Centre for Data Analytics



# Background Knowledge Injection for Interpretable Sequence Classification

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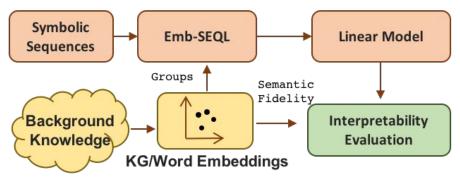








## Contributions



#### Groups:

Regex-like expansion of traditional k-mers

Emb-SEQL:

Injection of Background Knowledge into Sequence Learning Algorithm

Semantic Fidelity:

Metric to quantify interpretability

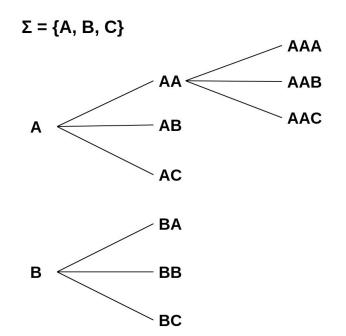
### Symbolic Sequence Classification

Sequence	Class	
ABBCBAABCBABCBABBBCBABBABBCB	+1	
CCBBABACAABBABBAAABBBCCBBABA	-1	Σ = {A, B, C}
ACBBCACCCBAABCBABCCABCAABCCA	+1	
BABACCBABCTABCBABBCAABCBBBCA	?	

<i>k</i> -mers: Consecutive sequences <i>k</i> of symbols					
<i>2</i> -mer:	AB				
<i>5</i> -mer:	BCTCB				

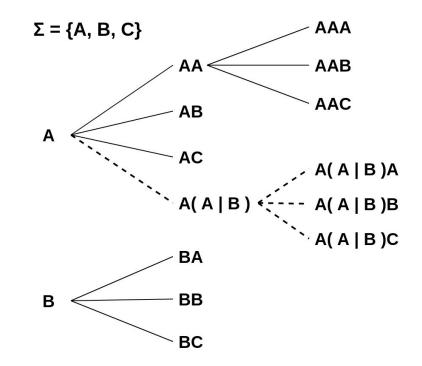
### SEQL - Sequence Learner

- Integrated approach
- Learns sparse *k*-mer based linear models
- Feature space of all possible *k*-mers
- Gauss-Southwell coordinate descent
- Iteratively add best *k*-mer to model
- Exploits structure in feature space

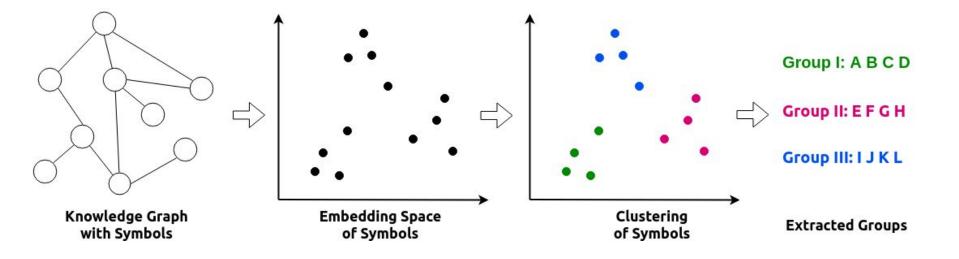


### SEQL - Sequence Learner with Groups

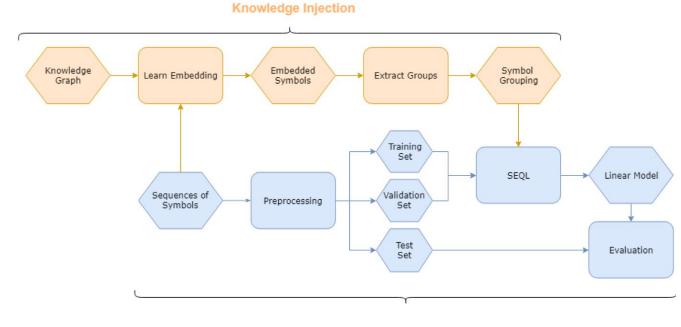
- Exploit structure in symbol space
- Use groups to gain more flexibility
- *Groups* are built by combining basic symbols with OR
- Groups predefined by user or automatically generated



### Automatic Group Generation



### Emb-SEQL Pipeline



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Sequence Learning

### Interpretability

- Interpretability is crucial in some problems
- Accuracy-interpretability trade-off
- Measuring interpretability of models is an open question

Semantic Fidelity intuition:

- Positive features should be "close" to target class
- Negative features should be "close" to non-target class

Functional grounded protocol as proxy measurement

### Semantic Fidelity

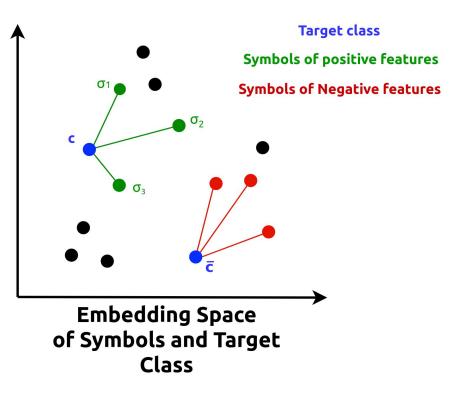
### *k*-mer - Target Class Distance

$$d_c(\phi, c) = \frac{1}{n_{\phi}} \sum_{\sigma_j \in \phi} \|\mathbf{E}_{\sigma_j} - \mathbf{e}_c\|$$

Weighted Target Class Distance $h(\phi) = |w| \begin{cases} d(\phi, c) & \text{if } w \ge 0\\ d(\phi, \bar{c}) & \text{otherwise} \end{cases}$ 

### **Semantic Fidelity**

$$SF = 1 - \frac{1}{2n} \sum_{\phi_i \in \Phi} h(\phi_i)$$



### Experiment

**Opportunity** - Human Composite Activity Recognition (HAR) [1]:

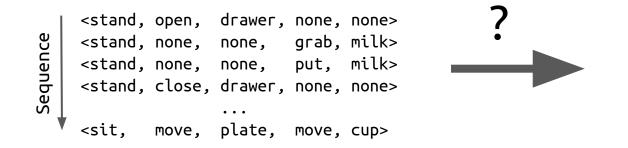
- Predict Composite Activity
- Multiclass classification problem
- Combinations of 5 low level features categories ( $|\Sigma| > 1400$  symbols)

### **PhosphoELM** - Protein Classification [2]:

- Binary classification problem
- Predict Kinase group
- Amino acid sequences ( $|\Sigma| = 21$  symbols; 438 sequences)

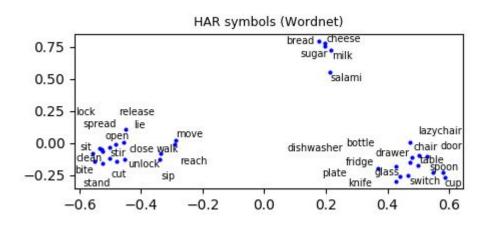
### **Composite Activity Recognition**

Predict composite activity based on sequence of low-level activity



Coffee time Early morning Cleanup Sandwich time Relaxing

### **Composite Activity Recognition**



#### Atomic symbol embeddings

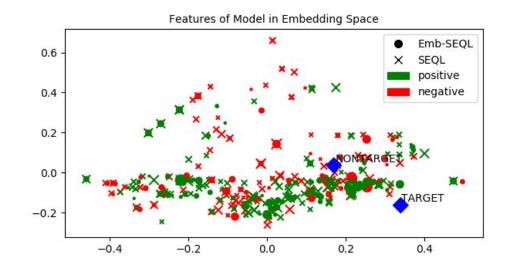
Weight	Feature
1.0	<ul> <li>([sit, release, cheese, move, knife cheese]</li> <li>OR [stand, move, plate, move, plate]</li> <li>OR [stand, move, plate, reach, drawer1]</li> <li>OR [stand, move, plate, open, drawer1]</li> <li>OR [stand, reach, bread, open, drawer3]) </li> </ul>
-0.867	<ul> <li></li> <li>〈 ([stand, open, fridge, move, milk]</li> <li>OR [stand, none, none, release, milk]</li> <li>OR [walk, move, plate, none, none]</li> <li>OR [walk, move, plate, release, bread]</li> <li>OR [walk, none, none, move, plate]</li> <li>OR [stand, reach, sugar, reach, spoon]) ,</li> <li>[stand, none, none, none] &gt;</li> </ul>

#### Sandwich time model

### **Results - Semantic Fidelity**

Dataset	Embeddings	Model	$\overline{SF}$	std	Class 1	Class 2	Class 3	Class 4	Class 5
HAR	GloVe	SEQL Emb-SEQL	0.902 <b>0.923</b>	0.028 0.025	0.930 0.958	$0.871 \\ 0.888$	0.925 0.931	0.865 0.901	0.921 0.938
	ConceptNet	SEQL Emb-SEQL	0.871 <b>0.875</b>	0.033 0.025	0.908 0.903	0.828 0.853	0.895 0.887	0.833 0.836	$0.889 \\ 0.894$
	YAGO-41	SEQL Emb-SEQL	<b>0.867</b> 0.835	0.029 0.043	0.899 0.897	$0.847 \\ 0.824$	0.893 0.861	0.823 0.767	0.872 0.827
	WordNet	SEQL Emb-SEQL	0.894 <b>0.936</b>	0.025 0.010	0.921 0.937	0.879 0.945	0.918 0.943	0.857 0.917	0.895 0.939
Protein	ChEBI-ChEMBL	SEQL Emb-SEQL	0.708 <b>0.719</b>	-					

### **PCA Visualization**



Target: Coffee time Embedding: WordNet

### Results - Classification Quality

Dataset	Model	Embeddings	F1	Accuracy	
HAR	SVM		0.502	0.564	
	LSTM		0.767	0.810	
	SEQL		0.973	0.961	
		ConceptNet	0.965	0.951	
	Emb-SEQL	GloVe	0.961	0.945	
		WordNet	0.968	0.955	
		YAGO-41	0.957	0.941	
Protein	SCIS_MA		_	0.948	
	HMM		-	0.918	SCIS_MA and HMM
	LSTM		0.797	0.796	results from [2]
	SEQL		0.902	0.903	
	Emb-SEQL	ChEBI-ChEMBL	0.898	0.901	

### Achievements & Conclusion

- Introduction of *Groups*, regex like k-mer symbols
- Generation of *Groups* from background knowledge sources
- **Emb-SEQL**, a method to learn sparse linear models
- Semantic Fidelity a way to measure interpretability

• Background knowledge injection improves interpretability measured by Semantic Fidelity without hurting accuracy of learned model

### Limitations & Future Work

- High memory demand of Emb-SEQL for large *Groups*
- Clustering method and *Group* size is crucial
- Background knowledge source is needed

- Semantic Fidelity for non-linear models
- Human-based evaluation of Semantic Fidelity

## Thank you!

Please email severin.gsponer@insight-centre.org if you have further questions

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