Interpretable components and graph neural networks

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Graph neural networks

Machine learning

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Metric learning

$$f \in \Lambda(\mathcal{O} \times \mathcal{O}, \mathbb{R})$$

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$$f \in \Lambda\left(\mathbb{R}^N \times \mathbb{R}^N, \mathbb{R}^M\right)$$

- naturally computers cannot operate on real objects and concepts, so they need to be properly encoded $\Lambda\left(\mathcal{O}, \mathbb{R}^N\right)$ (feature extraction) and model outputs need to be decoded $\Lambda\left(\mathbb{R}^M, \{1, \ldots, L\}\right)$ or $\Lambda\left(\mathbb{R}^M, \mathbb{R}\right)$

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Linear classifiers can be applied in $\mathbb{R}^N$ only if feature vectors are in fact linearly separable in that feature space.

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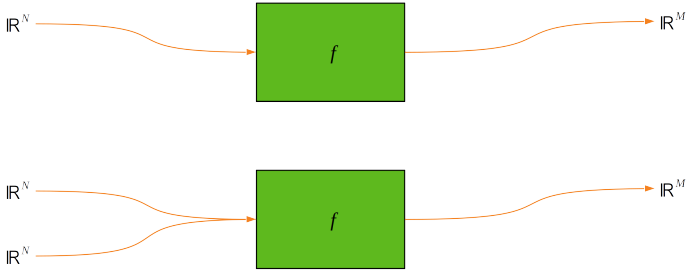

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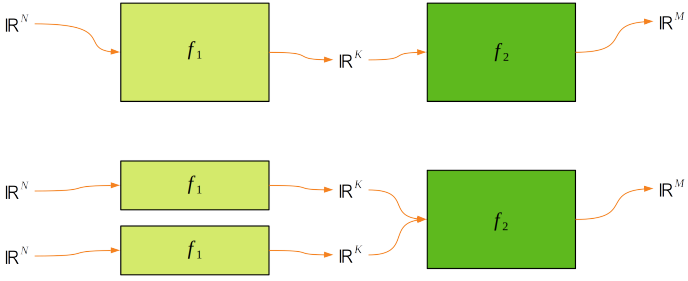

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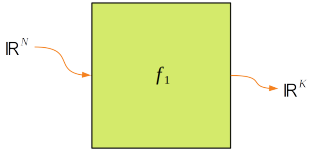

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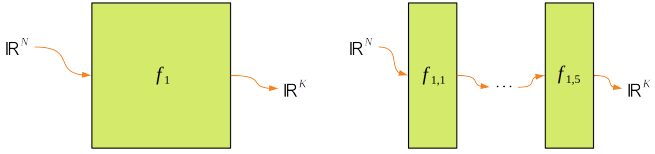

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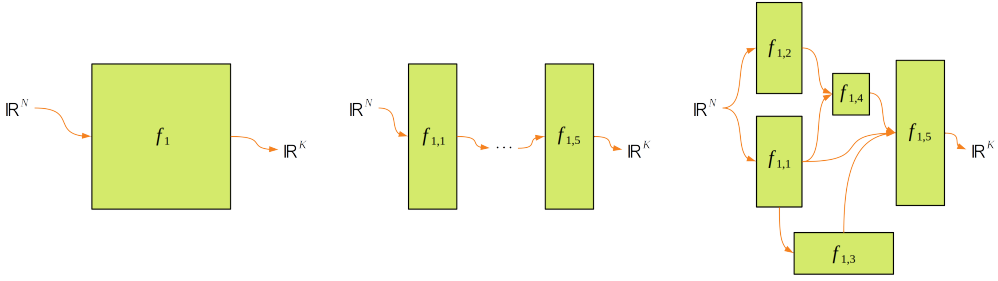

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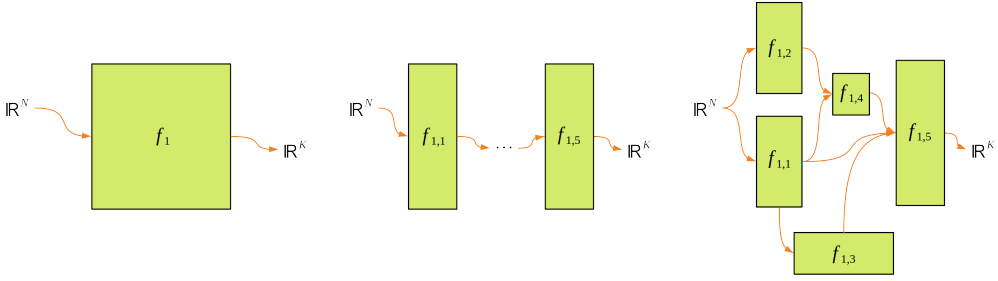

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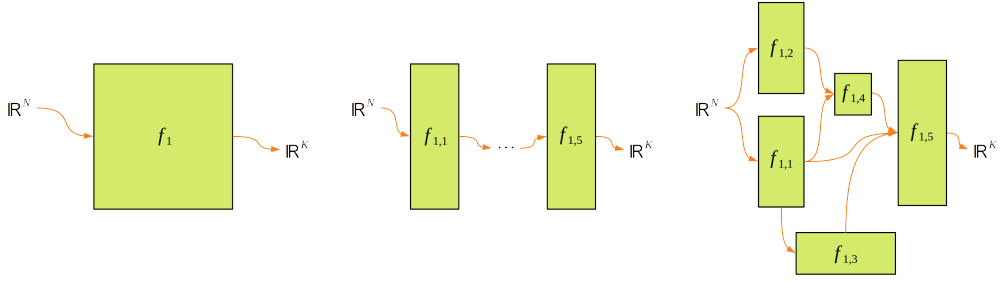

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- mainly we are interested in feedforward architectures (no cycles and loops)
- all blocks can be trainable or not, but all of them should be differentiable with respect to their inputs and parameters (possible end-to-end training)

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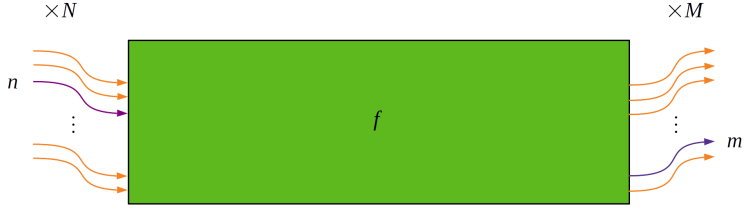
- it is hard to assess quality of explanations
- explanations can lead to knowldge discovery

Attributions

- attribution method assigns scores to inputs based on their contribution to model output



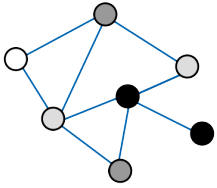
Attributions

- attibutions can be assigned to interpretable components and not to specific inputs

LIME ([10])

Graphs

- there are many problems where input objects $\mathcal{O}$ are graphs $G = (\mathcal{V}, \mathcal{E})$ with nodes $\mathcal{V}$ and connecting them edges $\mathcal{E}$



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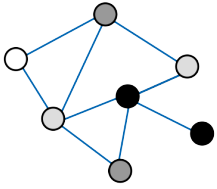

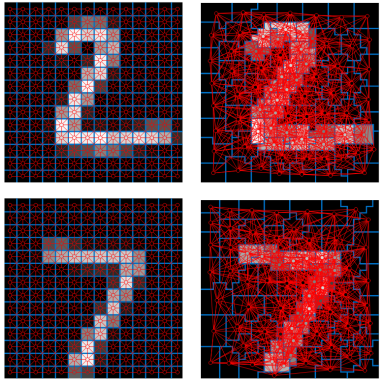

Images ([4])

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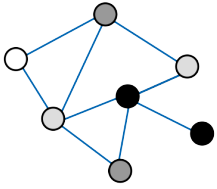

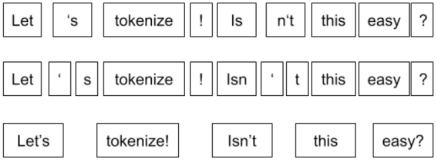

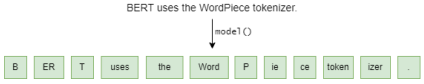

Sentences ([8, 2])

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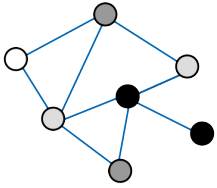

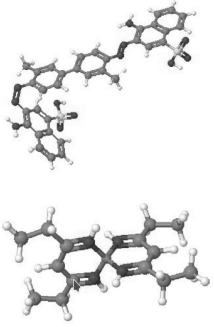

Chemical molecules ([11])

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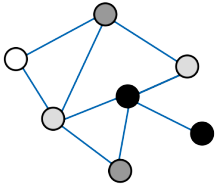

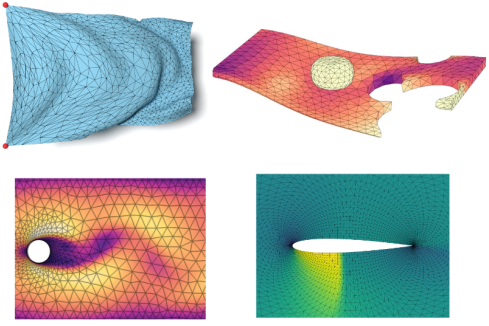

Meshes ([7])

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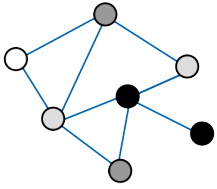

Point clouds ([12])

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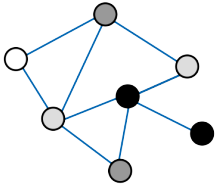

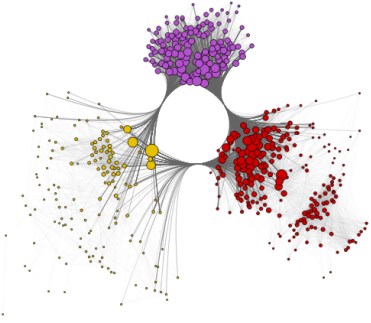

Social networks ([6])

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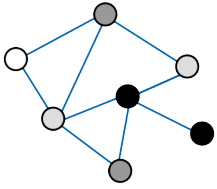

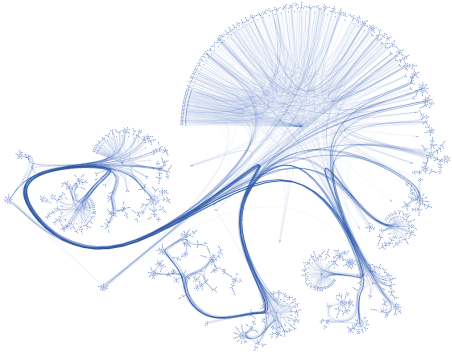

Citation networks ([1])

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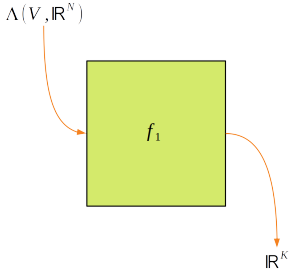

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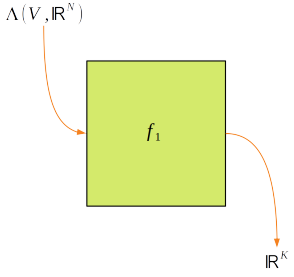

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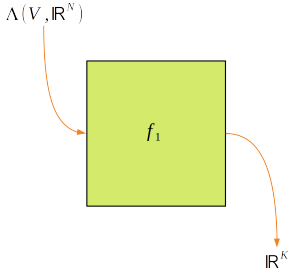

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- in some tasks edge features can also be considered but it is out of scope of this presentation

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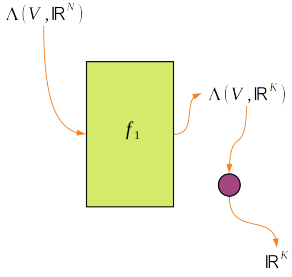

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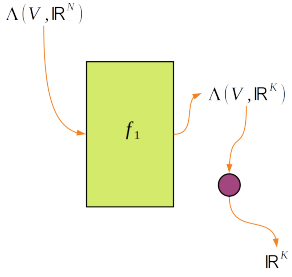

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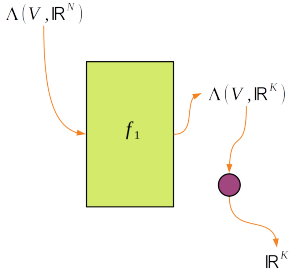

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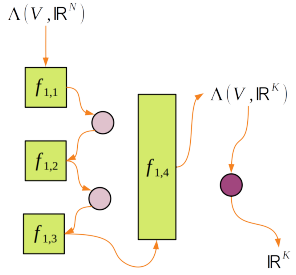

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- modification of graph structure (local pooling) can be an element of processing

Structure

- calculating node embedding we cannot take into account its features only since nodes are elements of a structure

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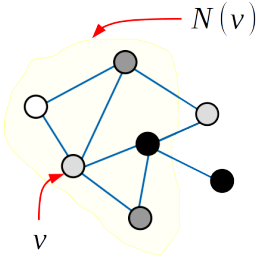

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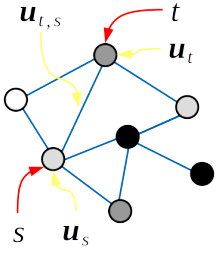

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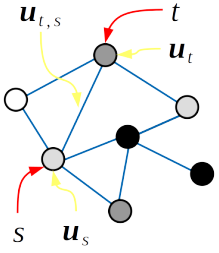
- node position may be taken into account as an additional information assigned either to nodes (global) $\mathbf{u}_s \in \mathbb{R}^d$ or edges (relative) $\mathbf{u}_{t,s} = \mathbf{u}_t - \mathbf{u}_s \in \mathbb{R}^d$



Tasks

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Metric learning

Measuring similarity between nodes may lead to link prediction.

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- here representation learning for graph elements becomes an obvious choice

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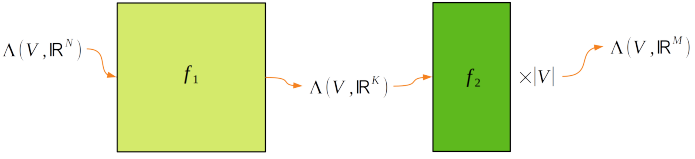
- here representation learning for graph elements becomes an obvious choice

Structured prediction

Classification of nodes leads to segmentation.

Metric learning

Measuring similarity between nodes may lead to link prediction.



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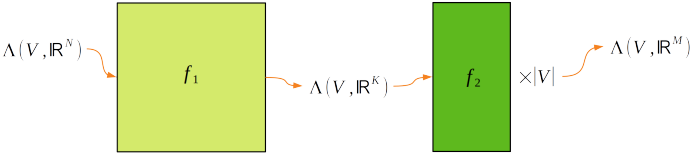

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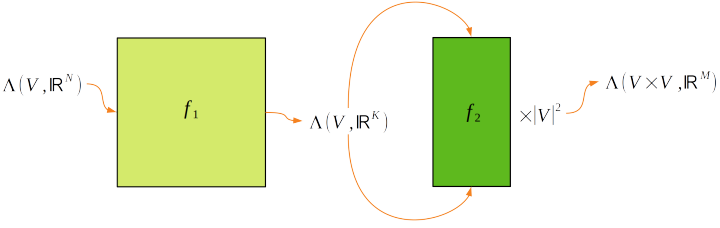
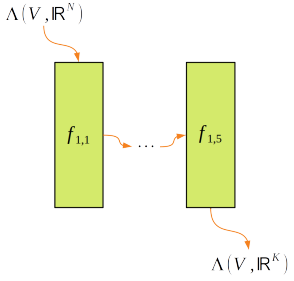


Graph neural networks



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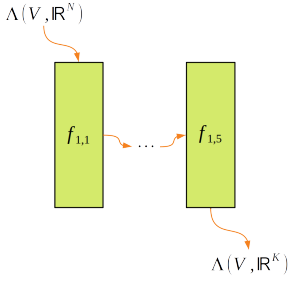
Graph neural networks



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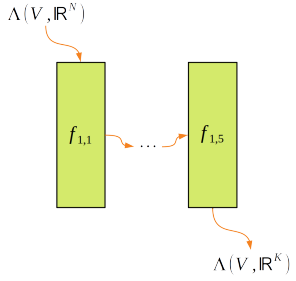

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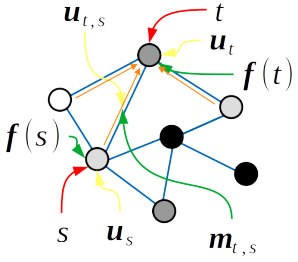
- graph operators are not the only components of those networks (local pooling, non-linear activation functions, etc.)
- the general scheme of graph operator working can be expressed using so called message passing mechanism

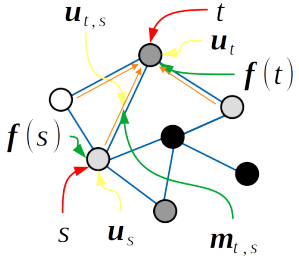
Message passing



Message

$$\mathbf{m}_{t,s} = \mathrm{MSG}(\mathbf{f}(t), \mathbf{f}(s), \mathbf{u}_t, \mathbf{u}_s)$$

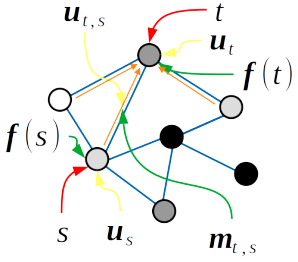
Message passing



Aggregation

$$\mathbf{m}_t = \mathsf{AGG}(\mathbf{m}_{t,s} : s \in \mathcal{N}(t))$$

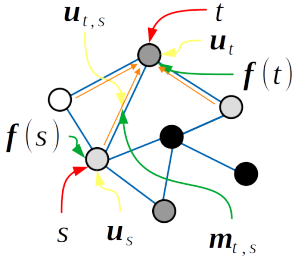
Message passing



Update

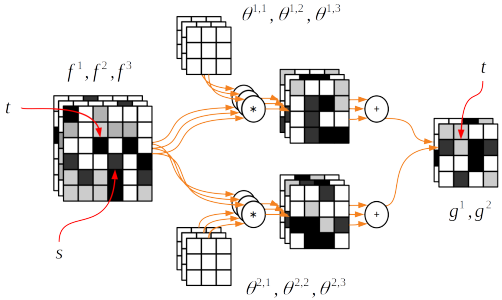
$$\mathbf{g}(t) = \text{UPDATE}(\mathbf{f}(t), \mathbf{m}_t)$$

Message passing



- commonly used graph operators, taking into account spatial ordering of nodes, base on concepts taken from computer vision (convolutional neural networks) and natural language processing domain (transformers)
- naturally, there are also operators designed for specific graph-based tasks (e.g. GCN, GarpgSAGE)

Convolutional neural networks



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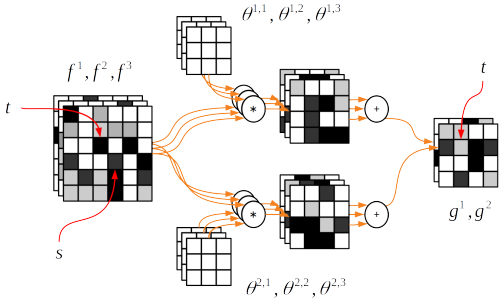

- Mixture Model Network (MoNet) defines continous filters using a trainable gaussian mixture model, taking into account relative coordinates $\mathbf{u}_{t,s} \in \mathbb{R}^d$ which can be defined almost arbitrarily

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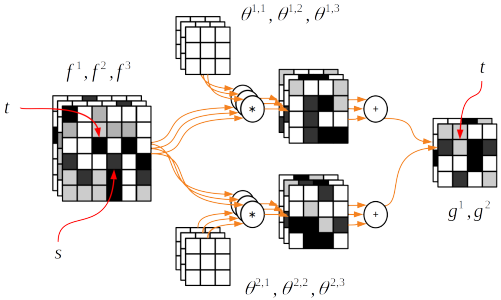
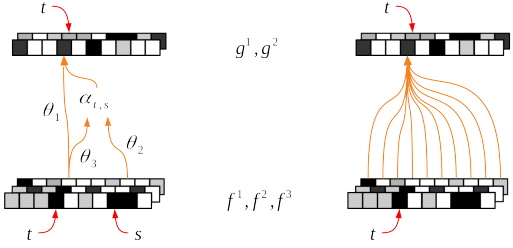


- Mixture Model Network (MoNet) defines continous filters using a trainable gaussian mixture model, taking into account relative coordinates $\mathbf{u}_{t,s} \in \mathbb{R}^d$ which can be defined almost arbitrarily
- Filter weights do not depend on features of currently processed pixels

Transformer



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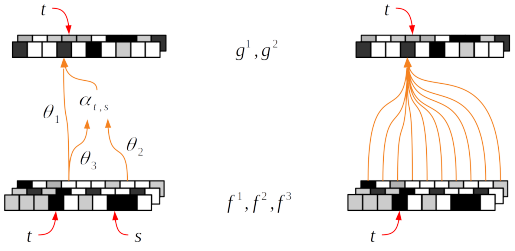

- Graph Transformer (GT) or Graph Attention Network (GAT, GATv2) need not to consider the fully connected graph ($\mathcal{N}$ is used) and uses either global $\mathbf{u}_s \in \mathbb{R}^d$ or relative node positions $\mathbf{u}_{t,s} \in \mathbb{R}^d$ to calculate attention weights

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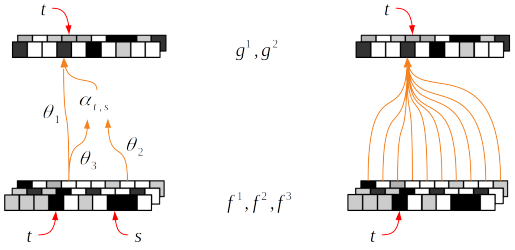

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Explainability

- although many classic attibution methods can be used for models operating on graphs, there are also some dedicated techniques

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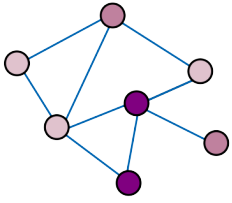
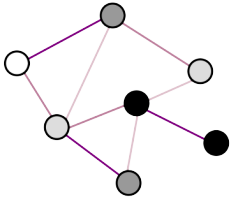
- although many classic attibution methods can be used for models operating on graphs, there are also some dedicated techniques
- since graphs have internal structure (nodes and edges), new interpretable components can be considered (separate or common features across all elements, whole elements)

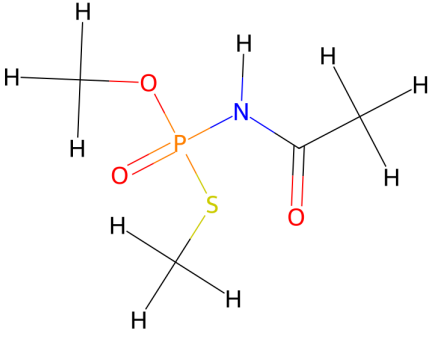




Chemistry

Chemical compounds

- we consider problems where the set of analysed objects $\mathcal{O}$ are chemical compounds



Acephate

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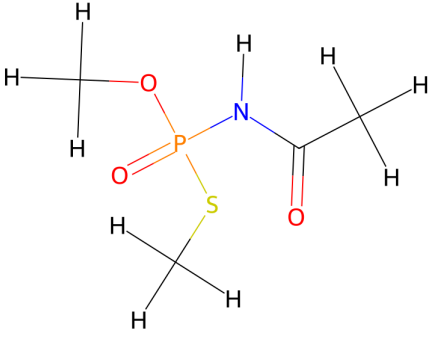
- this work was conducted with Bartosz Durys



Acephate

Prediction

Regression loss

In regression problems $\mathrm{M} = 1$ and loss function can be defined as:

$$\mathrm{L}^{prediction}(\mathbf{z}^j, y^j) = (\mathbf{z}^j - y^j)^2$$

where $\mathbf{z}^j = \mathrm{f}(G^j, \theta) \in \mathbb{R}^{\mathrm{M}}$

- selected MoleculeNet [14] datasets: ESOL, FreeSolv, and Lipophilicity
- feature vectors contained 9 numerical features describing atoms
- considered tasks: water solubility prediction, hydration free energy estimation, and finding octanol/water distribution coefficient

Prediction

Classification loss

In classification problems $\mathrm{M} = \mathrm{L}$ and loss function can be defined as:

$$\mathrm{L}^{prediction}(\mathbf{z}^j, y^j) = -\ln \frac{\exp \mathbf{z}^j_{y^j}}{\sum_{l=1}^{L} \exp \mathbf{z}^j_l}$$

where $\mathbf{z}^j = \mathrm{f}(G^j, \theta)\mathbb{R}^{\mathrm{M}}$

- selected TUDataset [5] datasets: AIDS, ENZYMES, and PROTEINS
- feature vectors were one-hot encoded representation of node class: chcemical element for AIDS, secondary structure element for ENZYMES and PROTEINS
- considered tasks: identification of molecule activity against HIV, assigning a molecule to one of the six Enzyme Commission top-level classes, and predicting if a protein is an enzyme

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$$\mathrm{L}^{explain}(\mathbf{z}^j, y^j) = \sum_{t \in \mathcal{V}} \left(1 - \max_{s \in \mathcal{N}(t)} \alpha_{t,s}(\theta)\right)$$

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- the final loss function used during training is $\mathrm{L} = \mathrm{L}^{prediction} + \lambda \cdot \mathrm{L}^{explain}$, where λ controls the trade-off between the two components

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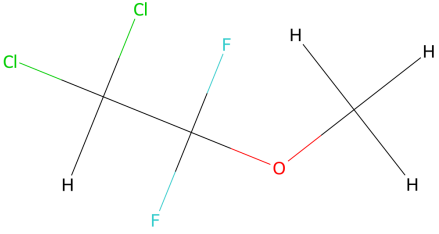
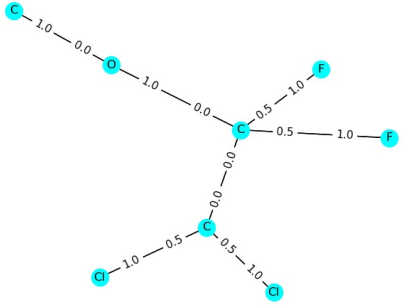
- λ was set to 0.1 experimentally.
- every experiment was repeated 50 times with 500 epochs per repeat, and the results were averaged using the best epoch on the validation set.

Explanations



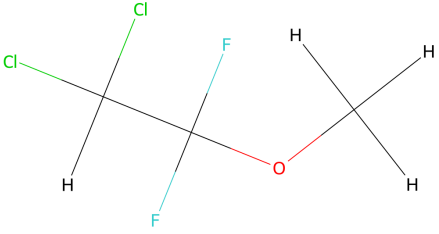
(a)



(b) normal

Methoxyflurane from the FreeSolv dataset

Explanations



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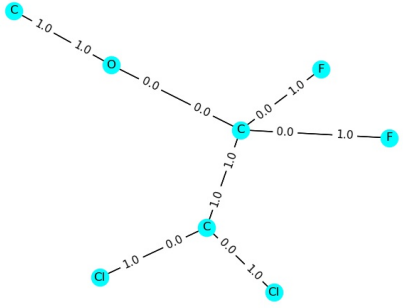

(b) with $\mathrm{L}^{explain}$

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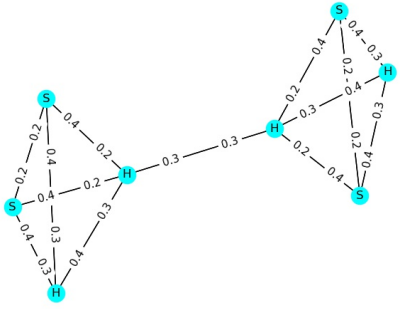
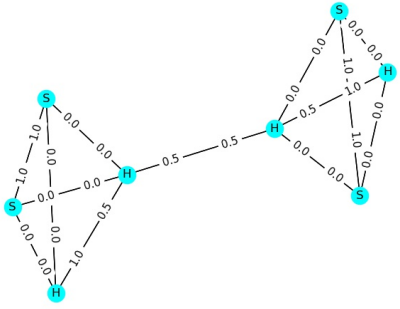
Explanations



(a) normal

Protein from the PROTEINS set

Explanations



(a) with $\mathrm{L}^{explain}$

Protein from the PROTEINS set

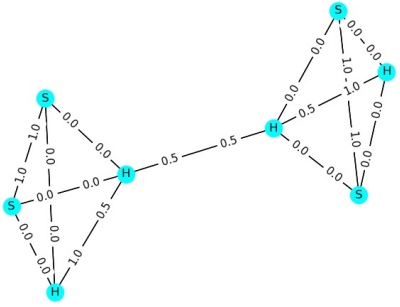
Regression

Dataset	Operator	Validation set			Test set		
		MSE	Standard deviation	Best	MSE	Standard deviation	Best
ESOL	GCN	35.24	9.11	8.15	35.24	8.80	8.11
	GAT	**11.76**	**5.09**	4.62	**11.01**	**5.04**	**4.46**
	GT	32.07	18.40	5.61	31.58	17.80	5.41
	GT with $L^{explain}$	17.87	11.29	**4.53**	17.25	11.11	**4.46**
FreeSolv	GCN	78.64	38.21	17.42	75.11	34.37	17.01
	GAT	36.02	16.94	14.42	**33.95**	**15.02**	14.17
	GT	44.30	26.35	**13.91**	41.87	25.38	14.01
	GT with $L^{explain}$	**34.71**	**11.35**	14.14	34.11	17.25	**13.86**
Lipophilicity	GCN	12.65	6.75	2.34	12.69	6.84	2.35
	GAT	10.67	4.54	2.12	10.64	4.58	2.16
	GT	12.51	9.19	2.44	12.44	9.15	2.46
	GT with $L^{explain}$	**2.62**	**0.80**	**1.62**	**2.56**	**0.77**	**1.64**

Classification

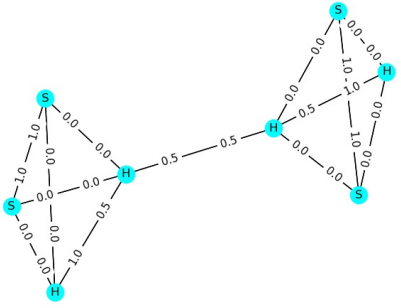
Dataset	Operator	Validation set			Test set		
		Accuracy	Standard deviation	Best	Accuracy	Standard deviation	Best
AIDS	GCN	80.22	2.81	**88.50**	79.84	**2.27** width=6cm	84.00
	GAT	79.84	**2.74**	85.50	79.91	2.55	86.00
	GT	**81.05**	2.80	86.00	**80.49**	2.46	**87.00**
	GT with $L^{explain}$	79.75	2.76	86.00	80.03	2.42	86.00
ENZYMES	GCN	30.90	4.14	43.33	20.87	5.69	35.00
	GAT	32.03	4.79	**46.67**	21.43	**5.56**	35.00
	GT	35.17	**3.45**	43.33	24.03	5.80	**40.00**
	GT with $L^{explain}$	**36.77**	3.81	45.00	**24.33**	5.74	35.00
PROTEINS	GCN	73.69	3.99	81.08	68.88	5.27	78.57
	GAT	73.39	**3.43**	81.08	68.55	4.63	76.79
	GT	**74.29**	3.97	**81.98**	**69.20**	5.04	**79.46**
	GT with $L^{explain}$	74.22	3.64	**81.98**	68.66	**4.50**	78.57

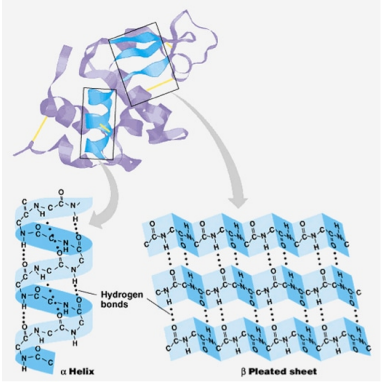
Interpretable components



Protein secondary structure ([9])

Interpretable components





Protein secondary structure ([9])

Image analysis

Research problem

How to use domain knowledge in image analysis?

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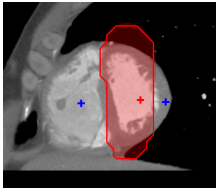

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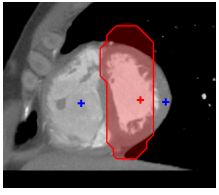

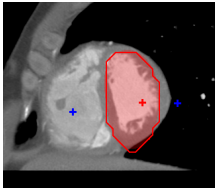

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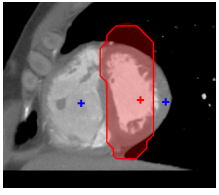
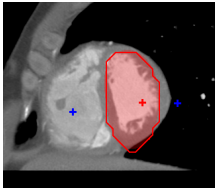
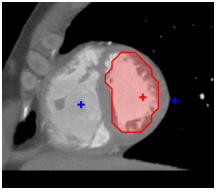
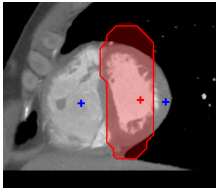
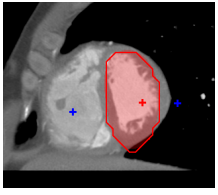
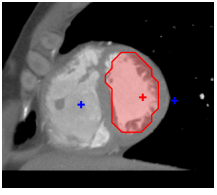
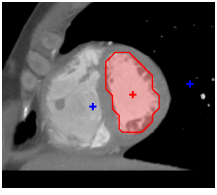




Research problem

How to use domain knowledge in image analysis?

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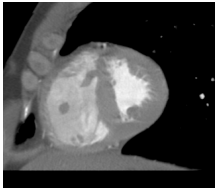

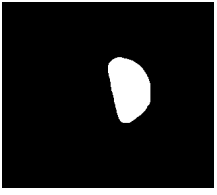

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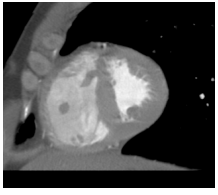
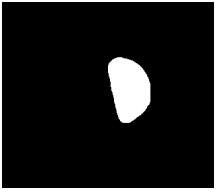
- images have their internal structure since they are composed of pixels $\mathcal{V}$ organized in a grid structure





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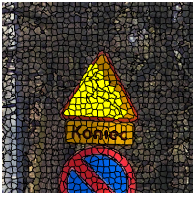

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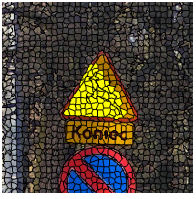
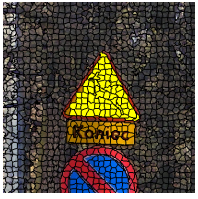

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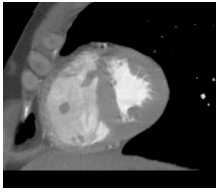

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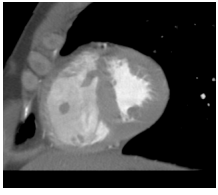

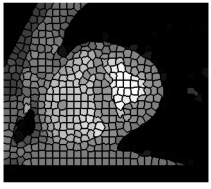

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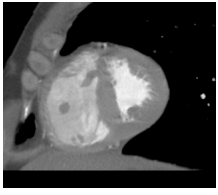

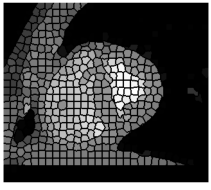

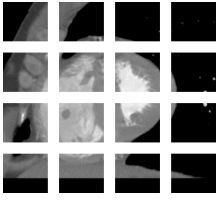

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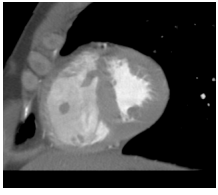
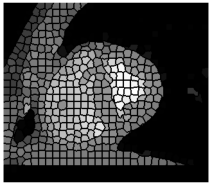
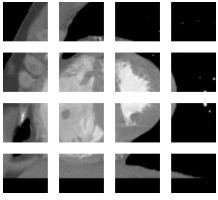
- graph neual networks are a tool allowing to process that kind of data







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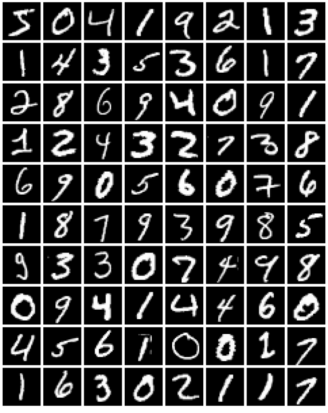

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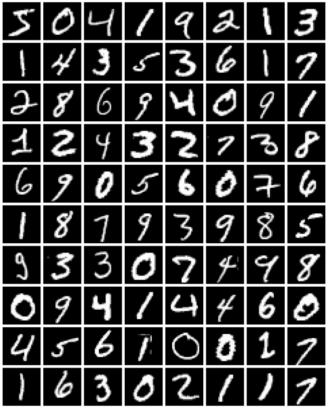

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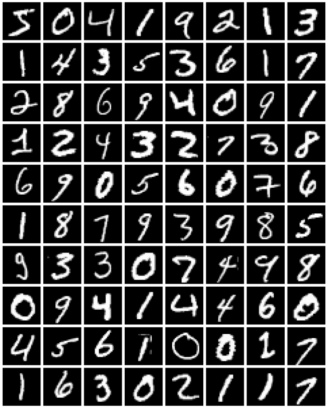

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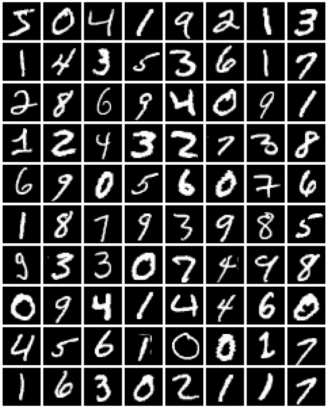

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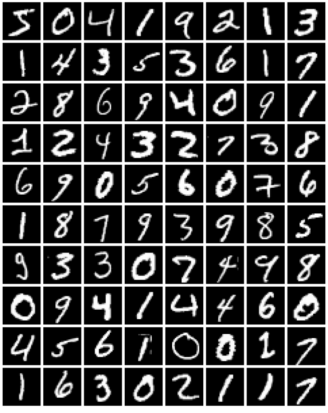

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- they achieved also 97.30% for 300 superpixels and 91.11% for 75 superpixels

Sparse coding

Convolutional sparse coding

$$\arg\min_{\{\mathbf{c}_i\}} \| \sum_i \mathbf{d}_i * \mathbf{c}_i - \mathbf{o} \|_2^2 + \lambda \sum_i \|\mathbf{c}_i\|_1$$

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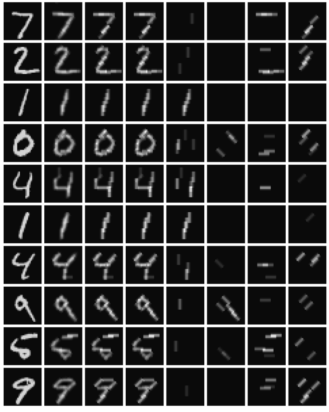
- to increase sparsity thresholding and non-maximum suppression were applied

Interpretable components

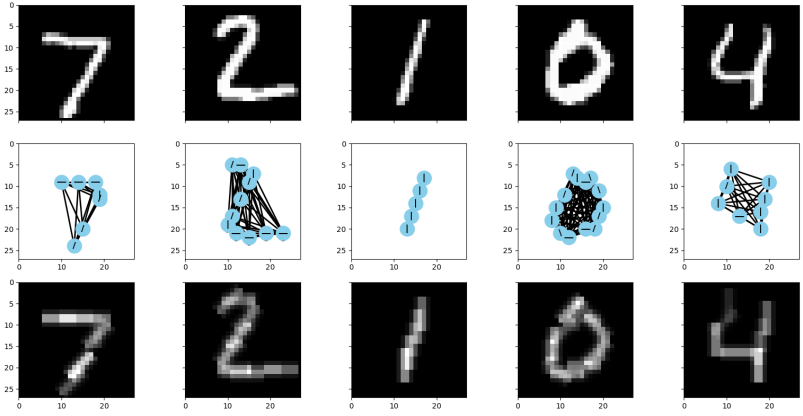


fixed dictionary

Interpretable components

trained dictionary

Graphs



fully connected graph was considered where $\mathcal{N}(v) = \mathcal{V}$ for every $v \in \mathcal{V}$

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method	50	100	200	1000	ALL
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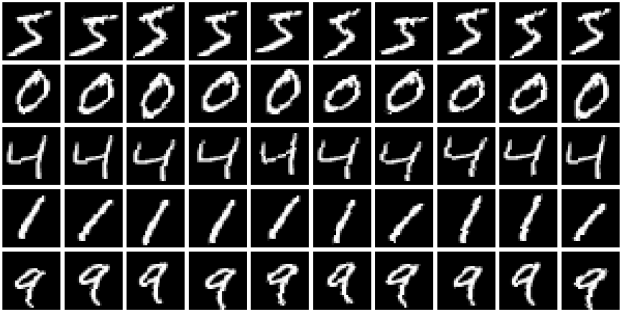

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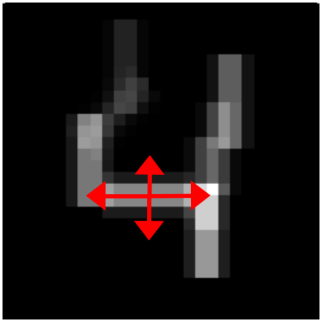

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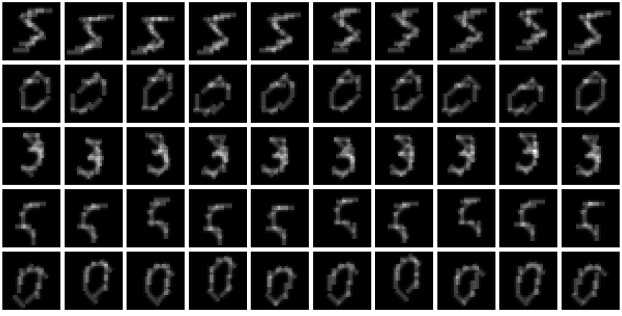

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Knowledge

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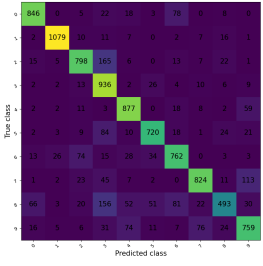

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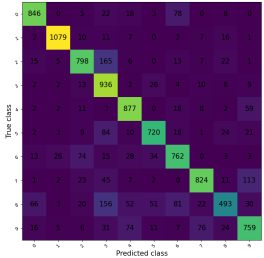

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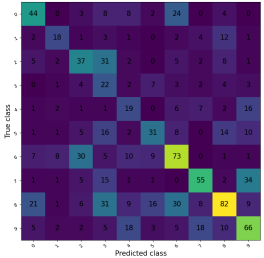

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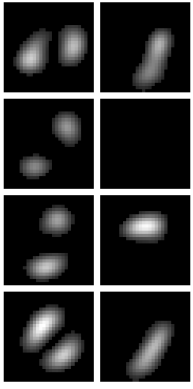

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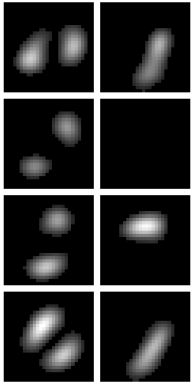
- those expectations can have form of rules or some visual guidelines
- they can be used to measure the coarse similarity w_l^j of given training sample to considered concepts



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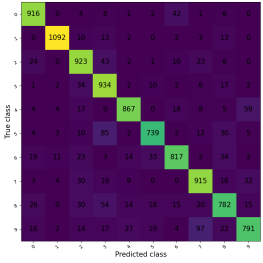

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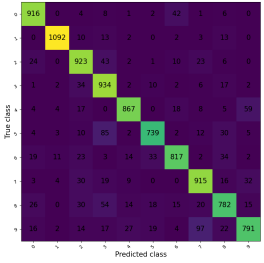
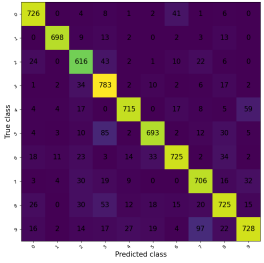


confusion matrix

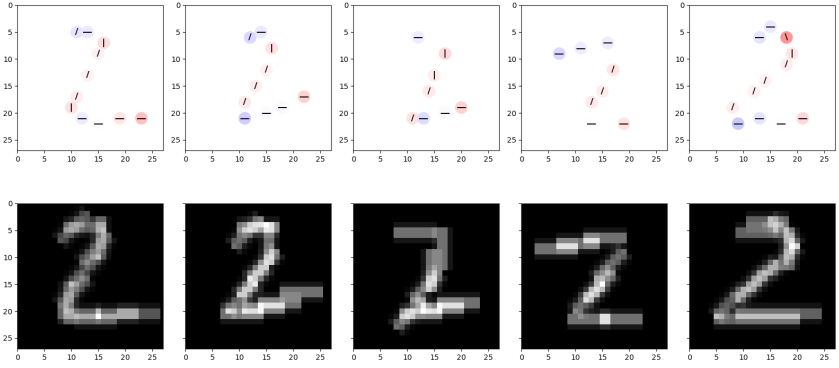


uncertainity

Knowledge

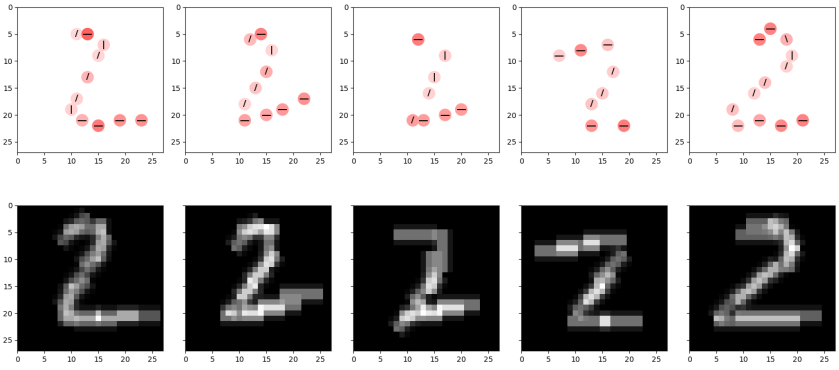
method	50	100	200	1000	ALL
CNN	33.51	55.77	71.62	90.67	99.21
MoNet	16.41	58.79	71.77	85.11	97.38
GT	47.94	66.52	77.02	88.87	96.52
CNN with augmentation	39.61	61.97	76.94	**93.75**	**99.31**
MoNet ($\alpha = 0.5$)	57.21	67.92	81.60	91.09	97.75
MoNet with augmentation ($\alpha = 0.5$)	56.25	71.21	82.29	92.34	97.56
GT ($\alpha = 0.5$)	60.30	75.21	81.84	91.61	96.87
GT with augmentation ($\alpha = 0.5$)	**67.43**	**78.00**	**87.76**	93.26	97.12
MoNet ($\alpha = 1.0$)	44.67	56.98	63.87	75.12	76.87
MoNet with augmentation ($\alpha = 1.0$)	46.88	59.21	66.14	75.93	77.91
GT ($\alpha = 1.0$)	50.30	59.57	68.54	74.12	77.15
GT with augmentation ($\alpha = 1.0$)	58.64	67.11	70.23	77.06	77.81

Explanations



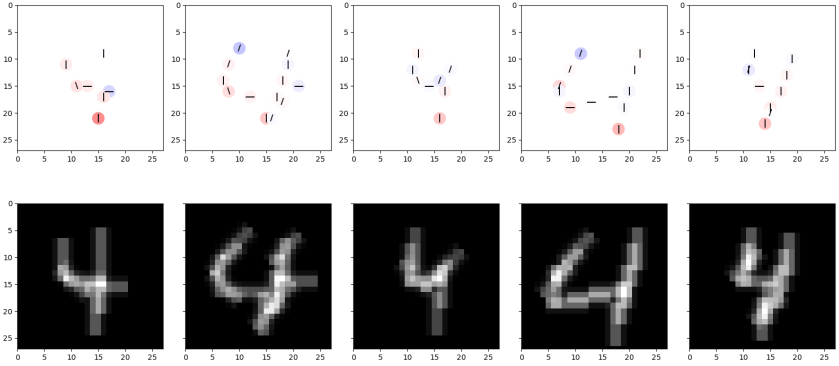
integrated gradients

Explanations



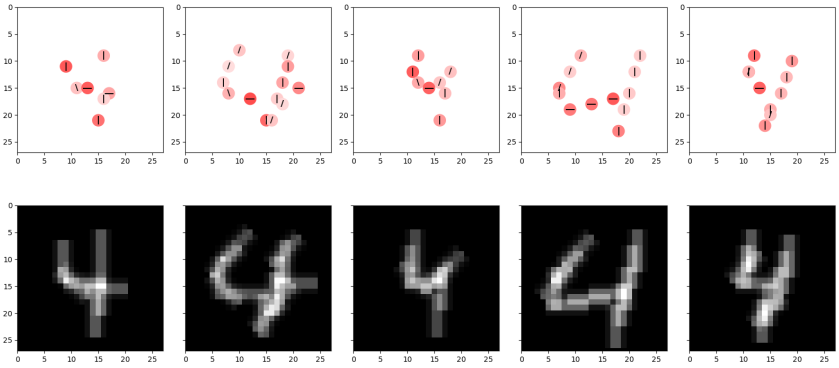
gnn explainer

Explanations



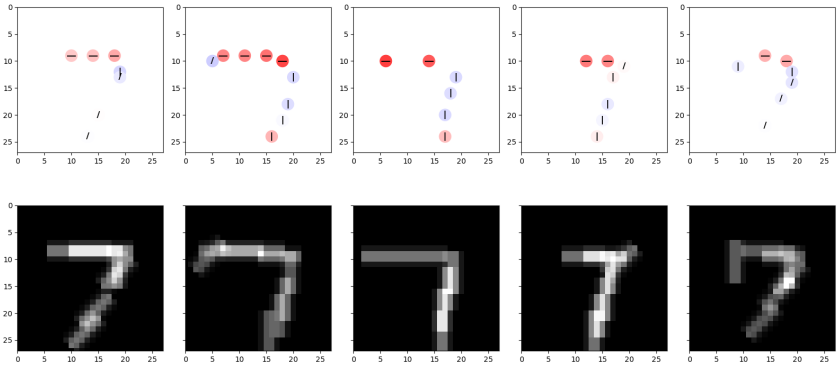
integrated gradients

Explanations



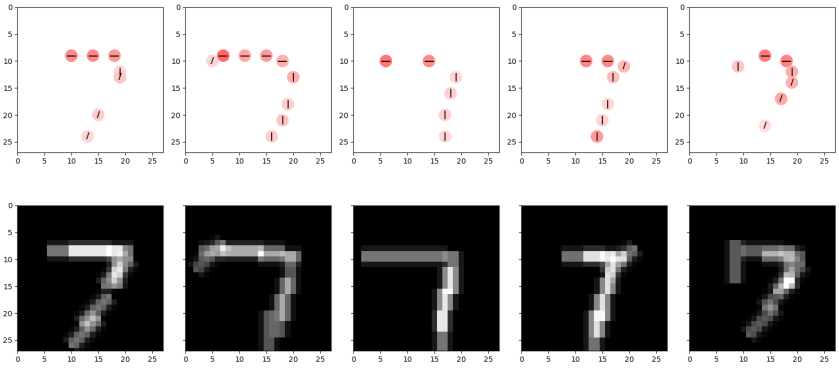
gnn explainer

Explanations



integrated gradients

Explanations



gnn explainer

Summary

Interpretable components allow to:

- use domain knowledge other then annotated set of training data
- explain results using domain specific concepts, which may lead to knowledge discovery

Summary

Open questions:

- should interpretable components be universal or task specific?
- should interpretable components be carefully designed or trainable?
- are interpretable components only useful in image analysis?

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