Structural Bioinformatics Training Workshop & Hackathon 2018

Spark Machine Learning

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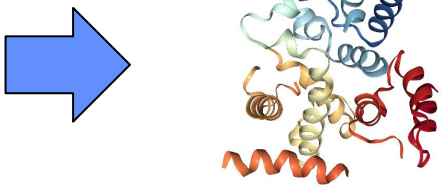
Example Problem

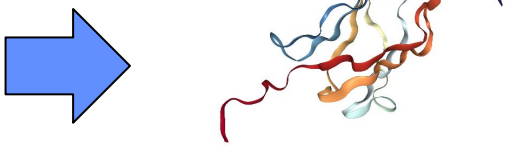
Classify protein fold as either all alpha or all beta given the protein sequence.

MHHHHHHSSGRENLYFQGMTVREKTRLEKFRQLLSSQNTDLDELRKCSW
PGVPREVRPITWRLLSGYLPANTERRKLTLQRKREEYFGFIEQYYDSRNEE
HHQDTYRQIHIDIPRTNPLIPLFQQPLVQEIFERILFIWAIRHPASGYVQGIND
LVTPFFVVFLSEYVEEDVENFDVTNLSQDMLRSIEADSFWCMSKLLDGIQD
NYTFAQPGIQKKVKALEELVSRIDEQVHNHFRRYEVEYLQFAFRWMNNLL
MRELPLRCTIRLWDTYQSEPEGFSHFHLYVCAAFLIKWRKEILDEEDFQGLL
MLLQNLPTIHWGNEEIGLLLAEAYRLKYMFADAPNHYRR



PDB ID: 3DZX – all alpha

GSSGSSGLPQVEAYSPSACSVRGGEELVLTGSNFLPDSKVVFIERGPDGK
LQWEEEATVNRLQSNEVTLTLTVPEYSNKRVSRPVQVYFYVSNGRRKRSPT
QSFRFLPVICKEE



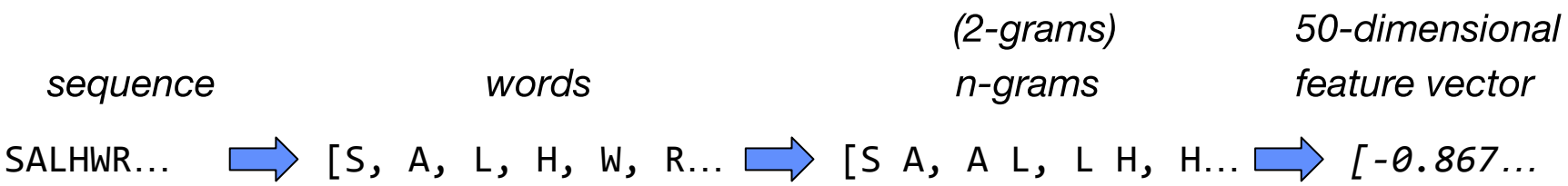
PDB ID: 2YRP – all beta

PySpark Machine Learning

- **pyspark.ml**
  - Uses Dataset
- **pyspark.mllib (maintenance mode)**
  - Uses RDD

http://spark.apache.org/docs/latest/api/python/pyspark.ml

Feature Vector Creation



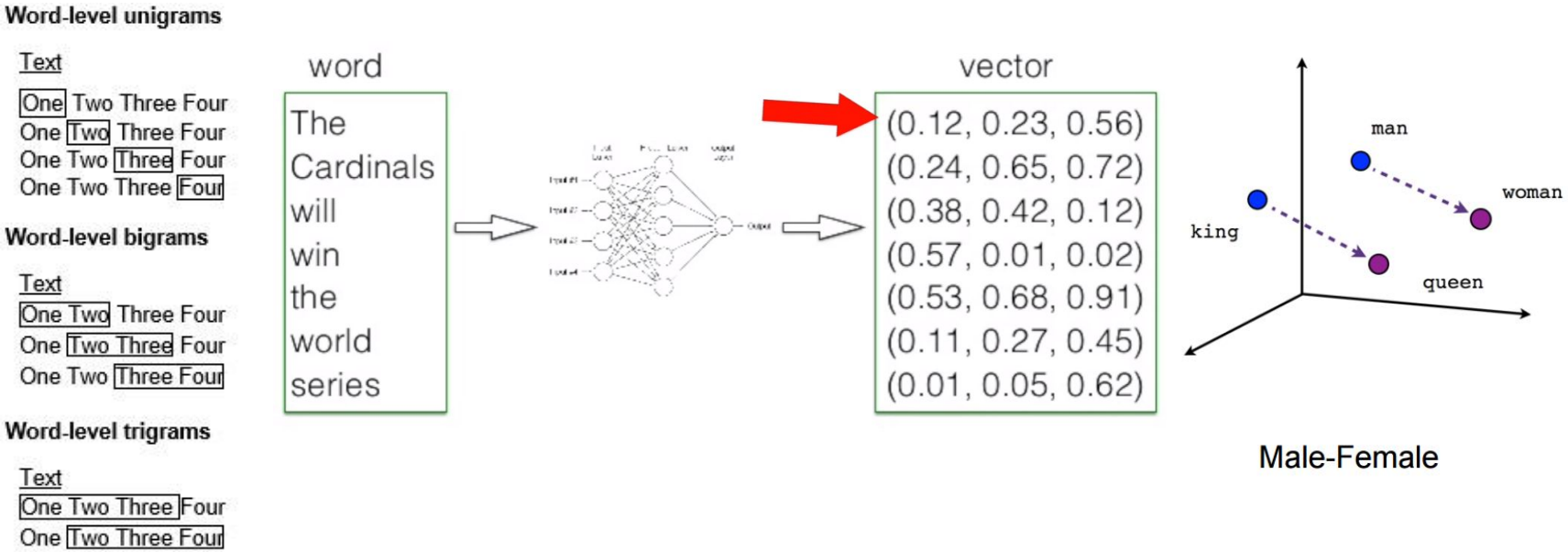
Feature Engineering Pipeline: ***NGram*** ***Word2Vec***

alpha	beta	coil	foldType	words	ngram	features
0.7194245	0.0	0.28057554	alpha	[S, A, L, H, W, R...]	[S A, A L, L H, H...]	[-0.8678886349164...]
0.4090909	0.0	0.59090906	alpha	[S, H, L, K, S, K...]	[S H, H L, L K, K...]	[-0.2172588950821...]
0.015151516	0.5808081	0.4040404	beta	[M, A, H, H, H, H...]	[M A, A H, H H, H...]	[-0.6485012823101...]
0.7916667	0.0	0.20833333	alpha	[M, G, S, S, H, H...]	[M G, G S, S S, S...]	[-0.7672874573129...]
0.028846154	0.52884614	0.44230768	beta	[M, E, K, A, T, K...]	[M E, E K, K A, A...]	[-0.7308713050851...]
0.6904762	0.011904762	0.29761904	alpha	[P, T, I, H, D, H...]	[P T, T I, I H, H...]	[-0.7869252321949...]
0.8108108	0.0	0.1891892	alpha	[G, A, M, E, P, E...]	[G A, A M, M E, E...]	[-0.8350848566740...]
0.022900764	0.39694658	0.5801527	beta	[I, V, N, G, E, E...]	[I V, V N, N G, G...]	[-0.6840203473201...]
0.8021978	0.0	0.19780022	alpha	[M, T, P, D, V, L...]	[M T, T P, P D, D...]	[-0.7698143909806...]

https://github.com/sbl-sdsc/mmtf-pyspark/blob/master/mmtfPyspark/ml/proteinSequenceEncoder.py

N-gram, Word2Vec

- **N-gram: Slice and group a string with a window size of N**
- **Word2Vec: Projecting a string to an n-dimensional vector**



https://spark.apache.org/docs/latest/mllib-feature-extraction.html#word2vec

Create Class Labels

alpha	beta	coil	foldType
0.7194245	0.0	0.28057554	alpha
0.4090909	0.0	0.59090906	alpha
0.015151516	0.5808081	0.4040404	beta
0.7916667	0.0	0.20833333	alpha
0.028846154	0.52884614	0.44230768	beta
0.6904762	0.011904762	0.29761904	alpha
0.8108108	0.0	0.1891892	alpha
0.022900764	0.39694658	0.5801527	beta
0.8021978	0.0	0.19780022	alpha

The Dataset for Classification

We save this dataset as .parquet file:

```
data.write.mode("overwrite").format("parquet").save(filename);
```

class label ***features***

alpha	beta	coil	foldType	words	ngram	features
0.7194245	0.0	0.28057554	alpha	[S, A, L, H, W, R...	[S A, A L, L H, H...	[-0.8678886349164...
0.4090909	0.0	0.59090906	alpha	[S, H, L, K, S, K...	[S H, H L, L K, K...	[-0.2172588950821...
0.015151516	0.5808081	0.4040404	beta	[M, A, H, H, H, H...	[M A, A H, H H, H...	[-0.6485012823101...
0.7916667	0.0	0.20833333	alpha	[M, G, S, S, H, H...	[M G, G S, S S, S...	[-0.7672874573129...
0.028846154	0.52884614	0.44230768	beta	[M, E, K, A, T, K...	[M E, E K, K A, A...	[-0.7308713050851...
0.6904762	0.011904762	0.29761904	alpha	[P, T, I, H, D, H...	[P T, T I, I H, H...	[-0.7869252321949...
0.8108108	0.0	0.1891892	alpha	[G, A, M, E, P, E...	[G A, A M, M E, E...	[-0.8350848566740...
0.022900764	0.39694658	0.5801527	beta	[I, V, N, G, E, E...	[I V, V N, N G, G...	[-0.6840203473201...
0.8021978	0.0	0.19780022	alpha	[M, T, P, D, V, L...	[M T, T P, P D, D...	[-0.7698143909806...

Demos

- Create a dataset
- Fit several classification models with pyspark.ml
- Fit several classification models with scikit-learn

Problem 1

- **Change the code to a 3-state classification problem:**
  - alpha, beta, alpha+beta
- **Rerun the classification with Decision Tree Classifier**

Resources

- **Pyspark.ml API**
  - http://spark.apache.org/docs/latest/api/python/pyspark.ml.html
- **Extracting, transforming and selecting features**
  - http://spark.apache.org/docs/latest/api/python/pyspark.ml.html#module-pyspark.ml.feature
  - N-gram
    - http://spark.apache.org/docs/latest/api/python/pyspark.ml.html#pyspark.ml.feature.NGram
  - Word2Vec
    - http://spark.apache.org/docs/latest/api/python/pyspark.ml.html#pyspark.ml.feature.Word2Vec
- **Classification and regression**
  - https://spark.apache.org/docs/latest/ml-classification-regression.html
- **Parquet files (columnar format)**
  - https://spark.apache.org/docs/latest/sql-programming-guide.html#parquet-files

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