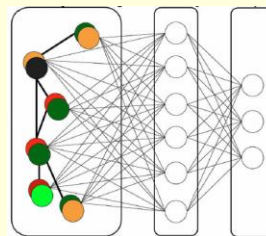


Deep Learning by Example on Biowulf

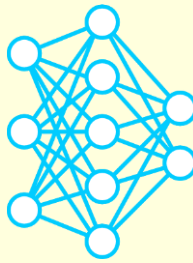
Class #6. Graph Convolutional Networks, handling imbalanced data and their application to classification of cancer types

Gennady Denisov, PhD

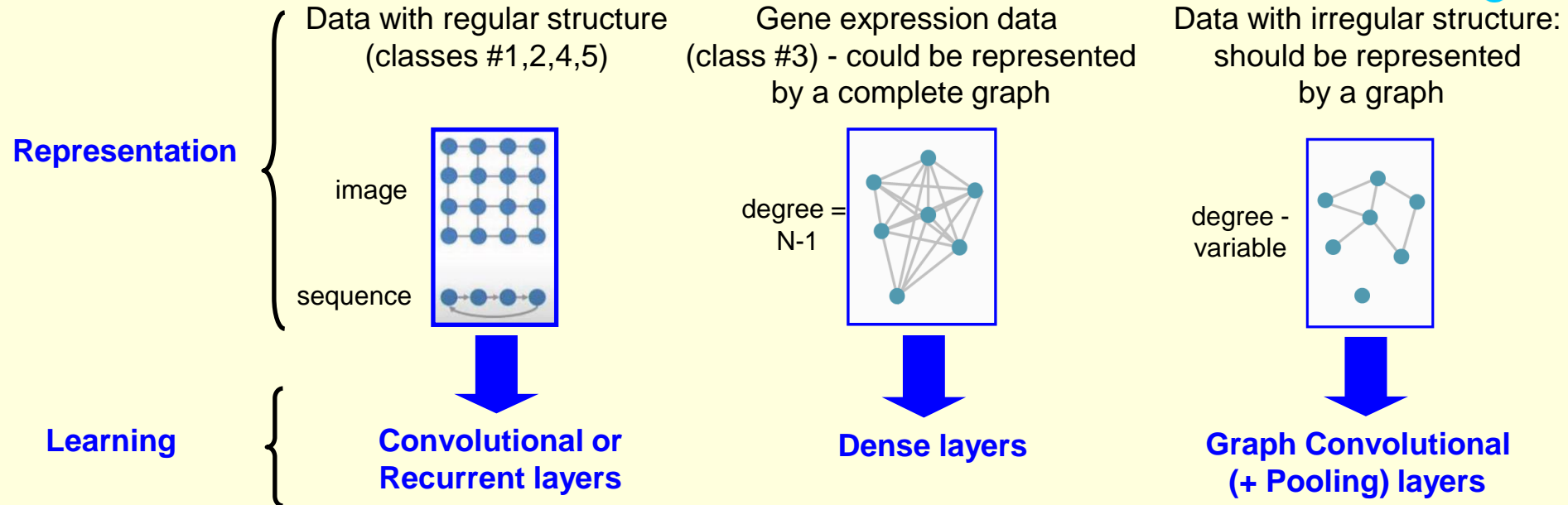


Intro and goals

graph, nodes / vertices, links / edges, feature, node degree



Question: how do we represent and learn the structure of data?

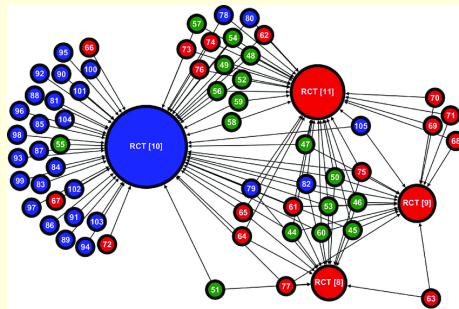


Non-bio examples:

Social network:
nodes = individuals,
edges = connections

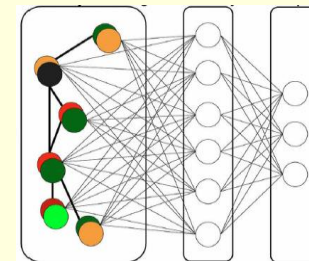


Citation network:
nodes = documents,
(directed) edges = citations



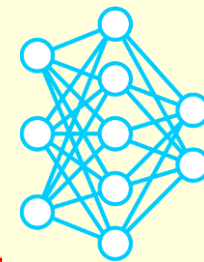
Bio example: GCN_Cancer

nodes = genes; edges = associations between genes; data similar to those of class #3, but the tasks / approaches are different



Examples overview

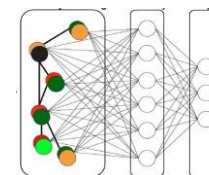
https://hpc.nih.gov/training/deep_learning_by_example.html



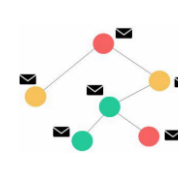
Class #	1	2	3	4	5	6	7
Bio app	Bioimage segmentation / fly brain connectome	Genomics / prediction of function of non-coding DNA	Genomics / reduction of dimensionality of cancer transcriptome	Bioimage synthesis / developmental biology	Drug molecule design	Genomics / classification of cancer types	Drug molecule property prediction
Neural network type	Convolutional	Recurrent or 1D-Convolutional	Autoencoder	Generative Adversarial	Reinforcement Learning	Graph Convolutional	Message Passing
ML type	Supervised	Supervised	Unsupervised	Unsupervised	Reinforcement	Supervised	Supervised

- **Supervised ML** like in classes #1 and #2, but the data are similar to those in #3
- Primary purpose: **demystifying** the Graph Neural Networks
- **“Transition” examples**: the more “traditional” MLP / DenseNet can still be used
- Graph imposes **constraints** / provides **additional knowledge** about the data, which may allow for **more accurate predictions** as compared to the constraint-agnostic models.

GCN



MPN

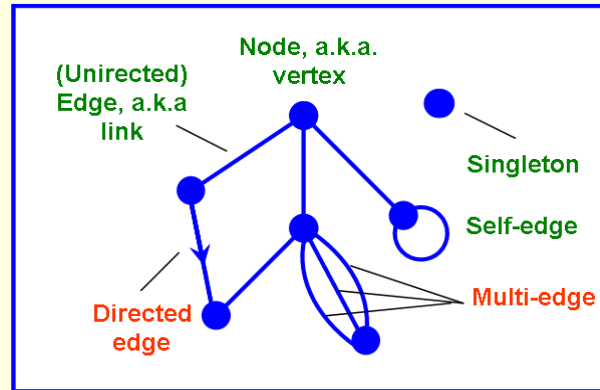


Prototype example #1: the graph classification task

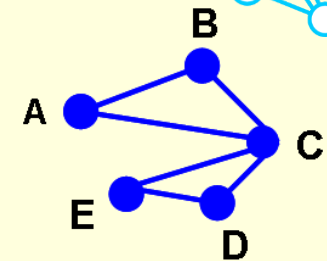
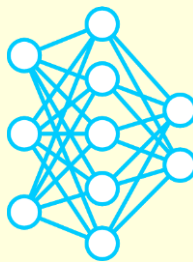
gene expression matrix, node features, undirected graph, singletons, adjacency matrix, graph classification task

		Genes						
		A	B	C	D	E		
Samples ↓	1	1	1	1	0	1	1	
	2	0	0	1	1	1	0	
	3	1	1	0	0	0	0	
	4	1	0	1	1	0	1	
	5	0	0	1	1	0	0	
	6	1	1	1	1	0	0	
	7	0	1	0	1	1	1	
	8	1	1	1	0	0	0	
	9	1	0	1	0	1	1	
	
		X (data)					Y (labels)	

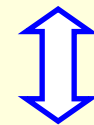
Modules = $[[0,0,0,1,1], [0,0,1,1,1]]$



Graph notation



Undirected graph:
Nodes = genes
Node feature = gene expression level
Edges = associations between genes



	A	B	C	D	E
A		1	1		
B	1		1		
C	1	1		1	1
D			1		1
E			1	1	

Adjacency matrix:

- symmetric (\Leftrightarrow no directed edges)
- values ≤ 1 (\Leftrightarrow no multi-edges)

Input:

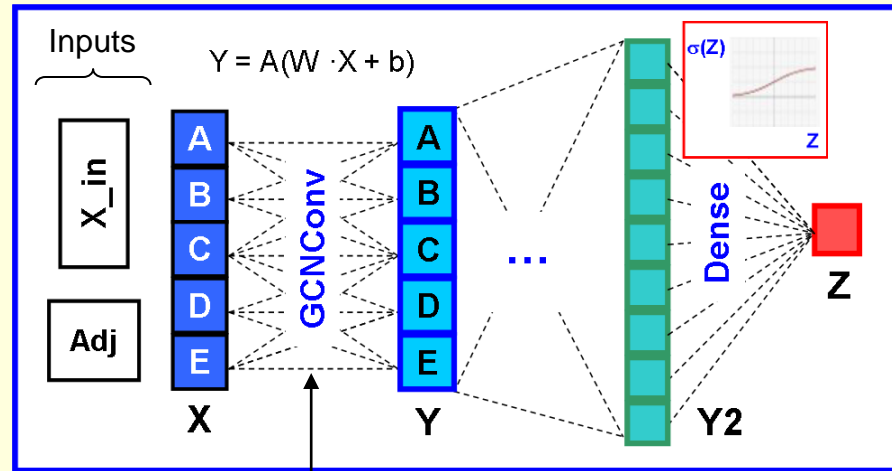
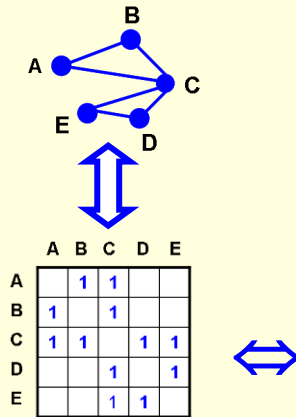
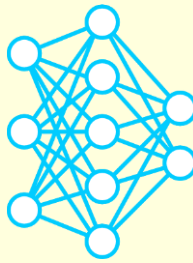
Gene expression data matrix generated randomly “on the fly”, with rows = **samples**, columns = **genes** and **values =1** (gene is expressed, shown in color) or **=0** (gene is unexpressed, shown as white). The samples can be of two types: “**normal**” (label=0) or “**tumor**” (label=1). In each the type of samples, genes are associated into **two modules**, designated 0 and 1, with the same probability of expression for all genes in a module, but different probabilities across different modules.

Task:

Train a graph convolutional **network model** on this data, so that it could **predict the class labels** for new, previously unseen samples.

Prototype example #1 (cont.): GCNConv vs Dense layer

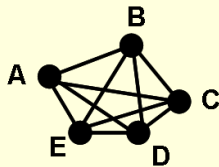
Vanilla Graph Convolution: Kipf, T.N., Welling, M.: arXiv preprint (2016)



Missing links: A-D, A-E, B-D, B-E, D-A, E-A, D-B, E-B.
The corresponding weights are constrained to 0

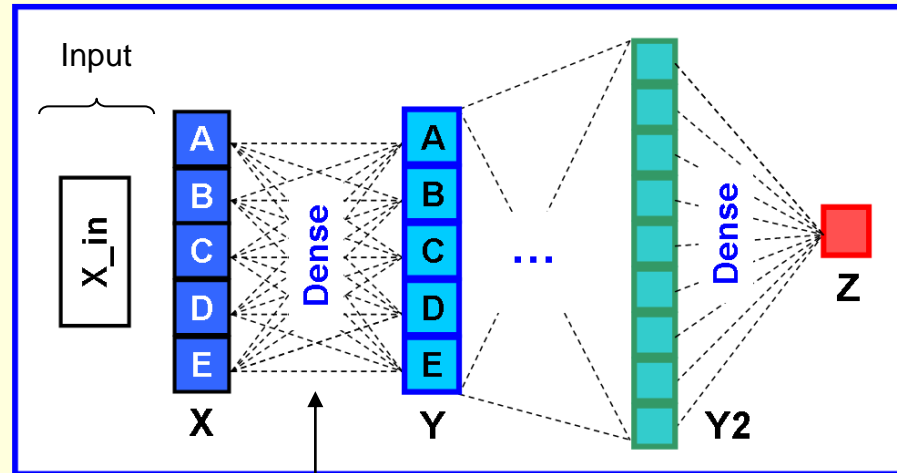
Graph
Convolutional
Network

Complete
graph



Adjacency
matrix
of ones

	A	B	C	D	E
A	1	1	1	1	1
B	1	1	1	1	1
C	1	1	1	1	1
D	1	1	1	1	1
E	1	1	1	1	1

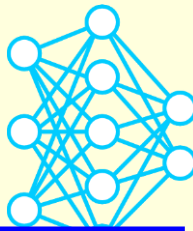


No missing links / zero weights in the fully connected layer.

MultiLayer
Perceptron
(MLP)

CONCLUSION: Dense layer can be regarded as GCNConv layer with adjacency matrix of ones.

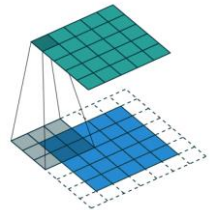
Prototype example #1 (cont.): GCNConv vs Conv1D / Conv2D layers



filtering, k-hop neighborhood, pooling, supernode, parent-child relationship

2D Convolution with 'same' padding

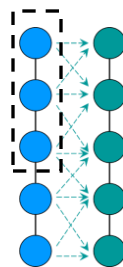
Output image



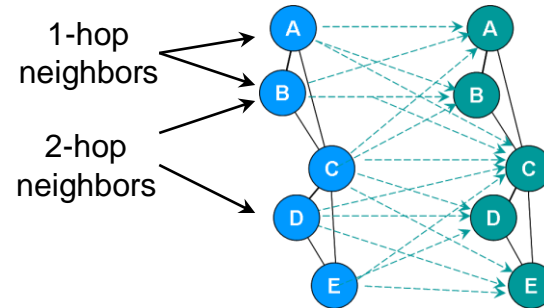
Input image

$$O = \sum_{\text{kernel}} w_i * I_i + b$$

1D Convolution with 'same' padding



Filtering, a.k.a. Graph Convolution in the narrow sense

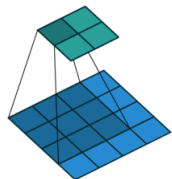


$$O = \sum_{\text{1-hop neighborhood}} w_i * I_i + b$$

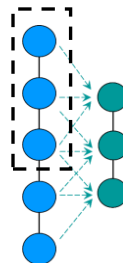
(only reassigns the node features, but does not change the number of nodes)

CONCLUSION: the filtering performed by the GCNConv layer is analogous to the Conv1D / Conv2D with 'same' padding and kernel of size = 3.

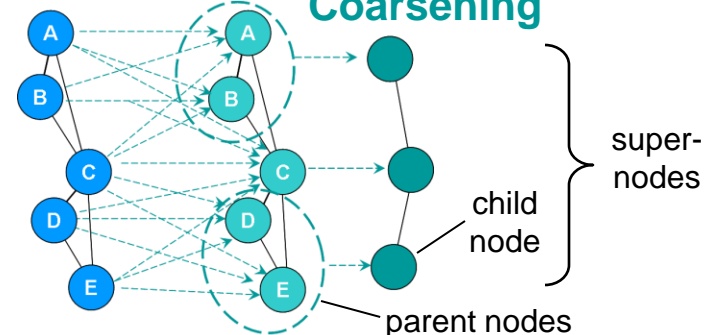
2D Convolution with 'valid' padding



1D Convolution with 'valid' padding

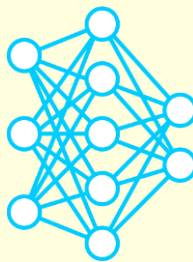


1) Filtering 2) Pooling, a.k.a. Coarsening



NOTE: an analog of the Conv1D / Conv2D with kernel of size > 3 would be a ChebConv layer, to be discussed later in this class, which employs a k-hop neighborhood of a node to update its value, with $k > 1$.

Prototype example #1 (cont.): training code



GCN: Kipf, T.N., Welling, M.: arXiv preprint (2016)

Spektral: <https://graphneural.network>

Header

- tensorflow
- spektral
- graph_net

Get data

- modules
- adj matrix
- samples and labels

```
denisovga@biowulf:/usr/local/apps/DLBio/class6/bin
#!/usr/bin/env python
import tensorflow as tf, spektral, numpy as np, scipy.stats as stats
graph_net, n_g, n_train, bsize, epochs, prob=1, 5, 700, 50, 100, 0.7
np.random.seed(1); tf.random.set_seed(1)

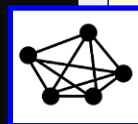
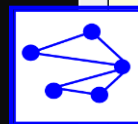
modules = [[0,0,0,1,1], [0,0,1,1,1]]
adj = np.zeros([n_g,n_g])
for k in range(2):
    for i in range(n_g):
        for j in range(n_g):
            if not i == j and modules[k][i] == modules[k][j]:
                adj[i][j] = 1

probs = [[prob,1.-prob],[prob,1.-prob]]
x_train,y_train = [],[]
for s in range(n_train):
    sample, t = [], np.random.choice([0,1], p=(0.5, 0.5))
    for g in range(n_g):
        sample.append(np.random.choice([0,1], 1,
                                       p=[probs[t][modules[t][g]],1.-probs[t][modules[t][g]]])[0])
    x_train.append(sample)
    y_train.append(t)
# 0 = green, 1 = red
x_train, y_train = np.array(x_train,dtype=float), np.array(y_train,dtype=float)
adj_train = np.array([adj for s in range(n_train)])
```

graph_net = $\begin{cases} 1 \Rightarrow \text{GCNNet} \\ 0 \Rightarrow \text{MLP} \end{cases}$

	1	1		
1		1		
1	1		1	1
			1	1
			1	1

1	0	0	0	0
0	1	0	0	0
0	0	1	0	0
0	0	0	1	0
0	0	0	0	1



Define a model:

- Functional API
- GCNConv vs Dense
- loss and optimizer

```
X = tf.keras.layers.Input(shape = (n_g,1))
A = tf.keras.layers.Input(shape = (n_g, n_g), sparse=False)

if graph_net == 1:
    Y = spektral.layers.GCNConv(n_g, activation='relu')([X,A])
else: # mlp
    Y = tf.keras.layers.Dense( n_g, activation='relu')( X)
Y_1 = tf.keras.layers.Flatten()(Y)
Y_2 = tf.keras.layers.Dropout(0.1)(Y_1)
Z = tf.keras.layers.Dense(1, activation='sigmoid')(Y_2)
model = tf.keras.models.Model(inputs=[X, A], outputs=Z)
model.compile(loss='bce', optimizer='adam')
model.summary()
```

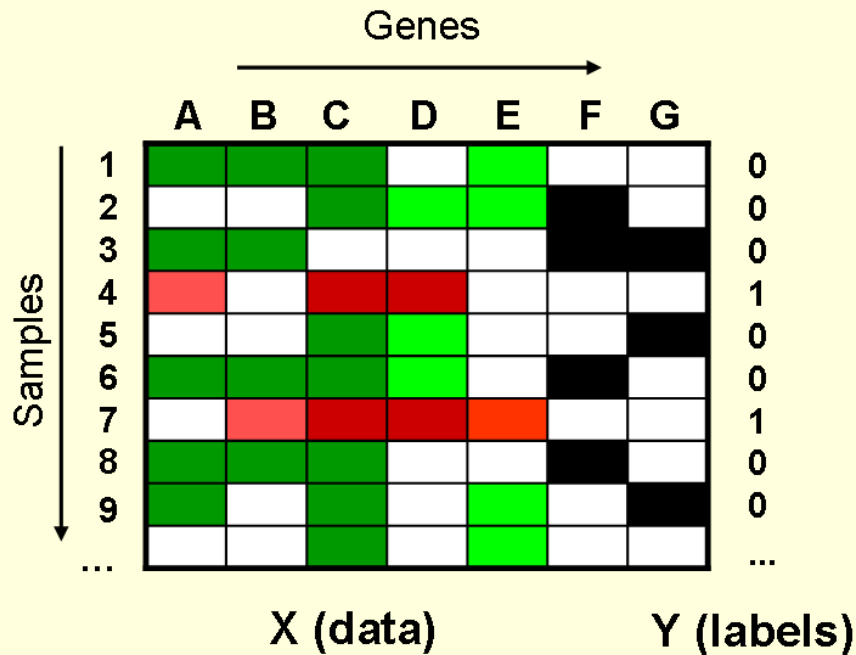
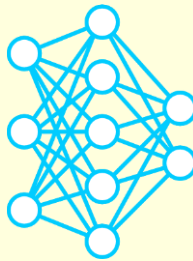
Run the model

```
model.fit([x_train, adj_train], y_train, epochs=epochs, batch_size=bsize)
```

38,76

Top

Prototype example #2: imbalanced input data containing singletons



Two additional hyperparameters:

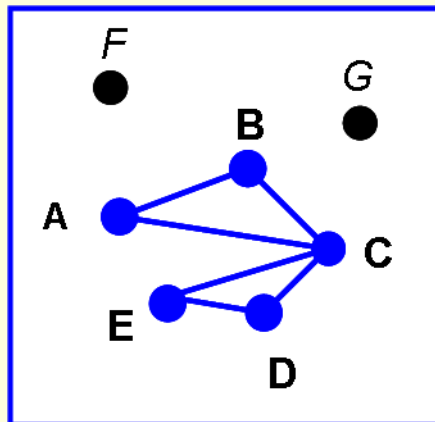
IR (imbalance ratio)

= # green samples / # red samples

n_s (# of singletons),

= genes that are not associated / co-expressed with other genes

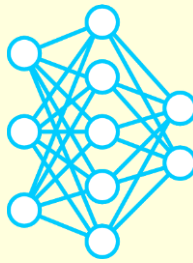
Undirected graph with singleton genes



	A	B	C	D	E	F	G
A		1	1				
B	1		1				
C	1	1		1	1		
D			1		1		
E			1	1			
F							
G							

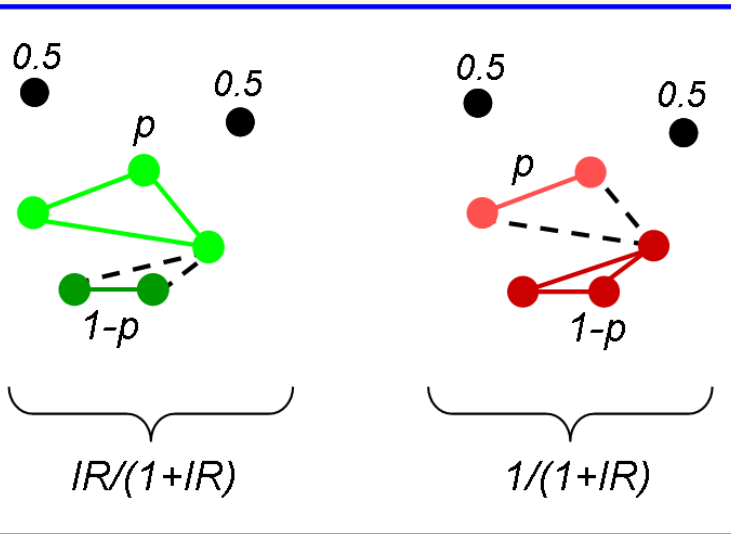
Adjacency matrix with singleton genes

Predictions from the prototype example #2



Parameterization of the gene expression probabilities

% correct predictions for $p = \text{prob} = 0.7$

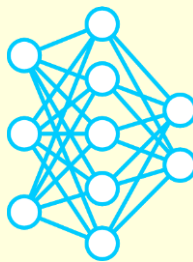


n_s	IR=1		IR=10	
	GCN	MLP	GCN	MLP
2	76	76	50.8	50.8
10	72	72	48.7	48.7
50	70.9	67.1	51.8	53.1
100	69.4	64.9	50.0	51.0
200	69	63.2	49.3	54.2

CONCLUSIONS:

- the constraints imposed on singletons by the adjacency matrix in GCN allow for attenuation of the effect of “noise” introduced by the presence of singletons, and hence for a better performance of the GCN over the constraint-agnostic MLP on balanced data
- since MLP possesses more adjustable parameters than GCN, it provides more flexibility in handling the challenge of data imbalance, and therefore can overperform the GCN on imbalanced data

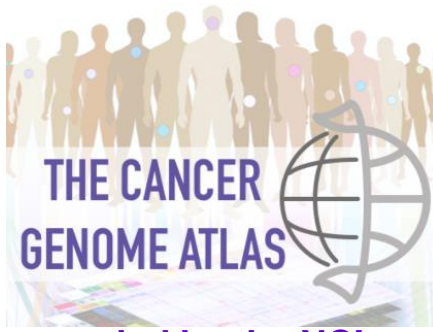
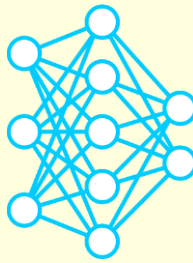
How to run the simple/prototype models on Biowulf?



```
denisovga@biowulf:/data/denisovga/1_DL_Course/0_Intro
sinteractive --gres=gpu:p100:1
module load DLBio/class6
...
ls $DLBIO_BIN
gcn_basic.py    gcn_imbalanced,singletons.py
gcn_basic.py
...
Epoch 500/500
20/20 [=====] - 0s 1ms/step - loss: 0.6122
...
correct= 696 / 1000
...
gcn_imbalanced,singletons.py
...
Epoch 500/500
20/20 [=====] - 0s 2ms/step - loss: 0.2572
...
correct= 508 / 1000
...
23,35 Top
```

Biological example #6: GCN_Cancer: Classification of Cancer Types Using Graph Convolutional Networks

R.Ramirez et al., Frontiers in Physics (2020)



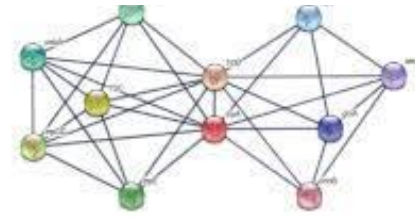
NIH program led by the NCI and NHGRI

GCN_Cancer input: RNA- seq data for

- 731 normal samples and
- 10,340 tumor samples representing 33 types of cancer

Goal: classify each sample as one of 34 types

The STRING database



STRING = Search Tool for the Retrieval of Interacting Genes/proteins

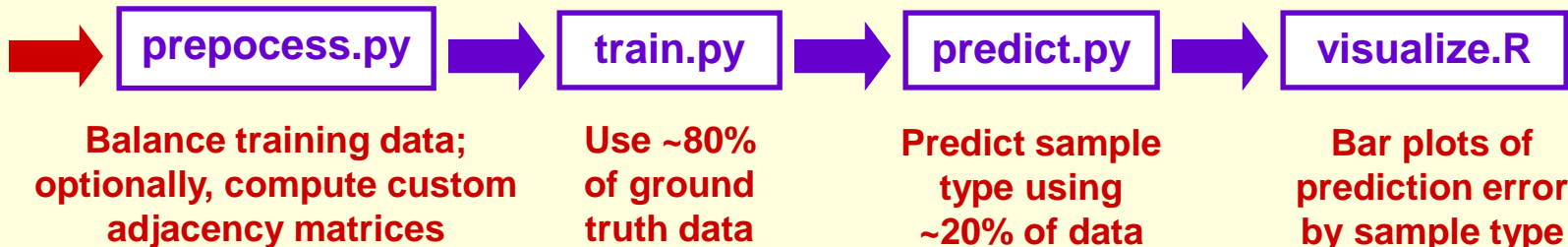
**Protein-protein interaction (PPI)
/ association confidence scores**

- used to generate adjacency matrices for the settings involving only protein coding genes

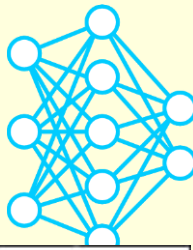
GCN_Cancer pipeline (reimplemented in Keras from Tensorflow):

Input data:

- GE levels
- adjacency matrices



Overview of the GCN_Cancer code



https://hpc.nih.gov/apps/GCN_Cancer.html

```
denisovga@biowulf:/data/denisovga/1_DL_Course/6_GCNS
#!/usr/bin/env python
import os, sys
import tensorflow as tf
import spektral
import options, data, models

if __name__ == '__main__':
    opt = options.parse_training_arguments()
    opt = options.parse_command_line_arguments("train")

    os.environ['CUDA_VISIBLE_DEVICES'] = "0"
    for j in range(1, opt.num_gpus):
        os.environ['CUDA_VISIBLE_DEVICES'] += "," + str(j)
    strategy = tf.distribute.MirroredStrategy()
    with strategy.scope():
        model = models.get_model(opt)

    opt, data_size, data_train = data.get_data(opt)
    if opt.load_weights:
        try:
            model.load_weights(opt.checkpoint_file)
        except:
            sys.exit("\nCannot read weights from: " + opt.checkpoint_file)

    checkpointer = tf.keras.callbacks.ModelCheckpoint(filepath=\
        opt.checkpoint_file, save_weights_only=True)
    num_steps = int(round(float(data_size)/float(opt.batch_size)))
    loader = spektral.data.BatchLoader(data_train, batch_size=opt.batch_size)
    model.fit(loader.load(), epochs=opt.num_epochs, steps_per_epoch=num_steps,
        batch_size=opt.batch_size, shuffle=True, callbacks=[checker])
```

Header

- imports, incl. Spektral
- parsing command line options

Define model(s)

- GCN_Cancer model
- GCNConv
- ChebConv
- MinCutPool
- DiffPool

Get data

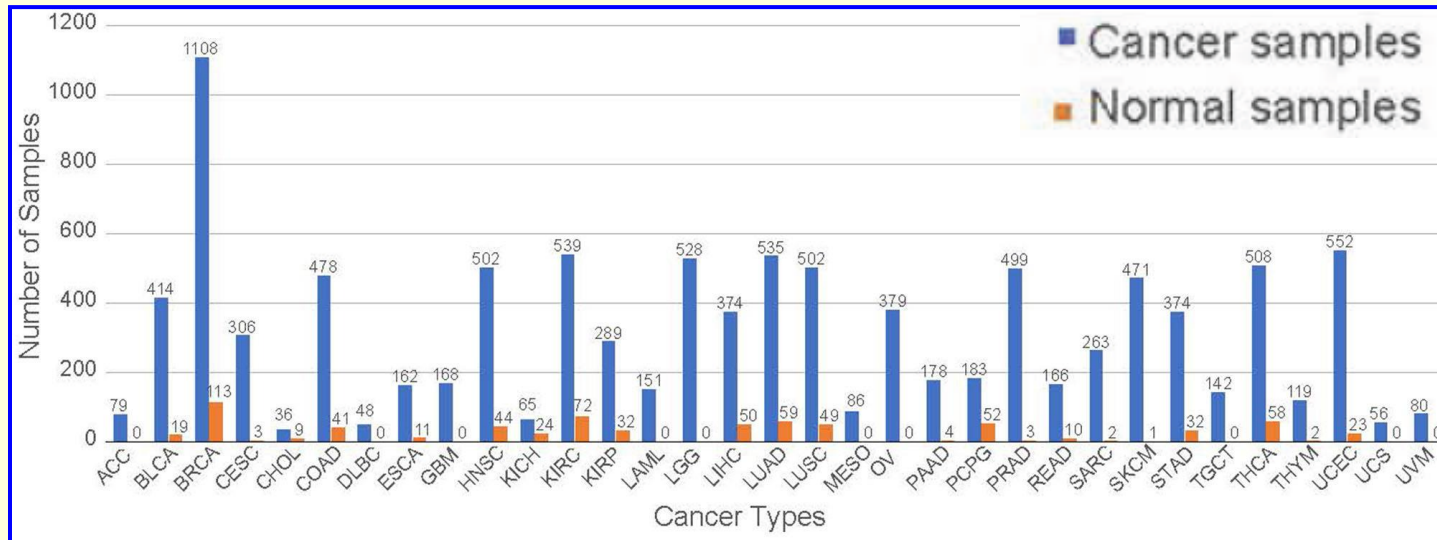
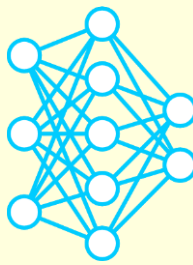
- GCE, GCES,
- PPI, PPIS

Run the models

- data balancing, SMOTE variants
- classification error

The GCN_Cancer data

R.Ramirez et al., Frontiers in Physics (2020)



RNA-seq data

- highly **imbalanced**
- **normal** samples from **23 tissues only**

Data matrices

GCE: genes of any type, no singletons
8850 samples x 3866 genes

GCES: genes of any type, including singletons;
8850 samples X 7091 genes

PPI: protein coding genes, no singletons;
8896 samples X 4444 genes

PPIS: protein coding genes, including singletons;
8850 samples x X 7091 genes

Adjacency matrices

GCE, GCES
gene expr. Spearman correlation coefficients
+ threshold=0.6
Size: 3866 x 3866

PPI, PPIS
STRING association
confidence scores
+ threshold=0.6
Size: 4444 x 4444

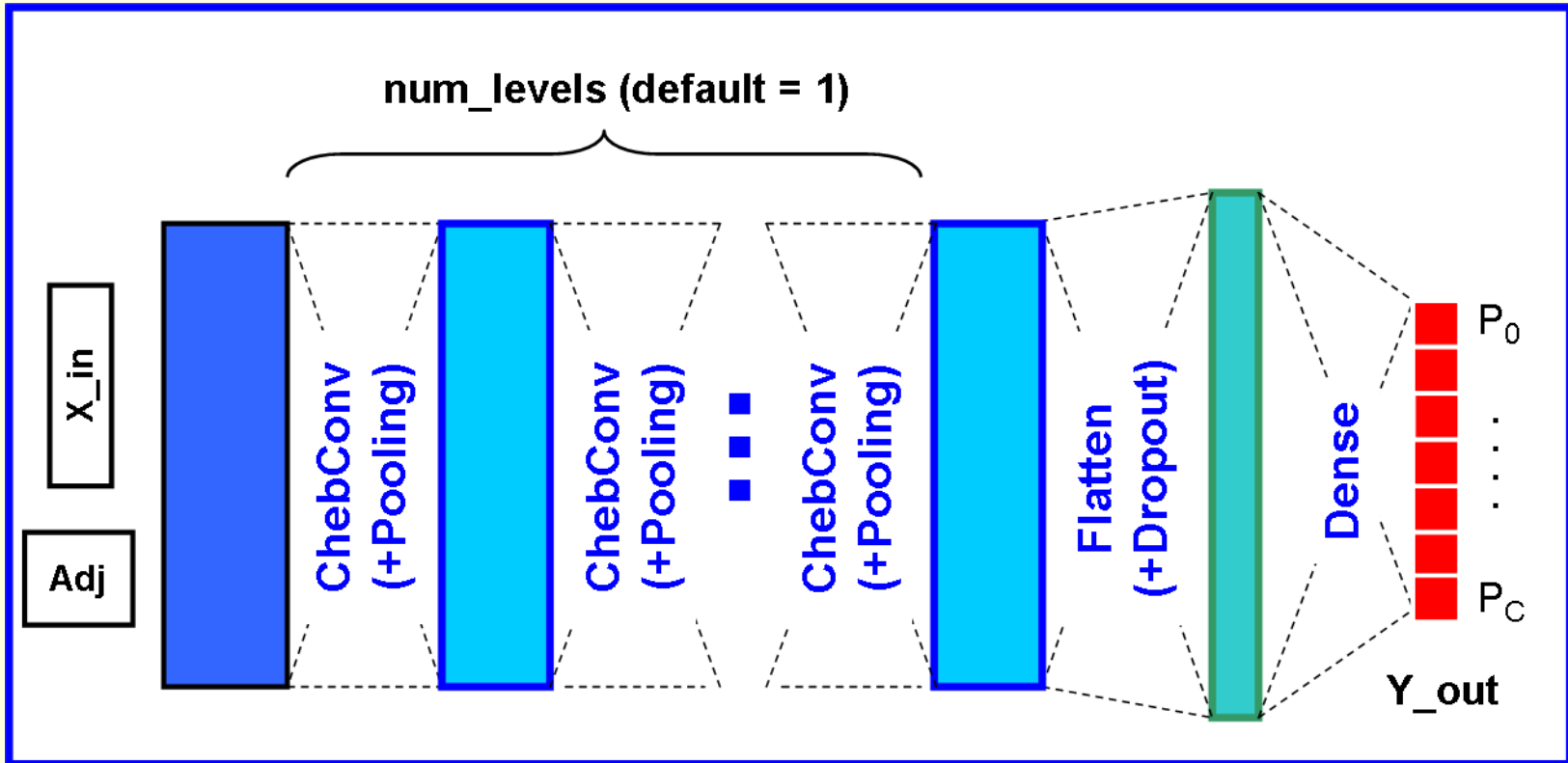
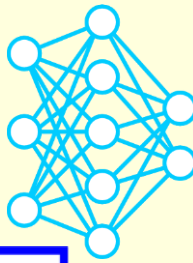
GCE: gene co-expression

PPI: protein-protein interaction

The GCN_Cancer model

Spektral: <https://graphneural.network>

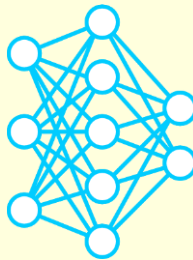
https://hpc.nih.gov/apps/GCN_Cancer.html



Features of the Keras implementation:

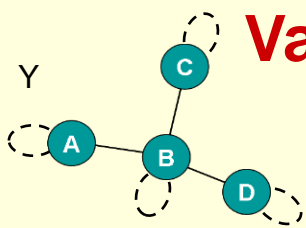
- classifies each sample as one of **C=34 types**
- supports GCNConv, **ChebConv** (=default) and Dense as the 1st layer in the network model
- **optionally**, allows for **balancing** of the number of training samples across different classes
- **optionally**, allows for **Pooling**, with two supported types of layers: MinCutPool and DiffPool
- **optionally**, allows for **multiple levels** of Filtering (+ Pooling)

Vanilla Graph Convolution: the GCNConv layer

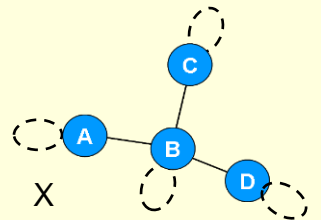


degree matrix, normalized adjacency matrix

Kipf, T.N., Welling, M.: arXiv preprint (2016)



GCNConv filtering



	A	B	C	D
A	0	1	0	0
B	1	0	1	1
C	0	1	0	0
D	0	1	0	0

$A = \{a_{ij}\}$
Adjacency matrix

	A	B	C	D
A	1	0	0	0
B	0	3	0	0
C	0	0	1	0
D	0	0	0	1

$D = \text{diag}(\sum_j a_{ij})$
Degree matrix

$I =$

	A	B	C	D
A	1	0	0	0
B	0	1	0	0
C	0	0	1	0
D	0	0	0	1

	A	B	C	D
A	1	1	0	0
B	1	1	1	1
C	0	1	1	0
D	0	1	0	1

$\tilde{A} = A + I$

	A	B	C	D
A	2	0	0	0
B	0	4	0	0
C	0	0	2	0
D	0	0	0	2

$\tilde{D} = D + I$

```
denisovga@biowulf:/data/denisovga/1_DL_Course/6_GCNS
module load GCN_Cancer
python
>>> import numpy as np
>>> import scipy.linalg as sl
>>> A = np.array([[0,1,0,0],[1,0,1,1],
...               [0,1,0,0],[0,1,0,0]])
>>> D = np.array([[1,0,0,0],[0,3,0,0],
...               [0,0,1,0],[0,0,0,1]])
>>> I = np.array([[1,0,0,0],[0,1,0,0],
...               [0,0,1,0],[0,0,0,1]])
>>> A_tilde = A + I
>>> D_tilde = D + I
>>> D_tilde_minus_one_half = \
... sl.fractional_matrix_power(D_tilde,-0.5)
>>> A_hat = D_tilde_minus_one_half * A_tilde \
...         * D_tilde_minus_one_half
...                               16,37 - Top
```

GCNConv transformation

$$Y_i = \frac{1}{\tilde{d}_i} \sum_{j \in \text{one-hop neighbors and self}} X_j \cdot w_j + b_i$$

\tilde{d}_i = number of immediate neighbors of the node i, incl. itself

including self-edges

$$Y = \hat{A} \cdot W \cdot X + b$$

GCNConv in matrix form

where: $\hat{A} = \tilde{D}^{-1/2} \cdot \tilde{A} \cdot \tilde{D}^{-1/2} =$
Normalized adjacency matrix

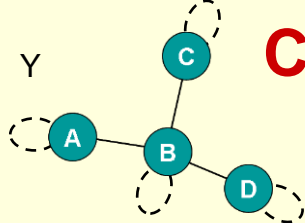
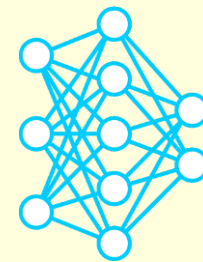
	A	B	C	D
A	0.5	0	0	0
B	0	0.25	0	0
C	0	0	0.5	0
D	0	0	0	0.5

spektral.layers.GCNConv(num_channels, activation=None, ...)

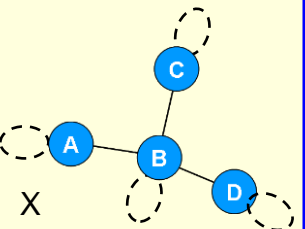
Chebyshev Convolution: the ChebConv layer

spectral approach, Convolution theorem, Fast Fourier transform, Graph Laplacian, eigenvectors, Chebyshev polynomials

M. Defferrard et al, arXiv preprint (2016)



ChebConv filtering ↑↑



Main ideas from convolution of discrete 1D signals:

“Regular” convolution in the time / spatial domain:

$$(f * g)[n] = \sum_{k=-\infty}^{\infty} f[n-k] \cdot g[k]$$

From the **Convolution theorem**: $f * g = F^{-1} \{ F \{ f \} \cdot F \{ g \} \}$, where $F \{ \}$ = Fourier transform

Fast Fourier transform: decomposing a signal into **eigenfunctions of Laplacian** $L = -d^2/dt^2$

$$x[k] = \sum_n [X_c[n] \cdot \cos(2\pi k n / N) + X_s[n] \cdot \sin(2\pi k n / N)]$$

Graph Convolution:

X = vector of node features

Graph Fourier transform:

$$\hat{X} = F(X) = U^T \cdot X,$$

inverse: $X = F^{-1}(\hat{X}) = U \cdot \hat{X}$

	A	B	C	D
A	1	-1	0	0
B	-1	3	-1	-1
C	0	-1	1	0
D	0	-1	0	1

Graph Laplacian:

$$L = D - A$$

4
0
1
1

Eigenvalues of L:

$$\lambda = \{\lambda_1, \lambda_2, \lambda_3, \lambda_4\}$$

-0.5	3e-4	-0.8	0.3
-0.5	0	0	-0.9
-0.5	-0.7	0.4	0.3
-0.5	0.7	0.4	0.3

Eigenvectors of L:

$$U = \{u_1, u_2, u_3, u_4\}$$

```
denisovga@biowulf:/data/denisovga/1_DL_Cou...
>>> L = D - A
>>> lambda = np.linalg.eigvals(L)
>>> _, U = np.linalg.eigh(L)
>>> D_minus_one_half = \
>>> sl.fractional_matrix_power(D, -0.5)
>>> L_hat = D_minus_one_half * L * \
>>> D_minus_one_half
>>> L_tilde = (2/max(lambda))*(I-L_hat)-I
8.42 A11
```

$$Y = \sum_{k=0}^K T^{(k)}(\tilde{L}) \cdot W \cdot X + b$$

$$\tilde{L} = (2/\lambda_{\max}) \cdot L - I = \text{normalized Graph Laplacian}$$

$T^{(k)}(x)$ = Chebyshev polynomials:

$$T^{(0)}(x) = I \quad T^{(1)}(x) = x$$

$$T^{(n+1)}(x) = 2x \cdot T^{(n)}(x) - T^{(n-1)}(x)$$

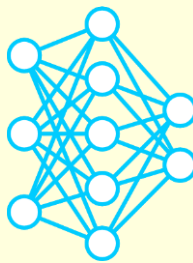
employs K-hop neighborhood of a node to update its value

spektral.layers.ChebConv(channels, K=1, ...)

Classification error: using the original / imbalanced input data

R.Ramirez et al., *Frontiers in Physics* (2020)

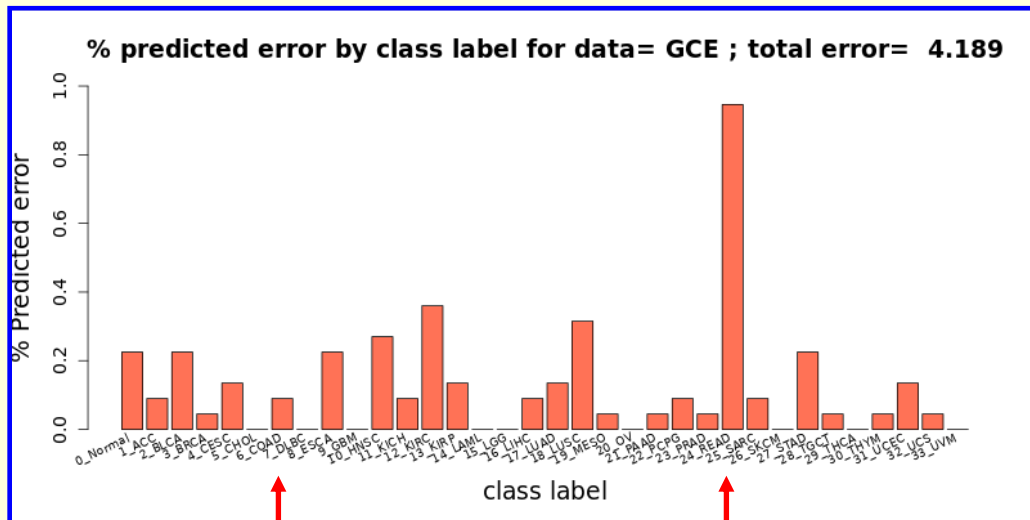
https://hpc.nih.gov/apps/GCN_Cancer.html



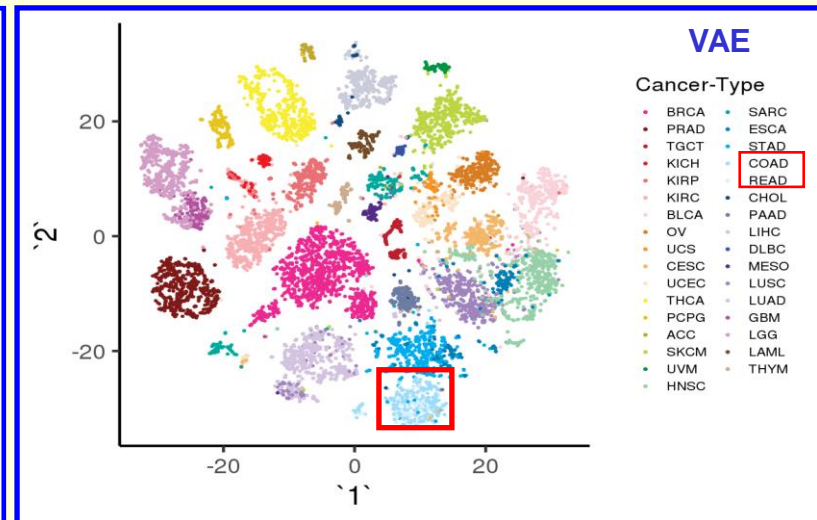
Data type	GCNNet	DenseNet	ChebNet, K=1	ChebNet, K=1 (orig. publication)
GCES	9.28%	5.7%	4.5%	$5.76 \pm 0.251\%$
GCE	6.4%	4.32%	4.19%	$5.77 \pm 0.146\%$
PPIS	7.79%	5.09%	4.37%	$5.39 \pm 0.107\%$
PPI	6.44%	5.06%	5.02%	$11.02 \pm 0.883\%$

CONCLUSIONS:

- 1) DenseNet overperforms GCNNet
- 2) ChebNet is the best
- 3) The ChebNet error is primarily due to misclassification of COAD / READ

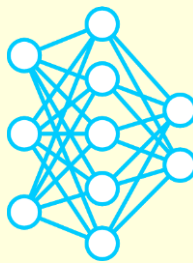


6_COAD Colon adenocarcinoma
24_READ Rectum adenocarcinoma



tSNE results from the class #3:
COAD and READ are not well separable

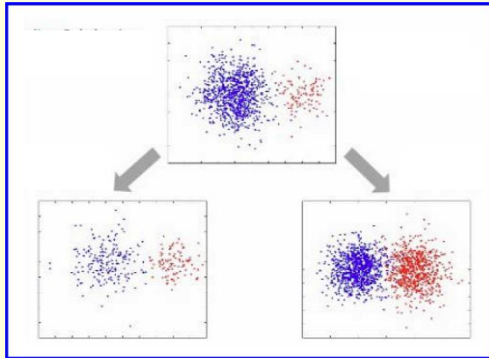
Classification error: using preprocessed / balanced input data



naïve balancing, synthetic minority oversampling technique (SMOTE)

SMOTE variants: G.Kovacs, SMOTE variants – Neurocomputing (2019)

Imbalanced data



Undersampling

Oversampling

- naïve balancing: duplicating randomly selected minority samples
- using **SMOTE variants** (total = 85): **MWMOTE** and **LLE_SMOTE** perform well

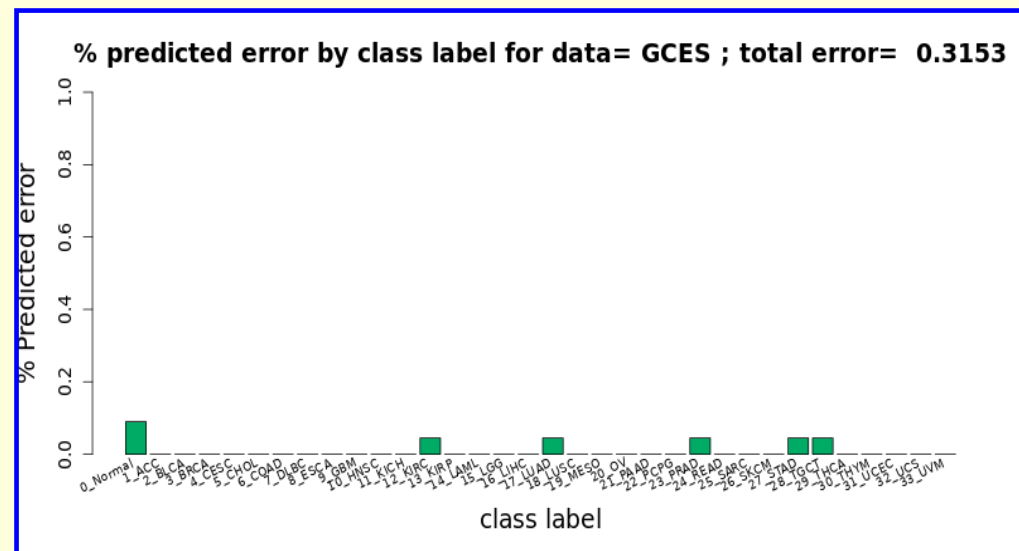
CONCLUSION:

1) balancing the # of training samples across classes and
2) using ChebNet at higher K can dramatically improve the accuracy of class predictions

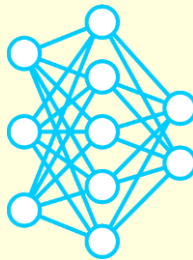
Data type	ChebNet, K = 1	ChebNet, K=10	ChebNet, K=20	ChebNet, K=100
GCE	0.09%	0%	0%	0%
GCES	0.54%	0.32%	0.32%	0.32%
PPI	0.18%	0.14%	0.046%	0.046%
PPIS	0.54%	0.41%	0.32%	0.14%

0 errors

1 error



How to run the GCN_Cancer app on Biowulf



https://hpc.nih.gov/apps/GCN_Cancer.html

```
denisovga@biowulf:/data/denisovga/1_DL_Course/6_GCNS
sinteractive --mem=120g --gres=gpu:p100:1,scratch:100 \
--cpus-per-task=14
module load gcn_cancer

ls $GCN_CANCER_SRC
data.py models.py options.py predict.py preprocess.py train.py visualize.R

cp -r $GCN_CANCER_DATA/* .

preprocess.py -h
preprocess.py -d GCE -B -S MWMOTE
preprocess.py -d PPI -B

train.py -h
train.py -d GCE -D 0.1
train.py -d GCE -K 100 -D 0.1 -B -S MWMOTE
train.py -d PPI -m DenseNet -D 0.1 -B

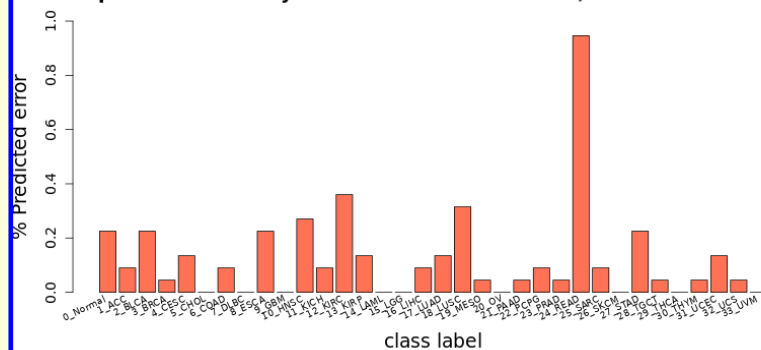
predict.py -h
predict.py -d GCE -D 0.1
predict.py -d GCE -K 100 -D 0.1 -B -S MWMOTE
predict.py -d PPI -m DenseNet -D 0.1 -B

visualize.R results/ChebNet.GCE.D_0.1.tsv
visualize.R results/chebnet.K_100.gces.D_0.1.B.S_MWMOTE.tsv
```

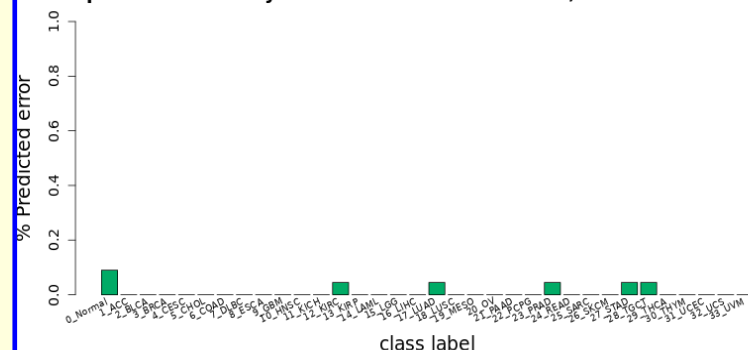
25,64

All

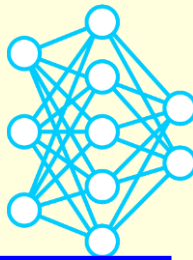
% predicted error by class label for data= GCE ; total error= 4.189



% predicted error by class label for data= GCEs ; total error= 0.3153



Summary

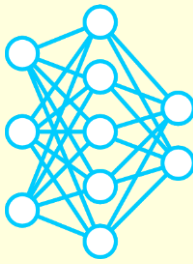


1) Intro using simple / prototype examples

- intro to the **graph classification task** and **graph-related terminology**
- GCNNet model requires a **second input** - the **adjacency matrix**
- GCNNet vs MLP: **Dense layer \approx GCNConv layer with adjacency matrix of ones**
- GCNConv vs Conv1D and Conv2D: **Filtering and Pooling**
- **GCNConv** is an analog of Conv1D / Conv2D with **filter of size = 3**
- **imbalanced** input data and the presence of **singletons** may reduce the classification accuracy

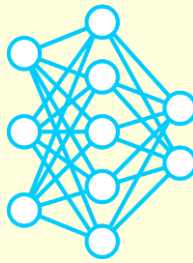
2) The GCN_Cancer application:

- **two types of gene association** in the GCN_Cancer data:
gene co-expression (GCE) and protein-protein interaction (PPI)
- **GCN_Cancer model outputs a vector of class probabilities**
- the **GCNConv layer implements a vanilla graph convolution**
- the meaning of hyperparameter **K** in the **ChebConv layer**
- the techniques for data balancing: **naïve balancing vs SMOTE variants**
- **data balancing dramatically reduces the classification error**
- the **ChebConv with higher K** allows further reduction in the classification error



BACKUP SLIDES

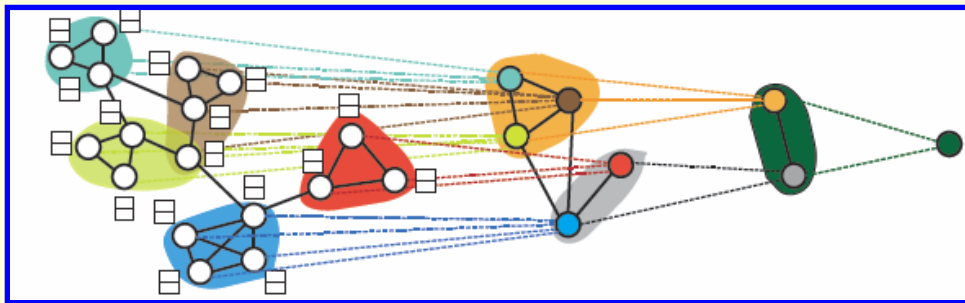
Pooling layers: DiffPool and MinCutPool



DiffPool: R. Ying et al, arXiv:1806.08804 (2019)

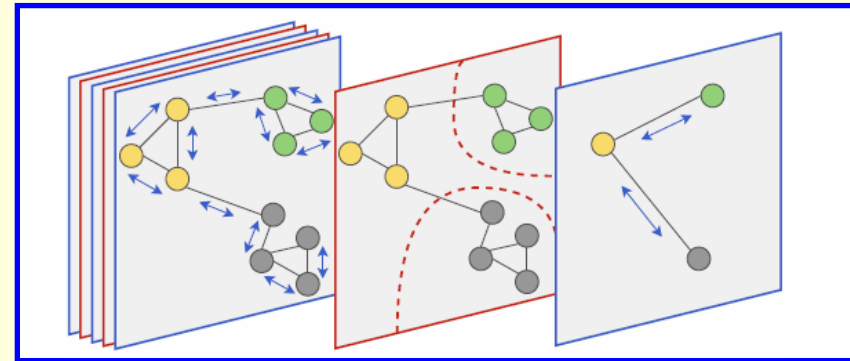
MinCutPool: F.M. Blanchi et al, arXiv:1907.00481 (2020)

Differentiable Pooling (agglomerative)



- iteratively **aggregate** “close” nodes
- compute a hierarchical representation of the graph
- stop when the target number of clusters is reached

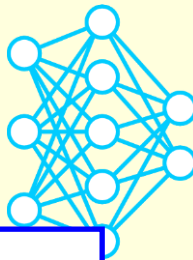
MinCutPool (divisive)



- **partition** nodes into a specified number C of clusters by removing the minimum # of links:

$$\frac{1}{K} \sum_{k=1}^K \frac{(\# \text{ links within cluster } k)}{(\# \text{ links between cluster } k \text{ and the rest of the graph})} \rightarrow \max$$

Graph convolution with polynomial filters



<https://distill.pub/2021/understanding-gnns>

<https://csustan.csustan.edu/~tom/Clustering/GraphLaplacian-tutorial.pdf>

- 1) **Polynomials of Laplacian** $p_w(L) = w_0 I_n + w_1 L + w_2 L^2 + \dots + w_d L^K = \sum_{i=0}^K w_i L^i$.

can be thought of as the **equivalents of filters in CNNs**

- 2) More specifically, if X = a vector of features of all nodes in a graph, then the convolved vector Y will be: $Y = p_w(L) X$. In particular, when $K = 1$, the v -th component of Y will be computed based on X_v and its **one-hop neighbors**:

$$Y_v = D_v X_v - \sum_{u \in \mathcal{N}(v)} X_u$$

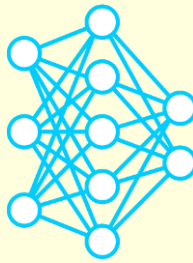
- 3) Likewise, it can be shown that for any K , the v -th component of Y will be computed based on the features of the nodes located at distance **no more than K -hops away** from the node v . This means that **polynomial filters are localized**.

- 4) ChebNet further refines this idea of polynomial filters by looking at polynomial filters of the form

$$p_w(L) = \sum_{i=1}^d w_i T_i(\tilde{L}) \quad \tilde{L} = \frac{2L}{\lambda_{\max}(L)} - I_n.$$

- 5) Eigenvalues of L are all non-negative, and one of them is always zero. \tilde{L} is effectively a scaled-down version of L , with **eigenvalues guaranteed to be in the range $[-1, 1]$**

The SMOTE variants LLE_SMOTE and MWMOTE

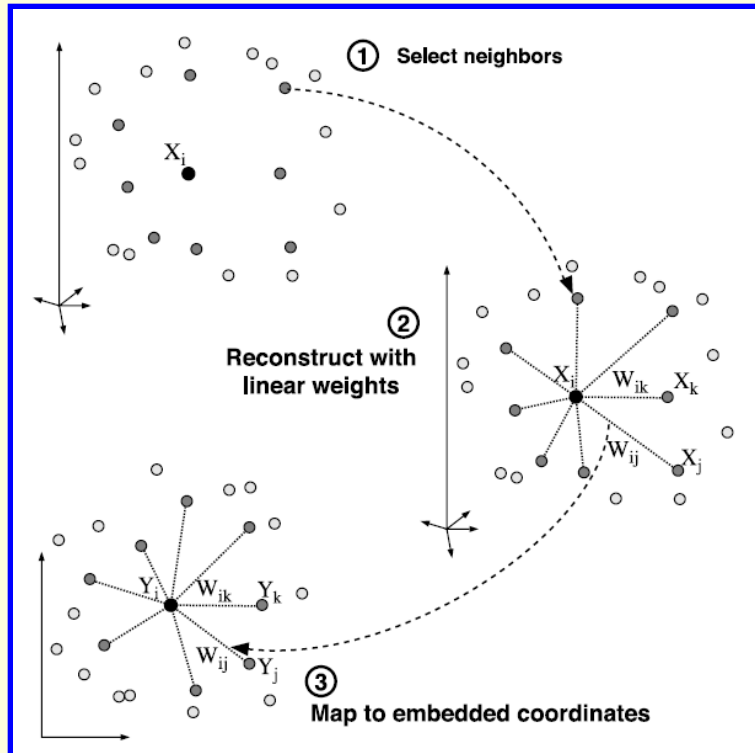


LLE SMOTE: J.Wang et al., ICSP 2006

MWMOTE: S.Barua et al, IEEE Trans. On Knowledge and Data Eng. (2014)

SMOTE variants: SMOTE, distance_SMOTE, SMOTE_D,
SMOTE_TomekLinks, **LLE_SMOTE**, **MWMOTE**,
NT_SMOTE, OUPS, Gazzah, ROSE, ...
(total = 85)

LLE SMOTE: Locally Linear
Embedding SMOTE



MWMOTE: Majority Weighted Minority
Oversampling Technique

