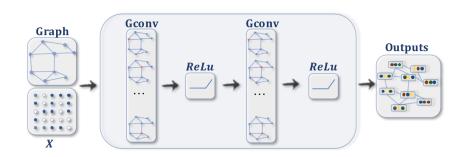
# **GCNN**

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## Зачем?

- Данные представлены в виде графа (например молекулы).
- Можно обучать классификаторы для multilabeling.
- Предсказание и распознавание действий.



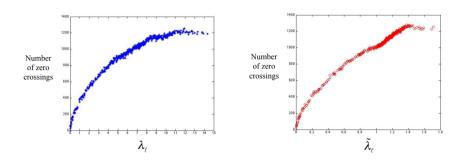
# Спектральные сети

$$L = D - A; L = I_N - D^{-0.5}AD^{-0.5}$$

$$\hat{f}(\lambda_I) = \sum_{i=1}^{N} f(i)u_I(i); f(i) = \sum_{l=0}^{N-1} \hat{f}(\lambda_l)u_I(i)$$

$$\mathcal{F}(x) = U^T x; \mathcal{F}^{-1}(x) = U\hat{x}$$

# Спектральные сети



$$\mathcal{Z}_{\mathcal{G}}(f) := e = (i,j) \in \mathcal{E} : f(i)f(j) < 0$$

# Спектральные сети

#### Свертка

$$x *_{G} g = \mathcal{F}^{-1}(\mathcal{F}(x) \odot \mathcal{F}(g)) = U(U^{T} x \odot U^{T} g) =$$
  
 $\{g_{\theta} = diag(U^{T} g)\} = Ug_{\theta}U^{T} x$ 

# T. N. Kipf and M. Welling 2017 ICLR

### Чебышев

$$T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x)$$

$$T_0(x) = 1 ; T_1(x) = x$$

$$x *_G g \approx \sum_{k=0}^K \theta_k T_k(L) x$$

#### GCN

$$x *_{G} g \approx \theta_{0}x + \theta_{1}(L - I_{N})x = \theta_{0}x - \theta_{1}D^{-0.5}AD^{-0.5}x$$

$$x *_{G} g \approx \theta(I_{N} + D^{0.5}AD^{-0.5})x$$

# T. N. Kipf and M. Welling 2017 ICLR

#### Renormalization trick

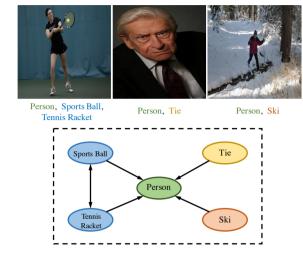
$$I_N + D^{-0.5}AD^{-0.5} \to \tilde{D}^{-0.5}\tilde{A}\tilde{D}^{-0.5}$$
 $\tilde{A} = A + I_N \; ; \tilde{D}_{ii} = \sum_j \tilde{A}_{ij}$ 
 $H^{(l+1)} = \sigma(\tilde{D}^{-0.5}\tilde{A}\tilde{D}^{-0.5}H^{(l)}W^{(l)})$ 

# T. N. Kipf and M. Welling 2017 ICLR

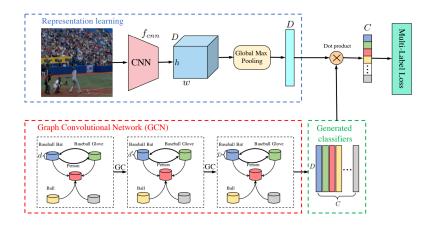


Рис.: Cora dataset t-SNE

#### Zhao-Min Chen, Xiu-Shen Wei, Peng Wang, Yanwen Guo 2019 CVPR



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# Adjacency matrix binary

$$P_i = M_i/N_i$$
 $A_{ij} = egin{cases} 0, & ext{if } P_{ij} < au \ 1, & ext{else} \end{cases}$ 

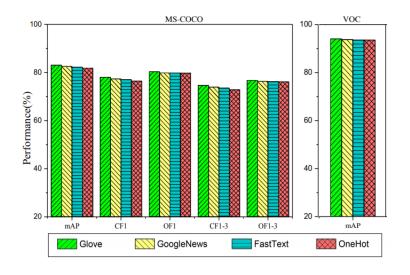
## Adjacency matrix reweighted

$$A_{ij} = egin{cases} p/\sum\limits_{j=1,\,j 
eq i}^C A_{ij} & ext{if } i 
eq j \ 1-p, & ext{else} \end{cases}$$

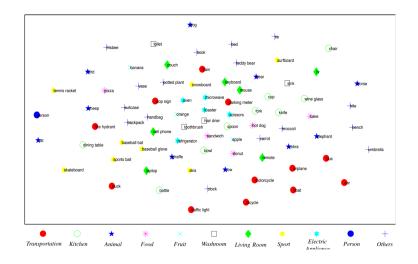
#### Zhao-Min Chen, Xiu-Shen Wei, Peng Wang, Yanwen Guo 2019 CVPR

```
def gen A(num classes, t, adi file):
   import pickle
   result = pickle.load(open(adj_file, 'rb'))
   adi = result['adi']
   nums = result['nums']
   nums = nums[:, np.newaxis]
   adj = adj / nums
   adi[adi < t] = 0
   _adj[_adj >= t] = 1
   _adj = _adj * 0.25 / (_adj.sum(0, keepdims=True) + 1e-6)
   _adj = _adj + np.identity(num_classes, np.int)
   return adi
def gen_adj(A):
   D = torch.pow(A.sum(1).float(), -0.5)
   D = torch.diag(D)
   adj = torch.matmul(torch.matmul(A, D).t(), D)
   return adj
```

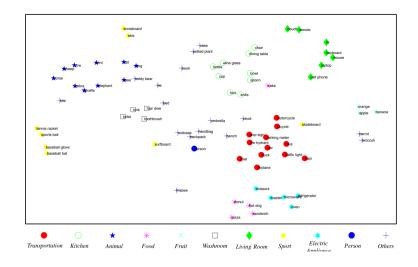
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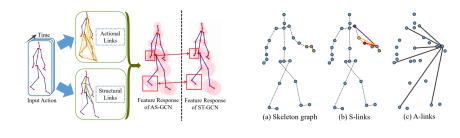


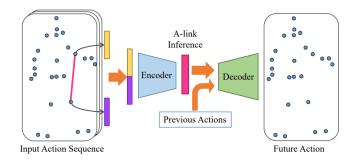
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### Encoder part

link features:  $Q_{ij}^{k+1} = f_e^k(f_v^k(p_i^k) \oplus f_v^k(p_j^k)),$ joint features:  $p_i^{k+1} = \mathcal{F}(Q^{k+1}) \oplus p_i^k$ 

$$\mathcal{A}_{i,j,:} = \mathsf{softmax}\left(rac{Q_{i,j}^K + r}{ au}
ight) \in \mathbb{R}^C$$

#### Decoder part

link features: 
$$\mathbf{Q}_{ij}^t = \sum_{c=1}^C \mathcal{A}_{i,j,c} f_e^c(f_v^c(\mathbf{x}_i^t) \oplus f_v^c(\mathbf{x}_j^t)),$$
 joint features:  $p_i^t = \mathcal{F}(Q_{i,:}^t) \oplus \mathbf{x}_i^t$  hidden state:  $S_i^{t+1} = GRU(S_i^t, p_i^t)$  expectation of position:  $\hat{\mu}_i^{t+1} = f_out(S_i^{t+1}) \in \mathbb{R}^3$ 

#### Loss

$$\mathcal{L}_{AIM}(\mathcal{A}) = -\sum_{i=1}^{n} \sum_{t=2}^{I} \frac{\|\mathbf{x}_{i}^{t} - \hat{\mu}_{i}^{t}\|^{2}}{2\sigma^{2}} + \sum_{c=1}^{C} \log \frac{\mathcal{A}_{:,:,c}}{\mathcal{A}_{:,:,c}^{0}}$$

#### Prior

$$\forall i, j, \ \mathcal{A}_{i,j,0} \sum_{c=1}^{C} \mathcal{A}_{i,j,c} = 1,$$

$$\mathcal{A}_{i,i,0}^{0} = P_{0}, \ \mathcal{A}_{i,i,c}^{0} = P_{0}/C, \ \hat{A}_{act}^{(c)} = D_{act}^{(c)^{-1}} A_{act}^{(c)}$$

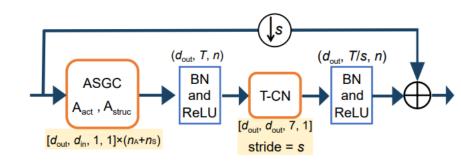
## AGC

$$X_{a}ct = AGC(X_{in}) = \sum^{C} \hat{A}_{act}^{(c)} X_{in} W_{act}^{(c)} \in \mathbb{R}^{n imes d_{out}}$$

#### Structural Convolution

$$\hat{A} = D^{-1}A$$

$$X_{s}truc = SGC(X_{i}n) = \sum_{l=1}^{L} \sum_{s \in \mathcal{D}} M_{struc}^{(p,l)} \odot \hat{A}^{(p)l} X_{in} W_{struc}^{(p,l)} \in \mathbb{R}^{n \times d_{out}}$$



$$\mathcal{L}_{recog} = -y^{T} \log(\hat{y}), \ \mathcal{L}_{predict} = \frac{1}{ndT'} \sum_{i=1}^{nd} \sum_{t=1}^{T'} \|\hat{\mathcal{X}}_{i,:,t} - \mathcal{X}_{i,:,t}\|_{2}^{2}$$

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