BroadProject

November 9, 2022

1 Broad Institute Project

1.1 Goals

- Generate a PCA value table for each sample from the call set
- Classify samples with missing ancestry labels
- Visualize PC values for each sample w/ labels for known and predicted classifications

1.1.1 Initial Filtering

- high callrate (95%)
- bi-allelic only (no haplotypes)
- common alleles (allele freq. > 0.01)
- linkage disequilibrium pruned to r2 < 0.1 (allelic independence)
- normalize genotypes after filtering

[3]:
```
# import libraries
import os
import numpy as np
import scipy
import pandas as pd
import matplotlib as mpl
import matplotlib.pyplot as plt
%matplotlib inline
import seaborn as sns
sns.set_style('white')
sns.set_style('ticks')
sns.set_context('notebook')

# hail packages
import hail as hl
hl.init(min_block_size=128)
from hail.plot import show
from pprint import pprint
import bokeh
from bokeh.io import output_notebook, show
hl.plot.output_notebook()
```

```
2022-04-06 13:26:06 WARN  Utils:69 - Your hostname, Jakes-MacBook-Air.local
```

```
resolves to a loopback address: 127.0.0.1; using 192.168.0.12 instead (on
interface en0)
2022-04-06 13:26:06 WARN  Utils:69 - Set SPARK_LOCAL_IP if you need to bind to
another address

WARNING: An illegal reflective access operation has occurred
WARNING: Illegal reflective access by org.apache.spark.unsafe.Platform
(file:/Users/jakeharris/opt/anaconda3/lib/python3.8/site-
packages/pyspark/jars/spark-unsafe_2.12-3.1.3.jar) to constructor
java.nio.DirectByteBuffer(long,int)
WARNING: Please consider reporting this to the maintainers of
org.apache.spark.unsafe.Platform
WARNING: Use --illegal-access=warn to enable warnings of further illegal
reflective access operations
WARNING: All illegal access operations will be denied in a future release

2022-04-06 13:26:07 WARN  NativeCodeLoader:60 - Unable to load native-hadoop
library for your platform… using builtin-java classes where applicable

Setting default log level to "WARN".
To adjust logging level use sc.setLogLevel(newLevel). For SparkR, use
setLogLevel(newLevel).

2022-04-06 13:26:07 WARN  Hail:43 - This Hail JAR was compiled for Spark 3.1.2,
running with Spark 3.1.3.
  Compatibility is not guaranteed.

Running on Apache Spark version 3.1.3
SparkUI available at http://192.168.0.12:4040
Welcome to
     __  __     <>__
    / /_/ /__  __/ /
   / __  / _ `/ / /
  /_/ /_/\_,_/_/_/   version 0.2.91-44b441376f9a
LOGGING: writing to /Users/jakeharris/Desktop/BroadProject/hail-20220406-1326-0.
2.91-44b441376f9a.log
```

[4]:
```
# Set working directory
print('Current wd:', os.getcwd())
desktop_dir = os.path.join('/Users', 'jakeharris', 'Desktop', 'BroadProject')
os.chdir(desktop_dir)
print('New wd:', os.getcwd())
```

```
Current wd: /Users/jakeharris/Desktop/BroadProject
New wd: /Users/jakeharris/Desktop/BroadProject
```

[3]:
```
# Run initial filter w/ VCFtools
    ## minor allele freq. >0.01
    ## bi-allelic only
    ## quality score >5
```

```
    ## max. allowable missing data < 0.1
!vcftools --gzvcf acs_mini_project.vcf.bgz --max-missing 0.9 --maf 0.01␣
 ↪--min-alleles 2 --max-alleles 2 \
--minQ 5 --recode --recode-INFO-all --out initial-vcf-filter
```

```
VCFtools - 0.1.16
(C) Adam Auton and Anthony Marcketta 2009

Parameters as interpreted:
        --gzvcf acs_mini_project.vcf.bgz
        --recode-INFO-all
        --maf 0.01
        --max-alleles 2
        --min-alleles 2
        --minQ 5
        --max-missing 0.9
        --out initial-vcf-filter
        --recode

Using zlib version: 1.2.11
After filtering, kept 1966 out of 1966 Individuals
Outputting VCF file…
After filtering, kept 92402 out of a possible 2203614 Sites
Run Time = 396.00 seconds
```

[4]:
```
# LD variant pruning for r2 < 0.1
    ## window size 50
    ## step size 5 variant ct
    ## r2 threshold < 0.1
!plink --vcf initial-vcf-filter.recode.vcf --indep-pairwise 50 5 0.1
!plink --vcf initial-vcf-filter.recode.vcf --extract plink.prune.in --make-bed␣
 ↪--out pruned-plink2
```

```
PLINK v1.90b6.21 64-bit (19 Oct 2020)          www.cog-genomics.org/plink/1.9/
(C) 2005-2020 Shaun Purcell, Christopher Chang   GNU General Public License v3
Logging to plink.log.
Options in effect:
  --indep-pairwise 50 5 0.1
  --vcf initial-vcf-filter.recode.vcf

8192 MB RAM detected; reserving 4096 MB for main workspace.
--vcf: plink-temporary.bed + plink-temporary.bim + plink-temporary.fam written.
92402 variants loaded from .bim file.
1966 people (0 males, 0 females, 1966 ambiguous) loaded from .fam.
Ambiguous sex IDs written to plink.nosex .
Using 1 thread (no multithreaded calculations invoked).
Before main variant filters, 1966 founders and 0 nonfounders present.
```

```
Calculating allele frequencies… 10111213141516171819202122232425262728293031 32
33343536373839404142434445464748495051525354555657585960616263646566676869707172
73747576777879808182838485868788899091929394959697989 done.
Total genotyping rate is 0.993399.
92402 variants and 1966 people pass filters and QC.
Note: No phenotypes present.
Pruned 6067 variants from chromosome 1, leaving 4339.
Pruned 3046 variants from chromosome 2, leaving 2473.
Pruned 2716 variants from chromosome 3, leaving 2185.
Pruned 1700 variants from chromosome 4, leaving 1648.
Pruned 2092 variants from chromosome 5, leaving 1827.
Pruned 3272 variants from chromosome 6, leaving 2212.
Pruned 2130 variants from chromosome 7, leaving 1928.
Pruned 1389 variants from chromosome 8, leaving 1365.
Pruned 2080 variants from chromosome 9, leaving 1745.
Pruned 2067 variants from chromosome 10, leaving 1822.
Pruned 3555 variants from chromosome 11, leaving 2284.
Pruned 2871 variants from chromosome 12, leaving 2063.
Pruned 727 variants from chromosome 13, leaving 817.
Pruned 1539 variants from chromosome 14, leaving 1244.
Pruned 1650 variants from chromosome 15, leaving 1279.
Pruned 2171 variants from chromosome 16, leaving 1462.
Pruned 3440 variants from chromosome 17, leaving 2218.
Pruned 632 variants from chromosome 18, leaving 758.
Pruned 4361 variants from chromosome 19, leaving 2783.
Pruned 1519 variants from chromosome 20, leaving 1145.
Pruned 604 variants from chromosome 21, leaving 550.
Pruned 1283 variants from chromosome 22, leaving 934.
Pruned 1131 variants from chromosome 23, leaving 1151.
Pruned 86 variants from chromosome 26, leaving 42.
Pruning complete.  52128 of 92402 variants removed.
Marker lists written to plink.prune.in and plink.prune.out .
PLINK v1.90b6.21 64-bit (19 Oct 2020)          www.cog-genomics.org/plink/1.9/
(C) 2005-2020 Shaun Purcell, Christopher Chang   GNU General Public License v3
Logging to pruned-plink2.log.
Options in effect:
  --extract plink.prune.in
  --make-bed
  --out pruned-plink2
  --vcf initial-vcf-filter.recode.vcf

8192 MB RAM detected; reserving 4096 MB for main workspace.
--vcf: pruned-plink2-temporary.bed + pruned-plink2-temporary.bim +
pruned-plink2-temporary.fam written.
92402 variants loaded from .bim file.
1966 people (0 males, 0 females, 1966 ambiguous) loaded from .fam.
Ambiguous sex IDs written to pruned-plink2.nosex .
--extract: 41616 variants remaining.
```

```
Warning: At least 2441 duplicate IDs in --extract file.
Using 1 thread (no multithreaded calculations invoked).
Before main variant filters, 1966 founders and 0 nonfounders present.
Calculating allele frequencies… 10111213141516171819202122232425262728293031323334
3536373839404142434445464748495051525354555657585960616263646566676869707172
7374757677787980818283848586878889909192939495969798 done.
Total genotyping rate is 0.992634.
41616 variants and 1966 people pass filters and QC.
Note: No phenotypes present.
--make-bed to pruned-plink2.bed + pruned-plink2.bim + pruned-plink2.fam …
1011121314151617181920212223242526272829303132333435363738394041424344454647484
9505152535455565758596061626364656667686970717273747576777879808182838485868788
909192939495969798 99done.
```

[4]:
```
# import Plink table to hail
hl.import_plink(bed='pruned-plink2.bed',
                bim='pruned-plink2.bim',
                fam='pruned-plink2.fam').write('BroadProject-plink2.mt',␣
 ↪overwrite=True)

mt = hl.read_matrix_table('BroadProject-plink2.mt')
mt.describe()
mt.GT.show(5)  # first 5 genotype entries
mt.aggregate_entries(hl.agg.counter(mt.GT.n_alt_alleles()))  # count␣
 ↪alt_alleles in GT
```

```
2022-04-06 13:26:17 Hail: INFO: Found 1966 samples in fam file.
2022-04-06 13:26:17 Hail: INFO: Found 41616 variants in bim file.
2022-04-06 13:26:28 Hail: INFO: wrote matrix table with 41616 rows and 1966
columns in 2 partitions to BroadProject-plink2.mt

----------------------------------------
Global fields:
    None
----------------------------------------
Column fields:
    's': str
    'fam_id': str
    'pat_id': str
    'mat_id': str
    'is_female': bool
    'is_case': bool
----------------------------------------
Row fields:
    'locus': locus<GRCh37>
    'alleles': array<str>
    'rsid': str
    'cm_position': float64
```

```
----------------------------------------
Entry fields:
    'GT': call
----------------------------------------
Column key: ['s']
Row key: ['locus', 'alleles']
----------------------------------------

+---------------+------------+--------+--------+--------+--------+
| locus         | alleles    | '1'.GT | '2'.GT | '3'.GT | '4'.GT |
+---------------+------------+--------+--------+--------+--------+
| locus<GRCh37> | array<str> | call   | call   | call   | call   |
+---------------+------------+--------+--------+--------+--------+
| 1:894573      | ["A","G"]  | 0/0    | 0/1    | 1/1    | 0/1    |
| 1:898323      | ["C","T"]  | 0/0    | 0/0    | 0/0    | 0/0    |
| 1:898852      | ["C","T"]  | 0/0    | 0/0    | 0/0    | 0/0    |
| 1:908275      | ["G","A"]  | 0/0    | 0/0    | 0/0    | 0/0    |
| 1:908749      | ["C","T"]  | 0/0    | 0/0    | 0/0    | 0/0    |
+---------------+------------+--------+--------+--------+--------+
showing top 5 rows
showing the first 4 of 1966 columns
[Stage 4:>                                                          (0 + 2) / 2]
```

[4]:
```
frozendict({0: 67233428, 1: 11148119, 2: 2832868, None: 602641})
```

[5]:
```
# edit sample_id labels in ancestry.txt file
anc_df = pd.read_csv('acs_mini_project_labels.txt', header=0, sep='\t')
for i in range(len(anc_df['sample_id'])):
    anc_df['sample_id'][i] = str(anc_df['sample_id'][i].split('_')[1])  #␣
 ↪remove 'TGG_'
anc_df.to_csv('ancestry_labels_edit.tsv', header=True, index=None, sep='\t',␣
 ↪na_rep='NA')

# import ancestry labels .txt file as Hail table & join w/ MatrixTable
anc_table = hl.import_table('ancestry_labels_edit.tsv',
                            key='sample_id',
                            types={'sample_id': hl.tstr, 'ancestry': hl.tstr})
mt = mt.annotate_cols(anc = anc_table[mt.s].ancestry)  # join ancestry labels␣
 ↪to mt
mt.anc.show(5)
pprint(mt.aggregate_cols(hl.agg.counter(mt.anc)))  # count ancestry labels
```

```
2022-04-06 13:26:33 Hail: INFO: Reading table without type imputation
  Loading field 'sample_id' as type str (user-supplied)
  Loading field 'ancestry' as type str (user-supplied)

+-----+-------+
| s   | anc   |
```

```
+-----+-------+
| str | str   |
+-----+-------+
| "1" | NA    |
| "2" | NA    |
| "3" | "eas" |
| "4" | NA    |
| "5" | "eas" |
+-----+-------+
showing top 5 rows
```

```
frozendict({'afr': 382, 'amr': 155, 'eas': 253, 'fin': 58, 'nfe': 210, 'sas':
228, None: 680})
```

[6]:
```
# further QC filters to MatrixTable
mt = hl.sample_qc(mt, name='sample_qc')
mt = hl.variant_qc(mt, name='variant_qc')
mt = mt.filter_cols(mt.sample_qc.call_rate >= 0.95)  # callrate >95%
mt = mt.filter_rows(mt.variant_qc.AF[1] > 0.01)  # variants w/ allele freq. >0.
↪01
mt.GT.summarize()  # most missing GTs are filtered
```

```
[Stage 12:>                                                         (0 + 2) / 2]
```

```
81687300 records.

- GT (call):
           Non-missing: 81085755 (99.26%)
               Missing: 601545 (0.74%)
  Homozygous Reference: 67106816
          Heterozygous: 11146395
    Homozygous Variant: 2832544
                Ploidy: frozendict({2: 81085755})
                Phased: frozendict({False: 81085755})
```

1.1.2 PCA

[7]:
```
# run Hardy-Weinberg normalized PCA on mt.GT (PCs=10) to reduce dimensionality
pca_eigen, pca_scores, _ = hl.hwe_normalized_pca(mt.GT)
pprint(pca_eigen)
pca_scores.show(5)
cumulative_pred = [sum(pca_eigen[0:i])/sum(pca_eigen) for i in range(1,11)]
```

```
2022-04-06 13:26:50 Hail: INFO: hwe_normalize: found 41550 variants after
filtering out monomorphic sites.
2022-04-06 13:26:53 Hail: INFO: pca: running PCA with 10 components… + 2) / 2]
[Stage 58:>                                                         (0 + 2) / 2]
```

```
[122.04221312954746,
```

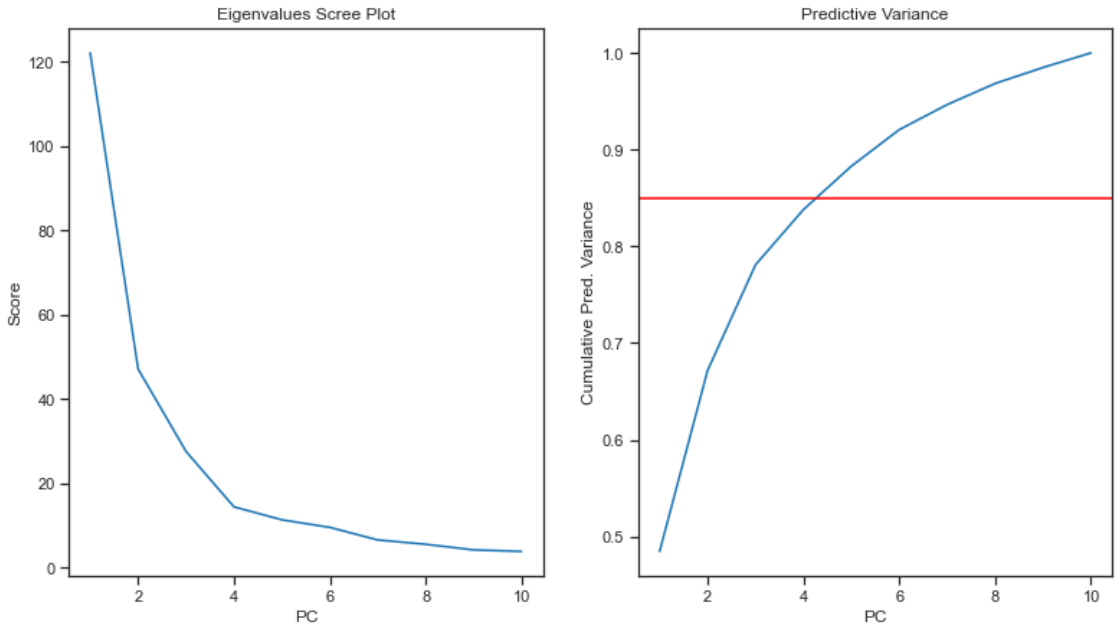
```
 47.0634740395591,
 27.502106042250052,
 14.368862825633087,
 11.301665907494064,
 9.499574336481622,
 6.523390529389579,
 5.492829804171036,
 4.160724102151552,
 3.803874125837476]
```

```
+--------+
| s      |
+--------+
| str    |
+--------+
| "1"    |
| "10"   |
| "100"  |
| "1000" |
| "1001" |
+--------+
```

```
+-----------------------------------------------------------------------------+
| scores                                                                      |
+-----------------------------------------------------------------------------+
| array<float64>                                                              |
+-----------------------------------------------------------------------------+
| [-1.09e-01,1.86e-01,3.79e-03,4.09e-02,7.29e-03,5.93e-02,-5.11e-02,2.15e-0… |
| [-1.36e-01,2.19e-01,2.42e-02,2.07e-02,1.53e-02,1.01e-01,-1.37e-02,1.59e-0… |
| [-1.36e-01,1.90e-01,5.92e-03,2.36e-02,2.58e-02,8.97e-02,-3.21e-03,1.20e-0… |
| [4.46e-01,-4.82e-02,1.15e-02,-9.48e-03,-4.91e-02,2.10e-02,-6.49e-03,-5.37… |
| [4.45e-01,-2.58e-02,-6.62e-03,2.64e-03,-1.06e-02,1.91e-02,2.66e-02,-1.06e… |
+-----------------------------------------------------------------------------+
showing top 5 rows
```

[8]:
```
# visualize for choosing num. of PCs
fig, (ax1, ax2) = plt.subplots(1,2, figsize=(13,7))
# scree plot
ax1.plot(range(1,11), pca_eigen)
ax1.set(xlabel='PC', ylabel='Score')
ax1.set_title('Eigenvalues Scree Plot')  # ~elbows at PC 4
ax1.plot()
# cumulative predictive variance
ax2.plot(range(1,11), cumulative_pred)
ax2.axhline(0.85, c='r')  # ~85% pred. variance at PC 4
ax2.set(xlabel='PC', ylabel='Cumulative Pred. Variance')
ax2.set_title('Predictive Variance')
ax2.plot()
```

[8]: []



[9]:
```
# convert PCA scores Table to pandas DF
scores_df = pca_scores.annotate(anc = anc_table[pca_scores.s].ancestry)  # add␣
 ↪ancestry labels
scores_df = scores_df.to_pandas()
scores_df['s'] = pd.to_numeric(scores_df['s'])
scores_df = scores_df.sort_values(by=['s']).reset_index(drop=True)
scores_df = scores_df.rename(columns={'s':'sample_id', 'anc':'ancestry'})

# split PCA scores lists into individual cols, join w/ scores_df
pc_cols = [f'PC{x}' for x in range(1,11)]
pca_df = pd.DataFrame(scores_df['scores'].tolist(), columns=pc_cols)
df = pd.concat([scores_df, pca_df], axis=1).drop('scores', axis=1)
df.head()
```

```
2022-04-06 13:28:22 Hail: INFO: Ordering unsorted dataset with network shuffle
2022-04-06 13:28:22 Hail: INFO: Ordering unsorted dataset with network shuffle
```

[9]:

	sample_id	ancestry	PC1	PC2	PC3	PC4	PC5	\
0	1	<NA>	-0.108950	0.185796	0.003794	0.040872	0.007293	
1	2	<NA>	-0.099430	0.167728	-0.008247	0.049278	-0.003240	
2	3	eas	-0.162769	-0.180516	-0.166356	0.031430	0.077520	
3	4	<NA>	-0.164679	-0.174732	-0.161684	0.037865	0.070457	
4	5	eas	-0.162195	-0.183088	-0.167374	0.045454	0.086184	

	PC6	PC7	PC8	PC9	PC10

```
0  0.059343 -0.051051  0.021510 -0.004269  0.023797
1  0.037837 -0.047196  0.011902 -0.005860  0.026438
2  0.051509 -0.060998  0.021161  0.007530  0.017163
3  0.052421 -0.063559  0.009929  0.020001  0.000998
4  0.049309 -0.054672  0.003709  0.012089  0.014168
```

1.1.3 Classification

- Supervised machine learning based on known ancestry labels and PCA values
- K Nearest Neighbor algorithm
  - relatively simple
  - label unknown samples based on distance in PCA dimensions
  - more accurate than Decision Tree
  - works with multiclass unlike SVM
  - consider other methods if using larger dataset due to computational burden

[10]:
```
# classification of unknown ancestry labels using KNN
from sklearn.neighbors import KNeighborsClassifier
from sklearn import metrics, preprocessing
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split

# split df based on known/unknown ancestry
known_df = df[~df['ancestry'].isna()]
known_df['predicted'] = False  # col. indicating anc. labels are already known
nan_df = df[df['ancestry'].isna()]
nan_df['predicted'] = True

# create instance of LabelEncoder to make numeric labels for ancestry
le = preprocessing.LabelEncoder()
anc_le = le.fit_transform(known_df['ancestry'])  # 6 anc. labels
lab = le.inverse_transform(anc_le)

# create features list of PCs 1-4
pc_features = list(zip(known_df['PC1'], known_df['PC2'], known_df['PC3'],␣
 ↪known_df['PC4']))
pprint(pc_features[:3])
```

```
[(-0.16276923591903478,
  -0.18051633198345443,
  -0.16635592774861477,
  0.03143020705319569),
 (-0.16219522188037347,
  -0.18308768876730674,
  -0.1673736731102984,
  0.04545390510526709),
 (-0.13615261077238494,
  0.22742118703088465,
```

```
  0.022659940859158748,
  0.012263961985858836)]
```

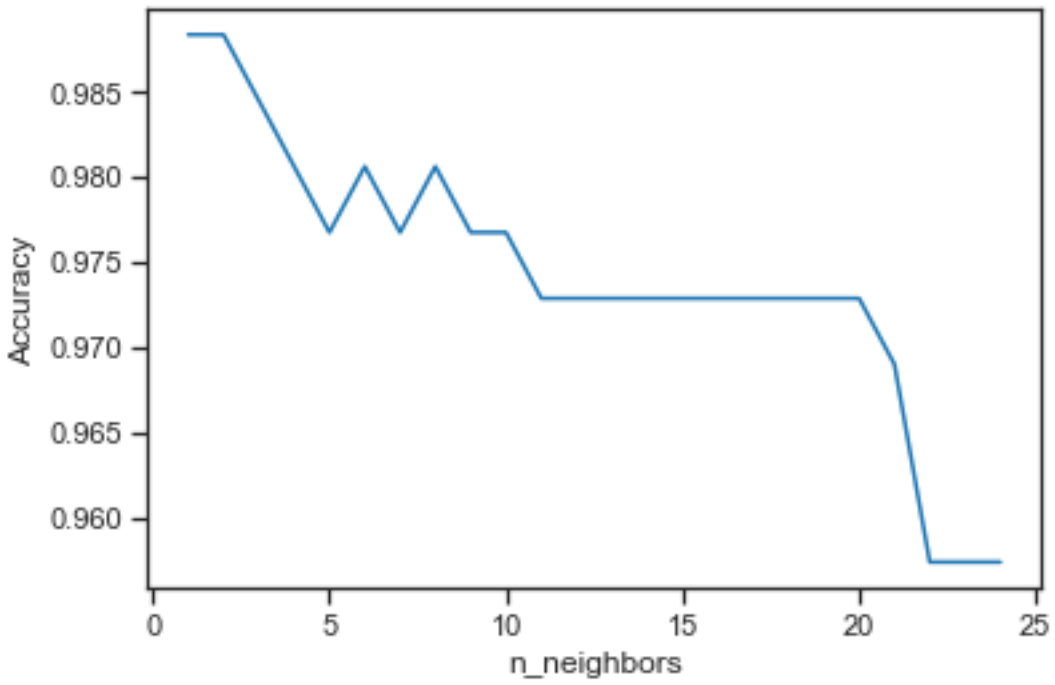
```
/var/folders/3v/3dcdttlj2xdgr3jcgn0mdt040000gn/T/ipykernel_1441/3704569124.py:9:
SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  known_df['predicted'] = False  # col. indicating anc. labels are already known
/var/folders/3v/3dcdttlj2xdgr3jcgn0mdt040000gn/T/ipykernel_1441/3704569124.py:11
: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  nan_df['predicted'] = True
```

[11]:
```
# train/test data for supervised learning (80% train/20% test split)
X_train, X_test, y_train, y_test = train_test_split(pc_features, anc_le,␣
 ↪test_size=0.2, random_state=4)

# run multiple KNN classifications to check for optimal n_neighbors
acc_scores = {}
for k in range(1,25):
    classifier = KNeighborsClassifier(n_neighbors=k)
    classifier.fit(X_train, y_train)
    y_pred = classifier.predict(X_test)
    acc_scores[k] = metrics.accuracy_score(y_test, y_pred)
pprint(acc_scores)

# plot of accuracy of k-neighbors -> k=3 is good choice because not even num,␣
 ↪high accuracy
plt.plot(range(1,25), acc_scores.values())
plt.xlabel('n_neighbors')
plt.ylabel('Accuracy')
```

```
{1: 0.9883720930232558,
 2: 0.9883720930232558,
 3: 0.9844961240310077,
 4: 0.9806201550387597,
 5: 0.9767441860465116,
 6: 0.9806201550387597,
 7: 0.9767441860465116,
 8: 0.9806201550387597,
 9: 0.9767441860465116,
```

```
10: 0.9767441860465116,
11: 0.9728682170542635,
12: 0.9728682170542635,
13: 0.9728682170542635,
14: 0.9728682170542635,
15: 0.9728682170542635,
16: 0.9728682170542635,
17: 0.9728682170542635,
18: 0.9728682170542635,
19: 0.9728682170542635,
20: 0.9728682170542635,
21: 0.9689922480620154,
22: 0.9573643410852714,
23: 0.9573643410852714,
24: 0.9573643410852714}
```

[11]:
```
Text(0, 0.5, 'Accuracy')
```



[12]:
```
# classify unknown ancestry samples in nan_df using kNN model
classifier = KNeighborsClassifier(n_neighbors=3)
classifier.fit(X_train, y_train)
anc_classes = {0: 'afr', 1: 'amr', 2: 'eas', 3: 'fin', 4: 'nfe', 5: 'sas'}
X_unknown = list(zip(nan_df['PC1'], nan_df['PC2'], nan_df['PC3'],␣
 ↪nan_df['PC4']))  # PC values
```

```
anc_predict = classifier.predict(X_unknown)  # list of pred. anc_class.keys()

# predict ancestries, add to nan_df
anc_list = []
for i in range(len(anc_predict)):
    anc_list.append(anc_classes[anc_predict[i]])
nan_df['ancestry'] = anc_list
nan_df.head()
```

```
/var/folders/3v/3dcdttlj2xdgr3jcgn0mdt040000gn/T/ipykernel_1441/2179299177.py:12
: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  nan_df['ancestry'] = anc_list
```

[12]:

	sample_id	ancestry	PC1	PC2	PC3	PC4	PC5	\
0	1	amr	-0.108950	0.185796	0.003794	0.040872	0.007293	
1	2	amr	-0.099430	0.167728	-0.008247	0.049278	-0.003240	
3	4	eas	-0.164679	-0.174732	-0.161684	0.037865	0.070457	
5	6	nfe	-0.182688	0.153385	0.286218	0.016470	0.214450	
10	11	nfe	-0.133551	0.205124	0.028771	0.019358	0.013979	

	PC6	PC7	PC8	PC9	PC10	predicted
0	0.059343	-0.051051	0.021510	-0.004269	0.023797	True
1	0.037837	-0.047196	0.011902	-0.005860	0.026438	True
3	0.052421	-0.063559	0.009929	0.020001	0.000998	True
5	-0.178499	-0.067623	0.083320	-0.028691	-0.064241	True
10	0.105923	-0.013851	0.002123	0.000936	-0.032794	True

[13]:
```
# concat known_df w/ nan_df, save to .csv
final_df = pd.concat([known_df, nan_df])
final_df = final_df.sort_values(by=['sample_id']).reset_index(drop=True)
final_df.to_csv('BroadProject_PCvalues.csv')  # save to .csv
final_df.head()
```

[13]:

	sample_id	ancestry	PC1	PC2	PC3	PC4	PC5	\
0	1	amr	-0.108950	0.185796	0.003794	0.040872	0.007293	
1	2	amr	-0.099430	0.167728	-0.008247	0.049278	-0.003240	
2	3	eas	-0.162769	-0.180516	-0.166356	0.031430	0.077520	
3	4	eas	-0.164679	-0.174732	-0.161684	0.037865	0.070457	
4	5	eas	-0.162195	-0.183088	-0.167374	0.045454	0.086184	

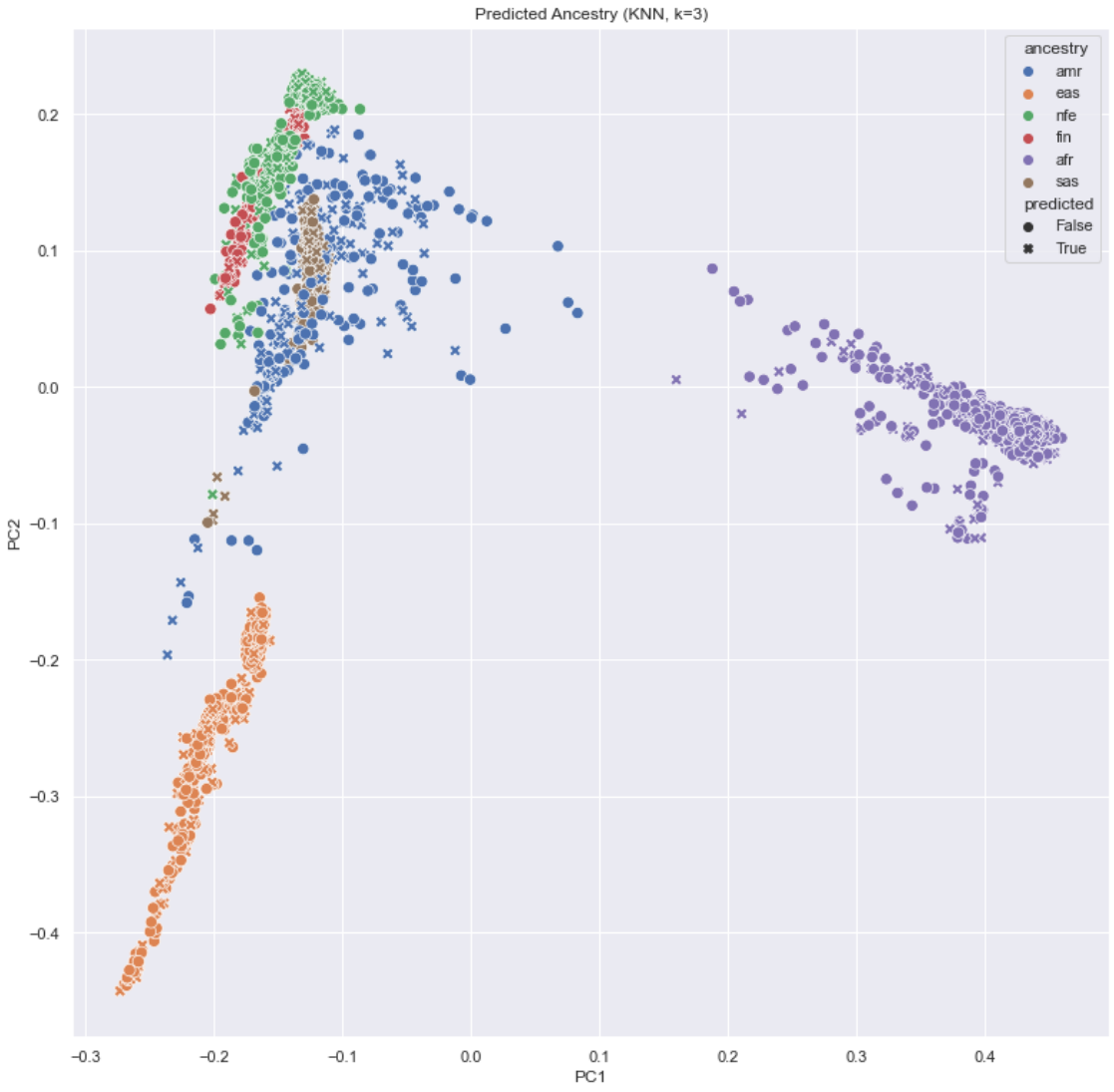
	PC6	PC7	PC8	PC9	PC10	predicted
0	0.059343	-0.051051	0.021510	-0.004269	0.023797	True
1	0.037837	-0.047196	0.011902	-0.005860	0.026438	True

```
2  0.051509 -0.060998  0.021161  0.007530  0.017163      False
3  0.052421 -0.063559  0.009929  0.020001  0.000998       True
4  0.049309 -0.054672  0.003709  0.012089  0.014168      False
```

1.1.4 Visualization

[14]:
```
# scatterplot of PCA values of known/predicted sample ancestry labels
sns.set(rc={'figure.figsize':(13,13)})
anc_plot = sns.scatterplot(data=final_df, x='PC1', y='PC2',
                           hue='ancestry', style='predicted',
                           s=70).set(title='Predicted Ancestry (KNN, k=3)',)
anc_plot
```

[14]:
```
[Text(0.5, 1.0, 'Predicted Ancestry (KNN, k=3)')]
```



[32]:
```
# 3D scatterplot
import plotly.express as px
fig = px.scatter_3d(final_df, x=final_df['PC1'], y=final_df['PC2'],␣
 ↪z=final_df['PC3'],
                    color=final_df['ancestry'], opacity=0.7, size_max=1)
fig.update_layout(margin=dict(l=100, r=100, t=20, b=20))
fig.update_traces(marker=dict(size=3))
fig.show()
```