

Mahdi_Anvari.compG_HW2

May 3, 2025

1 Computational Genomics - HW2

To identify five SNPs with significant allele frequency (AF) differences between two ethnic groups—while minimizing the risk of linkage disequilibrium (LD)—I plan to extract one SNP from each of five distinct genes. To achieve this, I first explored various genomic resources to select genes known for high population-specific variation. These genes will then be examined using the Iranome database to identify suitable SNPs.

```
[59]: GENE_LIST = {"G6PD": "https://www.iranome.com/gene/ENSG00000160211",
                  "LCT": "https://www.iranome.com/gene/ENSG00000115850",
                  "ABO": "https://www.iranome.com/gene/ENSG00000175164",
                  "CYP2D6": "https://www.iranome.com/gene/ENSG00000100197",
                  "HLA-B": "https://www.iranome.com/gene/ENSG00000234745"}
```

HLA-B: Highly polymorphic immune gene with strong ethnic differentiation.

CYP2D6: Key gene in drug metabolism, known for copy number and allele variability across populations.

LCT: Associated with lactase persistence; exhibits clear ancestral selection signals.

ABO: Determines blood type; shows distinct allele frequency patterns among populations.

G6PD: Enzyme gene with variants common in certain regions due to malaria-driven selection.

```
[60]: import pandas as pd
pd.DataFrame({
    "Gene_Name": ["HLA-B", "CYP2D6", "LCT", "ABO", "G6PD"],
    "SNP_Count": [449, 255, 568, 484, 145]
})
```

```
[60]:
```

	Gene_Name	SNP_Count
0	HLA-B	449
1	CYP2D6	255
2	LCT	568
3	ABO	484
4	G6PD	145

Manually checking each SNP within the selected genes is not feasible. Therefore, I used an automated approach with Selenium to extract all available SNPs for each gene from the Iranome

database. After gathering the data, I will apply several criteria to identify the most suitable SNP for each gene.

```
[61]: gene_variants = {"HLA-B": [],
                        "CYP2D6": [],
                        "LCT": [],
                        "ABO": [],
                        "G6PD": []}
```

```
[62]: gene_variants
```

```
[62]: {'HLA-B': [], 'CYP2D6': [], 'LCT': [], 'ABO': [], 'G6PD': []}
```

```
[7]: from selenium import webdriver
from selenium.webdriver.edge.service import Service
from selenium.webdriver.common.by import By
from selenium.webdriver.common.keys import Keys
from selenium.webdriver.support.ui import WebDriverWait
from selenium.webdriver.support import expected_conditions as EC
import time
import re
import pandas as pd
import warnings
warnings.filterwarnings("ignore")
```

```
[64]: options = webdriver.EdgeOptions()
options.add_argument("start-maximized")
service = Service()
driver = webdriver.Edge(service=service, options=options)

for gene_name in GENE_LIST:
    print(f"{gene_name} variants:")
    try:
        url = GENE_LIST[gene_name]
        driver.get(url)
        WebDriverWait(driver, 15).until(
            EC.presence_of_element_located((By.CSS_SELECTOR, "table tbody tr"))
        )

        rows = driver.find_elements(By.CSS_SELECTOR, "table tbody tr")
        for i in range(len(rows)):
            rows = driver.find_elements(By.CSS_SELECTOR, "table tbody tr")
            link = rows[i].find_element(By.CSS_SELECTOR, "td:nth-child(1) a")
            href = link.get_attribute("href")
            link_text = link.text
            driver.get(href)
            print(f"Visited: {href}")
```

```

html = driver.page_source
tables = pd.read_html(html)

if tables:
    df = tables[0]
    if link_text not in gene_variants[gene_name]:
        gene_variants[gene_name].append(link_text)
        df.to_csv("db/" + gene_name + "/" + re.sub(r'[\<>:"/\\"|?*]', '_',
↪'_', link_text) + ".csv", index=False)
    else:
        print("No table found on the page.")

    time.sleep(3)
    driver.back()
    WebDriverWait(driver, 15).until(
        EC.presence_of_element_located((By.CSS_SELECTOR, "table tbody_
↪tr"))
    )

finally:
    print(f"Done with gene {gene_name}.")

driver.quit()

```

G6PD variants:

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Done with gene G6PD.

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Visited: <https://www.iranome.com/variant/6-31324955-C-T>
Done with gene HLA-B.

```
[66]: import json
      with open('gene_variants.json', 'w') as json_file:
          json.dump(gene_variants, json_file, indent=4)
```

Now that all SNP variants for each selected gene have been successfully extracted from Iranome using automated Selenium scripts, the next step is to conduct a meta-analysis to identify the most informative SNPs for distinguishing between two specific ethnic groups.

2 1)

2.0.1 SNP Selection Strategy: Focus on Arab and Zartoshti Populations

In this analysis, the focus is on the Arab and Zartoshti populations, which have distinct historical and genetic backgrounds. These differences make them suitable candidates for identifying population-specific allele frequency divergence. The objective is to select one representative SNP per gene that shows the greatest allele frequency difference between these two groups. To ensure meaningful and reliable results, the following criteria are applied during SNP selection:

1. Considerable Allele Frequency (AF) Difference Purpose: Select SNPs with the largest absolute difference in allele frequency between the Arab and Zartoshti groups. This is the primary selection criterion.

2. Minor Allele Frequency (MAF) > 0.1 Rationale: Ensures that the SNP is not ultra-rare and has enough variability to be informative.

Application: Discard SNPs where the alternative allele frequency is less than 10% in both Arab and Zartoshti groups.

3. Sufficient Sample Support Criteria: - Allele count > 10 in both groups - At least 50 genotyped individuals per group

Rationale: Ensures statistical robustness and avoids unreliable frequency estimates due to sparse data.

4. Presence of Heterozygotes Rationale: The existence of both homozygous and heterozygous genotypes increases flexibility for downstream modeling, especially when simulating heterozygous individuals.

Application: Prefer SNPs with non-zero heterozygote counts in both groups.

5. Biallelic SNPs Only Rationale: Simplifies probabilistic modeling and interpretation. Tri-allelic variants and indels may introduce unnecessary complexity.

Application: Exclude SNPs with more than two alleles or complex indel patterns.

6. Coverage Across All 12 Iranome Ethnic Groups Rationale: To enable comprehensive allele frequency analysis across all populations included in the study.

Application: Discard SNPs that lack allele frequency data for any of the 12 Iranome ethnic groups.

```
[72]: rows = [(gene, variant) for gene, variants in gene_variants.items() for variant_
    ↪in variants]
SNPs_df = pd.DataFrame(rows, columns=["Gene_Name", "Variant_Name"])
SNPs_df
```

```
[72]:
```

	Gene_Name	Variant_Name
0	HLA-B	6:31321657 G / A (rs3177747)
1	HLA-B	6:31321681 C / T (rs1058067)
2	HLA-B	6:31321685 A / C (rs1058026)
3	HLA-B	6:31321686 A / C (rs1049268)
4	HLA-B	6:31321694 A / G (rs878941341)
...
1896	G6PD	X:153775343 A / C (rs3021074)
1897	G6PD	X:153775360 A / C (rs1390716946,rs3021072)
1898	G6PD	X:153775365 C / A
1899	G6PD	X:153775421 G / T (rs185623633)
1900	G6PD	X:153775785 T / C (rs111827785)

[1901 rows x 2 columns]

```
[111]: SNPs_df.to_excel("SNPs_table.xlsx", index=False)
```

I begin the filtering process by applying the primary selection criterion: identifying SNPs that show the **maximum allele frequency (AF) difference** between Arab and Zartoshti populations.

This step narrows down the candidate SNPs per gene by selecting those with the most pronounced divergence between these two ethnic groups.

Other criteria (e.g., sample support, heterozygosity, biallelic status, full population coverage) will be manually evaluated in subsequent steps after narrowing the list using this primary filter.

```
[103]: SNPs_df = pd.read_excel("SNPs_table.xlsx")
```

```
[104]: pop1 = "Arab"
pop2 = "Zartoshti"
def extract_AF_difference(gene_name, variant_name):
    df = pd.read_csv("db/"+ gene_name + "/" + re.sub(r'[\<: "\/ \\\|?*\']', '_ ',
    ↪variant_name) + ".csv")
    AF_difference = float(df[df["Population"]==pop1]["Allele_
    ↪Frequency"])-float(df[df["Population"]==pop2]["Allele Frequency"])
    return abs(AF_difference)

def extract_AF_divergance(gene_name, variant_name):
    df = pd.read_csv("db/"+ gene_name + "/" + re.sub(r'[\<: "\/ \\\|?*\']', '_ ',
    ↪variant_name) + ".csv")
    AF1_divergance = float(df[df["Population"]==pop1]["Allele Frequency"])-0.5
    AF2_divergance = float(df[df["Population"]==pop2]["Allele Frequency"])-0.5
    result1 = abs(AF1_divergance - AF2_divergance)
    result2 = abs(AF1_divergance + AF2_divergance)
    return min([result1, result2])
```

```
[105]: SNPs_df["AF_difference"] = SNPs_df.apply(lambda row:
    ↪extract_AF_difference(row['Gene_Name'], row['Variant_Name']), axis=1)
```

Because we aim to estimate the fractional ancestry of a heterozygous individual, an additional criterion is needed to ensure that the selected SNPs are informative for such inference. For example, although a SNP with a large allele frequency difference between two populations (e.g., 0.8 in population 1 and 0.2 in population 2) may appear ideal at first glance, it is actually not informative for a heterozygous individual. This is because both populations strongly favor opposite homozygous genotypes, making the presence of a heterozygote equally unlikely in either group. To address this, I introduce a criterion called allele frequency divergence, which captures how far the allele frequencies in both populations deviate from 0.5. This balance ensures that the SNP can meaningfully contribute to distinguishing ancestry while still being consistent with the heterozygous genotype observed.

```
[106]: SNPs_df["AF_divergance"] = SNPs_df.apply(lambda row:
    ↪extract_AF_divergance(row['Gene_Name'], row['Variant_Name']), axis=1)
```

```
[107]: SNPs_sorted_df = SNPs_df.sort_values(by="AF_divergance", ascending=False)
```

```
[108]: SNPs_sorted_df
```

```
[108]:
```

	Gene_Name	Variant_Name	AF_difference	AF_divergance
1070	LCT	2:136578703 A / G (rs4954451)	0.30250	0.30250
1607	ABO	9:136140462 C / T (rs1633513)	0.28710	0.28710
804	LCT	2:136554797 T / C (rs6430588)	0.28370	0.28370
1706	ABO	9:136146920 T / G (rs663054)	0.27657	0.27657
742	LCT	2:136550806 G / C (rs2083190)	0.27390	0.27390
...
1784	G6PD	X:153762330 G / A (rs781917123)	0.00000	0.00000
1785	G6PD	X:153762467 G / A (rs917134021)	0.00000	0.00000
1786	G6PD	X:153762472 C / T (rs782036244)	0.00000	0.00000
1787	G6PD	X:153762517 C / T	0.00000	0.00000
559	CYP2D6	22:42524478 C / G	0.00000	0.00000

[1901 rows x 4 columns]

```
[109]: selected_variants = {}
for i in SNPs_sorted_df.index:
    if SNPs_sorted_df.loc[i]["Gene_Name"] not in selected_variants:
        selected_variants[SNPs_sorted_df.loc[i]["Gene_Name"]] = SNPs_sorted_df.
        ↪loc[i]["Variant_Name"]
```

```
[110]: selected_variants
```

```
[110]: {'LCT': '2:136578703 A / G (rs4954451)',
'ABO': '9:136140462 C / T (rs1633513)',
'HLA-B': '6:31324201 C / G (rs1071652)',
'CYP2D6': '22:42526049 C / G (rs1931826324,rs28371701)',
'G6PD': 'X:153775343 A / C (rs3021074)'}

```

These are my selected variants. Let's save their tables into another folder and check the other criteria manually.

```
[111]: selected_variants_DFs = []
for gene in selected_variants:
    df = pd.read_csv("db/" + gene + "/" + re.sub(r' [<>: "/ \ | ? * ]', '_ ',
    ↪selected_variants[gene]) + ".csv")
    selected_variants_DFs.append(df)
    df.to_csv("db/SELECTED_SNPS/" + re.sub(r' [<>: "/ \ | ? * ]', '_ ',
    ↪selected_variants[gene]) + ".csv")
```

```
[112]: print(selected_variants["LCT"], "table:")
selected_variants_DFs[0]
```

2:136578703 A / G (rs4954451) table:

```
[112]:
```

	Population	Allele Count	Allele Number	Number of Homozygotes \
0	Mazani	90	200	45

1	Zartoshti	86	200	42
2	Baloch	66	202	33
3	Persian Gulf Islander	58	200	29
4	Sistani	47	200	23
5	Gilaki	38	198	19
6	Azeri	34	200	17
7	Kurd	28	200	14
8	Arab	26	204	13
9	Persian	14	200	7
10	Turkmen	14	200	7
11	Lur	12	200	6
12	Total	513	2404	255

	Number of Heterozygotes	Homozygous Genotype Freq. \
0	0	0.450000
1	2	0.420000
2	0	0.326700
3	0	0.290000
4	1	0.230000
5	0	0.191900
6	0	0.170000
7	0	0.140000
8	0	0.127500
9	0	0.070000
10	0	0.070000
11	0	0.060000
12	3	0.212146

	Heterozygous Genotype Freq.	Allele Frequency
0	0.000000	0.4500
1	0.020000	0.4300
2	0.000000	0.3267
3	0.000000	0.2900
4	0.010000	0.2350
5	0.000000	0.1919
6	0.000000	0.1700
7	0.000000	0.1400
8	0.000000	0.1275
9	0.000000	0.0700
10	0.000000	0.0700
11	0.000000	0.0600
12	0.002496	0.2134

```
[113]: print(selected_variants["ABO"], "table:")
selected_variants_DF[1]
```

9:136140462 C / T (rs1633513) table:

```
[113]:
```

	Population	Allele Count	Allele Number	Number of Homozygotes \
0	Zartoshti	78	200	38
1	Persian Gulf Islander	60	200	28
2	Mazani	56	200	27
3	Baloch	41	202	19
4	Sistani	26	200	12
5	Arab	21	204	10
6	Gilaki	20	198	10
7	Azeri	16	200	8
8	Turkmen	16	200	8
9	Lur	15	200	7
10	Kurd	8	200	4
11	Persian	6	200	3
12	Total	363	2404	174

	Number of Heterozygotes	Homozygous Genotype Freq. \
0	2	0.380000
1	4	0.280000
2	2	0.270000
3	3	0.188100
4	2	0.120000
5	1	0.098000
6	0	0.101000
7	0	0.080000
8	0	0.080000
9	1	0.070000
10	0	0.040000
11	0	0.030000
12	15	0.144759

	Heterozygous Genotype Freq.	Allele Frequency
0	0.020000	0.3900
1	0.040000	0.3000
2	0.020000	0.2800
3	0.029700	0.2030
4	0.020000	0.1300
5	0.009800	0.1029
6	0.000000	0.1010
7	0.000000	0.0800
8	0.000000	0.0800
9	0.010000	0.0750
10	0.000000	0.0400
11	0.000000	0.0300
12	0.012479	0.1510

```
[114]: print(selected_variants["CYP2D6"], "table:")
selected_variants_DFs[2]
```


22:42526049 C / G (rs1931826324,rs28371701) table:

[114]:

	Population	Allele Count	Allele Number	Number of Homozygotes \
0	Persian	84	200	27
1	Gilaki	83	198	28
2	Kurd	82	200	22
3	Zartoshti	81	200	22
4	Mazani	80	200	25
5	Lur	74	200	22
6	Persian Gulf Islander	73	200	20
7	Turkmen	72	200	26
8	Azeri	61	200	12
9	Baloch	58	202	9
10	Sistani	57	200	11
11	Arab	42	204	8
12	Total	847	2404	232

	Number of Heterozygotes	Homozygous Genotype Freq. \
0	30	0.270000
1	27	0.282800
2	38	0.220000
3	37	0.220000
4	30	0.250000
5	30	0.220000
6	33	0.200000
7	20	0.260000
8	37	0.120000
9	40	0.089100
10	35	0.110000
11	26	0.078400
12	383	0.193012

	Heterozygous Genotype Freq.	Allele Frequency
0	0.300000	0.4200
1	0.272700	0.4192
2	0.380000	0.4100
3	0.370000	0.4050
4	0.300000	0.4000
5	0.300000	0.3700
6	0.330000	0.3650
7	0.200000	0.3600
8	0.370000	0.3050
9	0.396000	0.2871
10	0.350000	0.2850
11	0.254900	0.2059
12	0.318636	0.3523

```
[115]: print(selected_variants["HLA-B"], "table:")
selected_variants_DFs[3]
```

6:31324201 C / G (rs1071652) table:

```
[115]:
```

	Population	Allele Count	Allele Number	Number of Homozygotes \
0	Baloch	73	202	29
1	Zartoshti	69	200	24
2	Mazani	68	200	24
3	Persian Gulf Islander	66	200	26
4	Sistani	64	200	22
5	Kurd	44	200	18
6	Arab	32	204	15
7	Azeri	31	200	14
8	Gilaki	30	198	14
9	Lur	16	200	6
10	Turkmen	8	200	3
11	Persian	7	200	3
12	Total	508	2404	198

	Number of Heterozygotes	Homozygous Genotype Freq. \
0	15	0.287100
1	21	0.240000
2	20	0.240000
3	14	0.260000
4	20	0.220000
5	8	0.180000
6	2	0.147100
7	3	0.140000
8	2	0.141400
9	4	0.060000
10	2	0.030000
11	1	0.030000
12	112	0.164725

	Heterozygous Genotype Freq.	Allele Frequency
0	0.148500	0.3614
1	0.210000	0.3450
2	0.200000	0.3400
3	0.140000	0.3300
4	0.200000	0.3200
5	0.080000	0.2200
6	0.019600	0.1569
7	0.030000	0.1550
8	0.020200	0.1515
9	0.040000	0.0800
10	0.020000	0.0400

11	0.010000	0.0350
12	0.093178	0.2113

```
[116]: print(selected_variants["G6PD"], "table:")
selected_variants_DF[4]
```

X:153775343 A / C (rs3021074) table:

```
[116]:
```

	Population	Allele Count	Allele Number	Number of Homozygotes \
0	Zartoshti	146	200	73
1	Mazani	142	200	71
2	Baloch	124	202	62
3	Persian Gulf Islander	118	200	59
4	Persian	94	200	47
5	Sistani	94	200	47
6	Azeri	90	200	45
7	Lur	88	200	44
8	Kurd	86	200	43
9	Arab	82	204	41
10	Turkmen	61	200	30
11	Gilaki	54	198	27
12	Total	1179	2404	589

	Number of Heterozygotes	Homozygous Genotype Freq. \
0	0	0.730000
1	0	0.710000
2	0	0.613900
3	0	0.590000
4	0	0.470000
5	0	0.470000
6	0	0.450000
7	0	0.440000
8	0	0.430000
9	0	0.402000
10	1	0.300000
11	0	0.272700
12	1	0.490017

	Heterozygous Genotype Freq.	Allele Frequency
0	0.000000	0.7300
1	0.000000	0.7100
2	0.000000	0.6139
3	0.000000	0.5900
4	0.000000	0.4700
5	0.000000	0.4700
6	0.000000	0.4500
7	0.000000	0.4400

8	0.000000	0.4300
9	0.000000	0.4020
10	0.010000	0.3050
11	0.000000	0.2727
12	0.000832	0.4904

3 2)

We now proceed to estimate the fractional ancestry of a newly observed individual who is heterozygous at all selected SNP loci

```
[141]: import numpy as np
Arab_Probs = np.array([])
Zartoshti_Probs = np.array([])
for df in selected_variants_DFs:
    Arab_Probs = np.append(Arab_Probs, float(df[df["Population"]==pop1]["Allele_Frequency"]))
    Zartoshti_Probs = np.append(Zartoshti_Probs, float(df[df["Population"]==pop2]["Allele_Frequency"]))
```

```
[142]: Arab_Probs
```

```
[142]: array([0.1275, 0.1029, 0.2059, 0.1569, 0.402 ])
```

```
[143]: Zartoshti_Probs
```

```
[143]: array([0.43 , 0.39 , 0.405, 0.345, 0.73 ])
```

```
[144]: import matplotlib.pyplot as plt
```

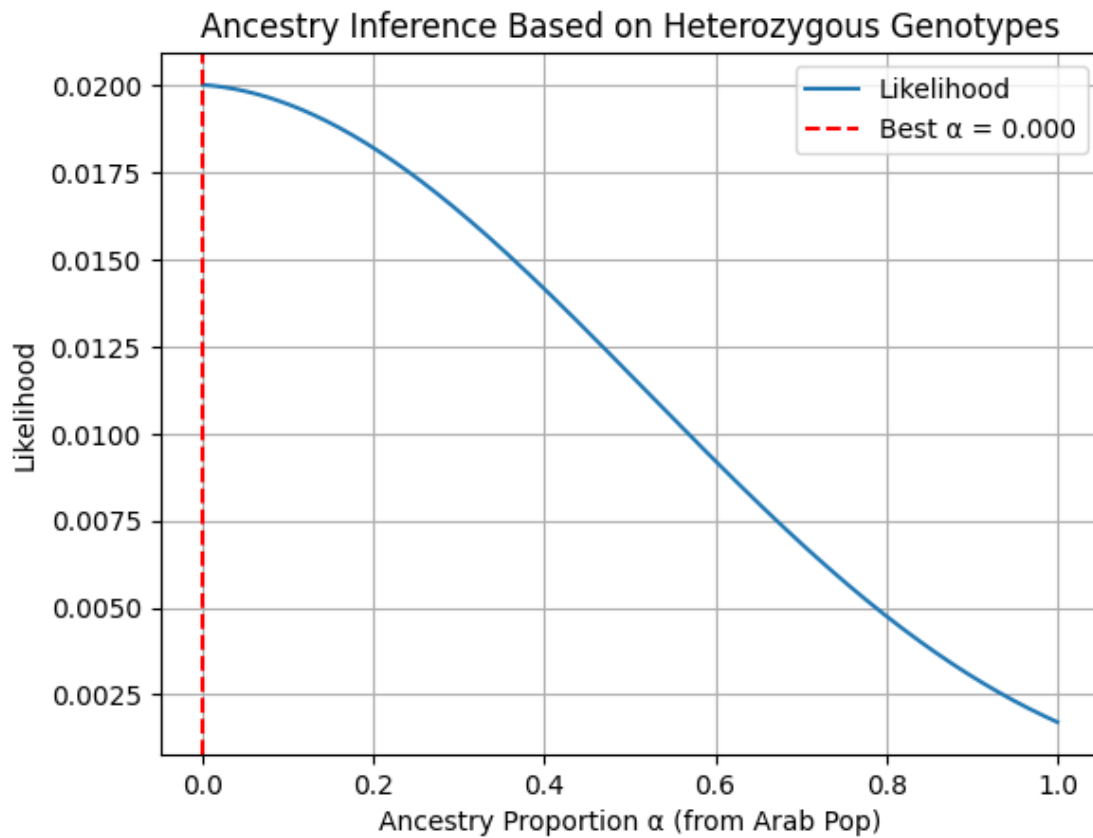
```
[145]: alphas = np.linspace(0, 1, 1000)
likelihoods = []

for alpha in alphas:
    probs = 2 * ((alpha * Arab_Probs + (1 - alpha) * Zartoshti_Probs) *
                 (1 - (alpha * Arab_Probs + (1 - alpha) * Zartoshti_Probs)))
    likelihood = np.prod(probs)
    likelihoods.append(likelihood)

likelihoods = np.array(likelihoods)
best_alpha = alphas[np.argmax(likelihoods)]

plt.plot(alphas, likelihoods, label="Likelihood")
plt.axvline(best_alpha, color='red', linestyle='--', label=f'Best = {best_alpha:.3f}')
plt.xlabel('Ancestry Proportion (from Arab Pop)')
```

```
plt.ylabel('Likelihood')
plt.title('Ancestry Inference Based on Heterozygous Genotypes')
plt.legend()
plt.grid(True)
plt.show()
```



Based on the genotype likelihood modeling, the analysis indicates that this individual has 0% ancestry from population 1 (Arab), suggesting that the selected SNPs effectively differentiate between the Arab and Zartoshti populations.