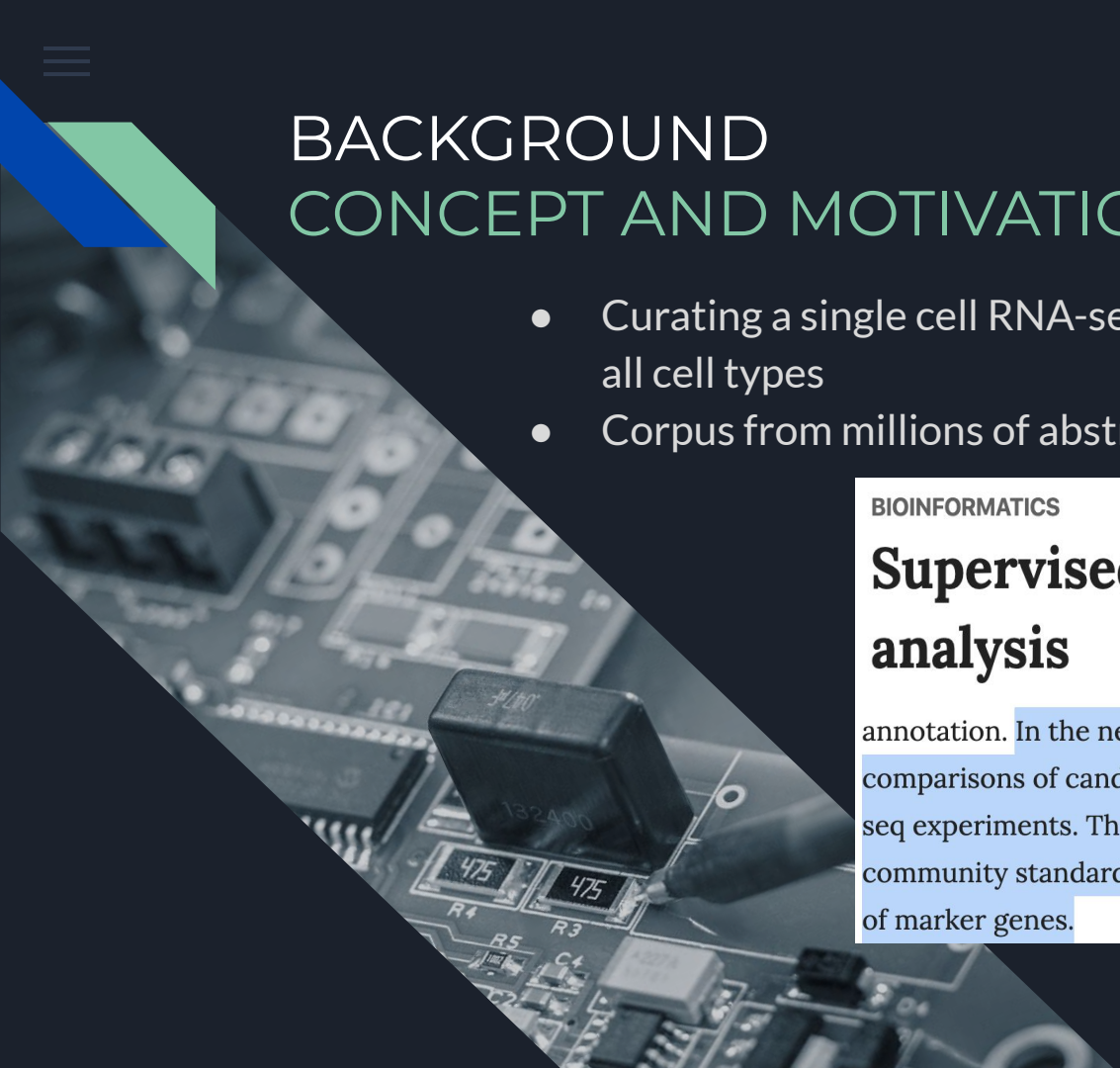
TYPER: Presentation

Steven Wu
Nicolas Cardozo
Samantha Borje

BACKGROUND
CONCEPT AND MOTIVATION

- Curating a single cell RNA-sequencing markers from across all cell types
- Corpus from millions of abstracts from pubmeds API



BIOINFORMATICS

Supervised clustering for single-cell analysis

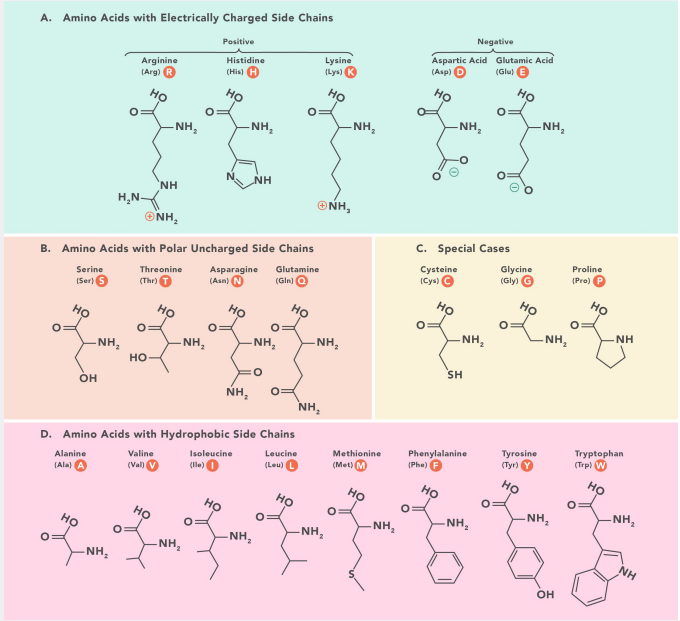
annotation. In the near future, we are likely to see large scale comparisons of candidate lists derived from the literature and scRNA-seq experiments. This will, in turn, drive the emergence of consistent community standards regarding the selection, evaluation and reporting of marker genes.

RESULTS
USE CASE

- The problem we are trying to solve is curating a list of single cell RNA-sequencing markers from across all cell types.

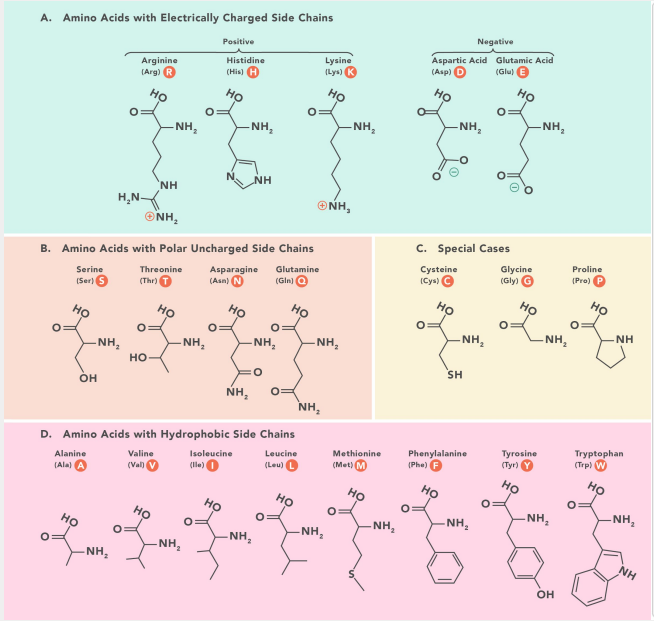
- We are going curate the corpus from millions of abstracts from pubmeds API.

RESULTS
PROOF OF CONCEPT



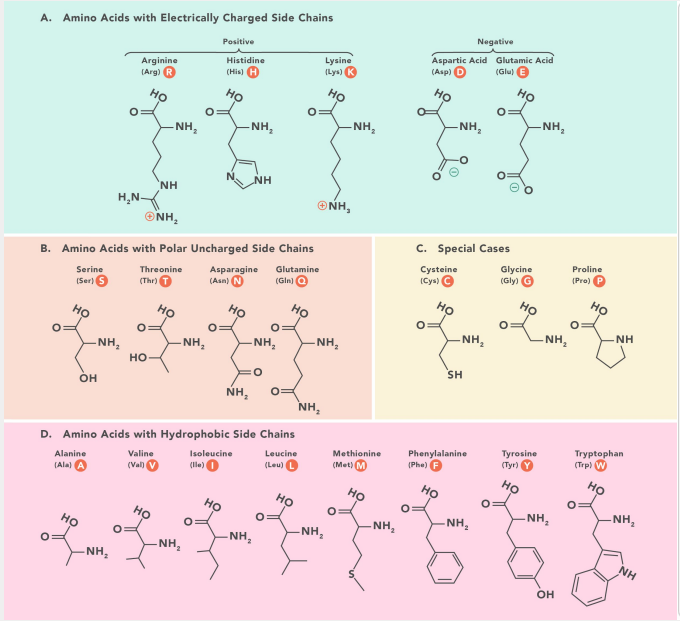

```
# load libraries
from gensim.models import
KeyedVectors
import numpy as np
import matplotlib.pyplot as plt
import umap
import pandas as pd
import seaborn as sns

# load word embeddings
word_vectors =
KeyedVectors.load_word2vec_format('pu
bmed2018_w2v_200D/pubmed2018_w2v_200D
.bin', binary=True)
```

RESULTS
PROOF OF CONCEPT



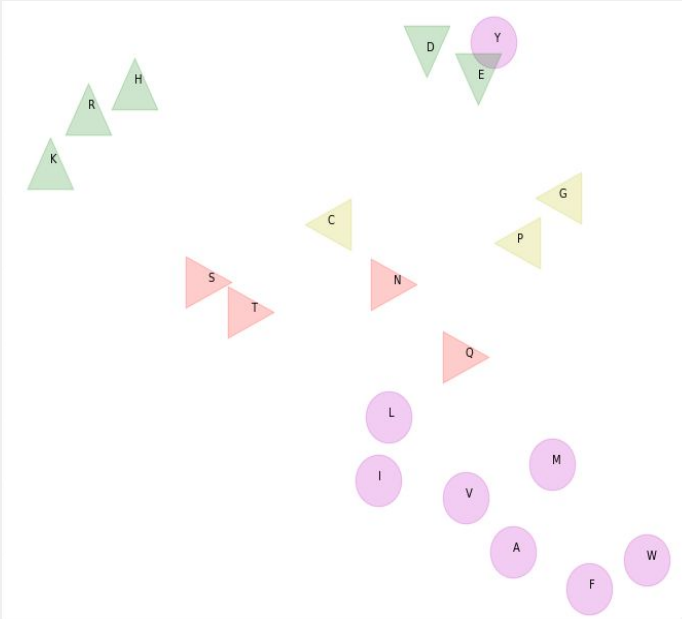

```
# 20 AMINO ACIDS to query and their properties
# define marker/shapes for each amino acid based off of proprty
aa = ['alanine', 'isoleucine', 'leucine', 'methionine',
      'valine', 'phenylalanine', 'tryptophan', 'tyrosine',
      'asparagine', 'cysteine', 'glutamine', 'serine',
      'threonine', 'aspartic-acid', 'glutamic-acid', 'arginine',
      'histidine', 'lysine', 'glycine', 'proline']

aa_properties = ['Hydrophobic', 'Hydrophobic', 'Hydrophobic', 'Hydrophobi
c',
                 'Hydrophobic', 'Hydrophobic', 'Hydrophobic', 'Hydrophobic',
                 'Polar', 'Special', 'Polar', 'Polar',
                 'Polar', 'Negative', 'Negative', 'Positive',
                 'Positive', 'Positive', 'Special', 'Special']

aa_short = ['A', 'I', 'L', 'M', 'V', 'F', 'W', 'Y',
            'N', 'C', 'Q', 'S', 'T', 'D', 'E', 'R',
            'H', 'K', 'G', 'P']

m = ['>', '<', '^', 'v', 'o']

cmap_dict = {'Polar': 'r',
             'Special': 'y',
             'Positive': 'g',
             'Negative': 'g',
             'Hydrophobic': 'm'}

m_dict = {'Positive': '^',
          'Negative': 'v',
          'Polar': '>',
          'Special': '<',
          'Hydrophobic': 'o'}
```

RESULTS
PROOF OF CONCEPT




```
# query each amino acid from loaded word2vec model
aa_vec = []
for i in aa:
        aa_vec.append(word_vectors[i])
aa_vec = np.array(aa_vec)

# reduce dimenions of the 200 dimension vector
umap_embed = umap.UMAP(n_neighbors=3, min_dist=0.01, random_state=42).fit_t
ransform(aa_vec)
df = pd.DataFrame([aa, aa_properties, aa_short, umap_embed[:,0], umap_embed
[:,1]]).T

# plot reduced dimensions
fig, ax = plt.subplots(figsize=(12,10))
for k, row in df.iterrows():
    ax.scatter(float(row[3]), float(row[4]), marker=m_dict[row[1]], c=cmap_
dict[row[1]], s=2000, alpha=0.2)

for i, txt in enumerate(df[2]):
    ax.annotate(txt, (umap_embed[i,0],umap_embed[i,1]))

plt.ylabel('UMAP 2', fontsize=15)
plt.xlabel('UMAP 1', fontsize=15)
```

RESULTS
PROOF OF CONCEPT




```
# query each amino acid from loaded word2vec model
aa_vec = []
for i in aa:
        aa_vec.append(word_vectors[i])
aa_vec = np.array(aa_vec)

# reduce dimenions of the 200 dimension vector
umap_embed = umap.UMAP(n_neighbors=3, min_dist=0.01, random_state=42).fit_t
ransform(aa_vec)
df = pd.DataFrame([aa, aa_properties, aa_short, umap_embed[:,0], umap_embed
[:,1]]).T

# plot reduced dimensions
fig, ax = plt.subplots(figsize=(12,10))
for k, row in df.iterrows():
    ax.scatter(float(row[3]), float(row[4]), marker=m_dict[row[1]], c=cmap_
dict[row[1]], s=2000, alpha=0.2)

for i, txt in enumerate(df[2]):
    ax.annotate(txt, (umap_embed[i,0],umap_embed[i,1]))

plt.ylabel('UMAP 2', fontsize=15)
plt.xlabel('UMAP 1', fontsize=15)
```

RESULTS
DEMONSTRATION

LOADING Libraries scRNA-seq data
gene2vec scores

```
# load libraries
import pickle
import umap
import umap.plot
import
matplotlib.pyplot as
plt
import numpy as np
import os
import scipy.io
import scanpy as sc
from scipy import
sparse
import pandas as pd

# import helper utils
for data-analysis
import utils
```

```
# load 10x datasets
data_path = '/Users/sjwu/nlp_CellMarkers/garnett/'
expr = scipy.io.mmread(os.path.join(data_path,
"matrix.mtx.gz"))
expr = expr.tocsr()

# load features and barcodes
pdata =
pd.read_csv(os.path.join(data_path,"barcodes.tsv"),
sep='\t')
fdata =
pd.read_csv(os.path.join(data_path,"genes.tsv"),
sep='\t')
N = expr.shape[0]

# downsample our data to avoid bias
idx_sample = utils.downsample(pdata)
expr_ds = expr[:, idx_sample]
pdata_ds = pdata.loc[idx_sample, :]
```

RESULTS
DEMONSTRATION

LOADING
Libraries
scRNA-seq
data
gene2vec
scores

```
# Load scores from gene2vec
with open('w2v_pbmc_m2vparams.scores', 'rb') as file:
    data = pickle.load(file)

# format data
data = utils.format_data(data, fdata)

# update keys to match ground_truth cell type label
data_update = {}
data_update['b_cells'] = data['325472302_b_lymphocytes']
data_update['cd14_monoctyes'] = data['325470302_monocytes']
data_update['cd34'] = data['cd34']
data_update['cd56_nk'] = data['nk_cell']
data_update['regulatory'] = data['treg']
data = data_update
del data_update

# update fdata with similarity scores
fdata = utils.update_fdata(fdata, data)

# print each datastructure to visualize what it looks like
print(fdata.head())
print(pdata_ds.head())
```

	ensembl	gene_id	b_cells	cd14_monoctyes	cd34	cd56_nk	\
0	ENSG00000243485	MIR1302-10	0.0	0.0	0.0	0.0	
1	ENSG00000237613	FAM138A	0.0	0.0	0.0	0.0	
2	ENSG00000186092	OR4F5	0.0	0.0	0.0	0.0	
3	ENSG00000238009	RP11-34P13.7	0.0	0.0	0.0	0.0	
4	ENSG00000239945	RP11-34P13.8	0.0	0.0	0.0	0.0	

	regulatory
0	0.0
1	0.0
2	0.0
3	0.0
4	0.0

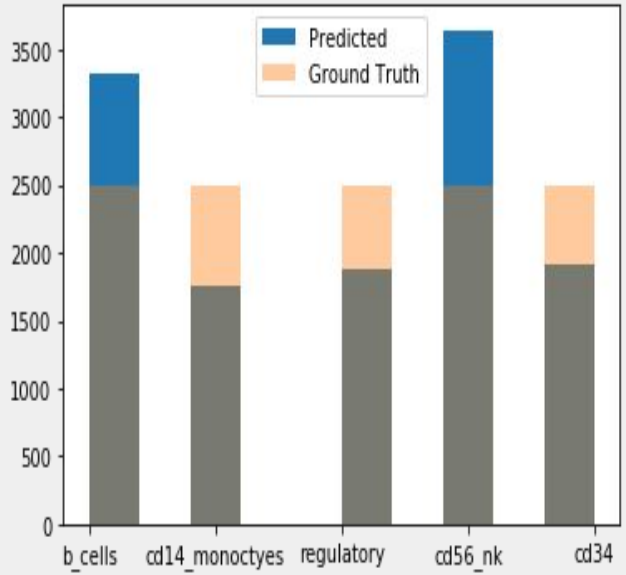
	barcode	celltype
5259	CTGTATACCCCAAA_1	b_cells
8860	TCGACCTGTATGGC_1	b_cells
3671	CATCAGGACGGAGA_1	b_cells
1300	ACTCAGGATCGCAA_1	b_cells
5264	CTGTGAGAGGTTTG_1	b_cells

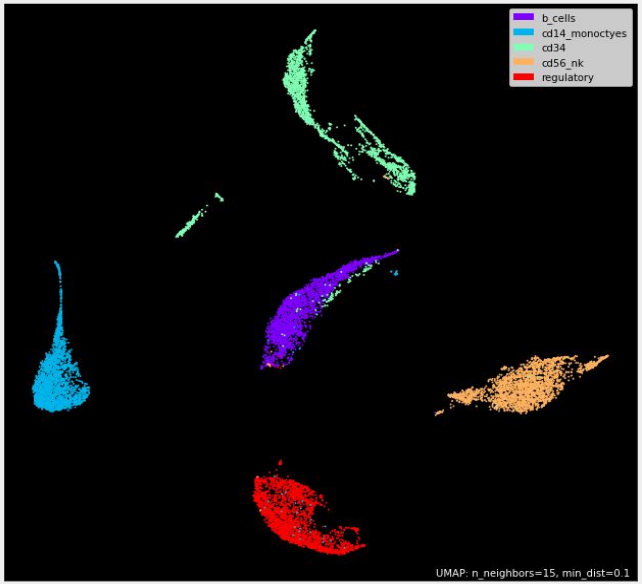
RESULTS
DEMONSTRATION

CLASSIFYING INDIVIDUAL CELLS

```
# generate a dictionary to map celltypes to index assignments
celltypes = ['b_cells', 'cd14_monoctyes', 'cd34', 'cd56_nk', 'regulatory']
ct_map = dict(zip([i for i in range(len(celltypes))], celltypes))

# normalize our scores from gene2vec
# Upweight higher ranked genes by taking the exponential of the scores.
arr_data = np.array(adata.var[celltypes])
arr_data = (1e5**(arr_data)-1)
arr_data = arr_data/np.sum(arr_data, axis=0)*1000
arr_data_sprse = sparse.csr_matrix(arr_data)

# calculate scores by dot product
scores = tfidf.dot(arr_data_sprse).argmax(axis=1)
scores = np.array(scores).squeeze()

# compute accuracy
acc = utils.accuracy_score([ct_map[i] for i in scores], adata.obs['celltype'])
print("A naive classification approach of single cells from scRNA-seq data yields:", acc)
```

RESULTS
DEMONSTRATION

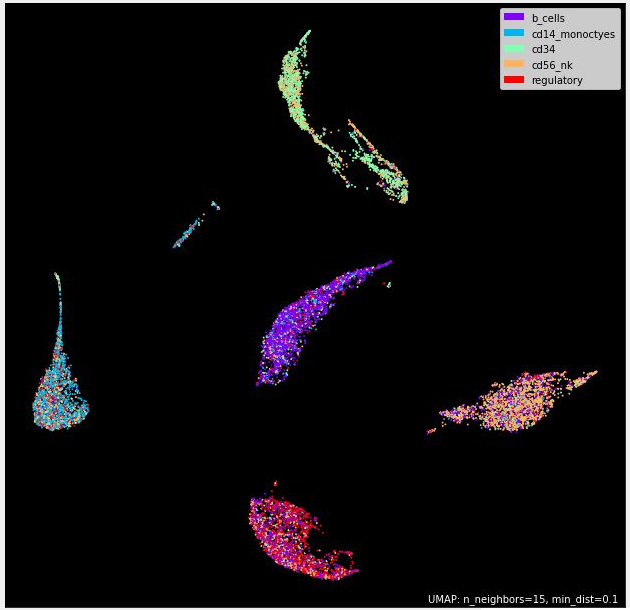


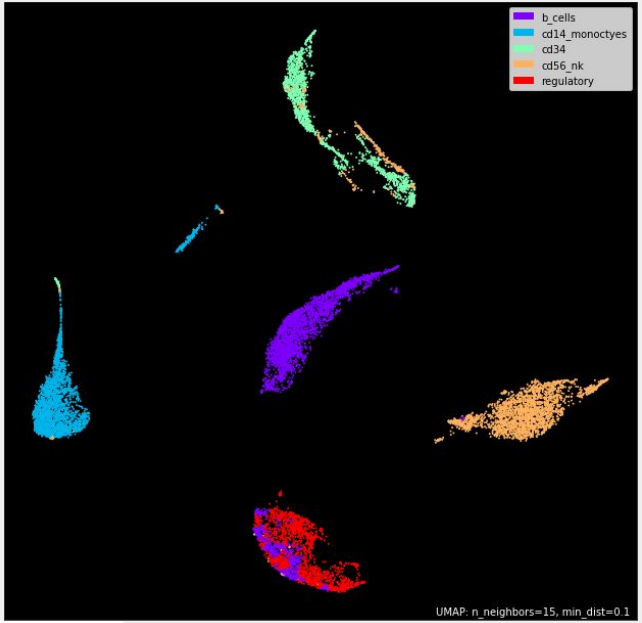


VISUALISATION

RESULTS
DEMONSTRATION

VISUALISATION





DISCUSSION
FUTURE DIRECTIONS

- Improved User Interface (Website? App?)
- Download data on SQL
- Implement the actual BERN algorithm

Thank you!