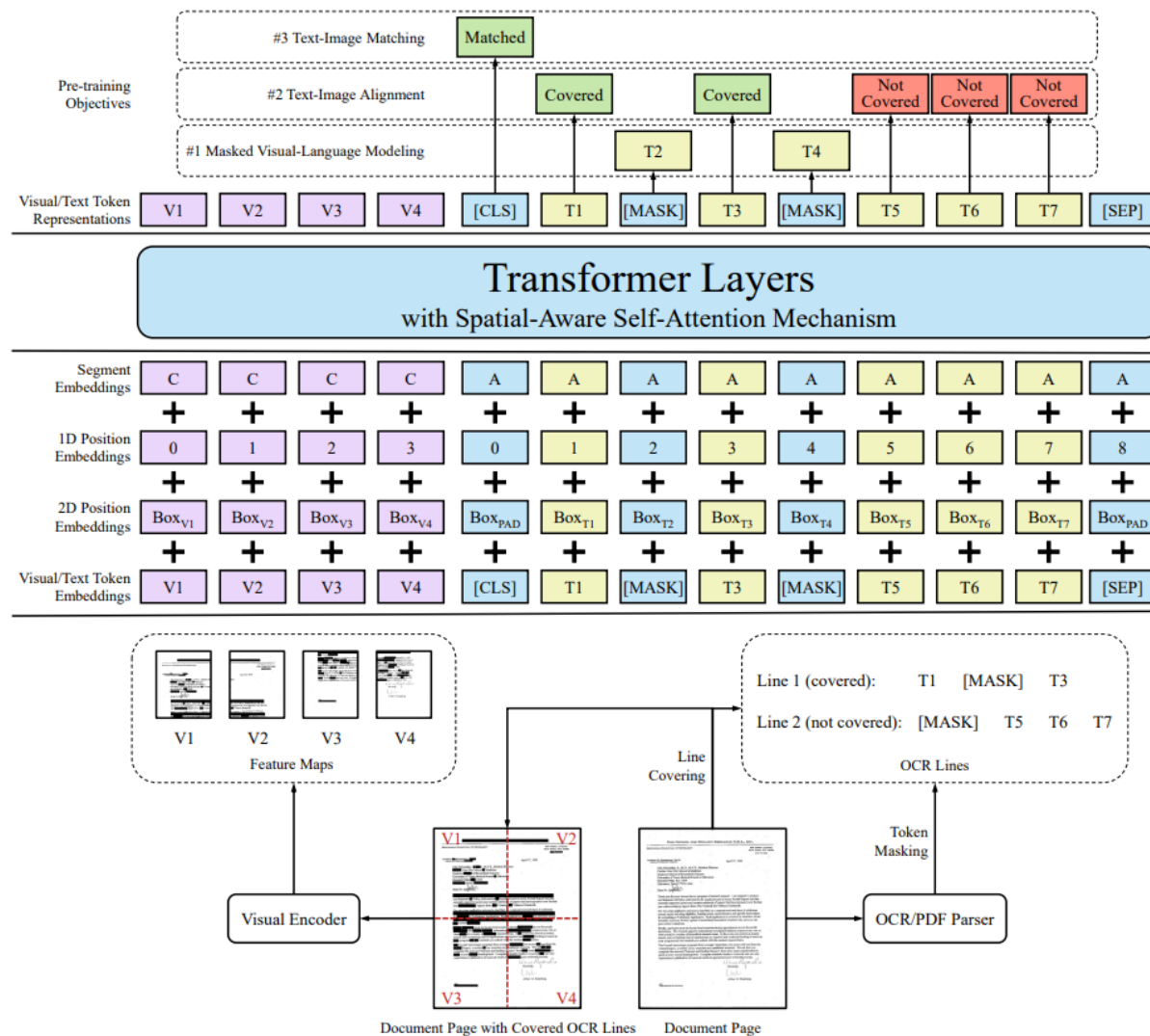


Figure 2: An illustration of the model architecture and pre-training strategies for LayoutLMv2