Exploratory and Predictive Analytics for Precision Medicine

Phu Dang (PACE Scholar) & **Leena Kang** (PATHS Scholar)
Data Science, Applied Mathematics
Mentor: Dr. Niema Moshiri
University of California San Diego

Outline - **FOR WORK/TIME DISTRIBUTION, WILL BE HIDDEN**

- Background (Phu) & Data + RQ (Leena)
- Exploratory Analysis
  - Uni-, Bi-, Multivariate Analyses (Phu)
  - Data Collection Bias Analysis (Phu)
- Predictive Analysis
  - Machine Learning Models (Leena)
  - Solutions to Imbalanced Data (Leena)
  - Performance Metrics & Assessment (Phu)
- Limitations (Leena) & Potential Applications (Phu)
- Conclusion & Closing

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  - Performance Metrics & Assessment
- Limitations
- Closing & Acknowledgements

Background

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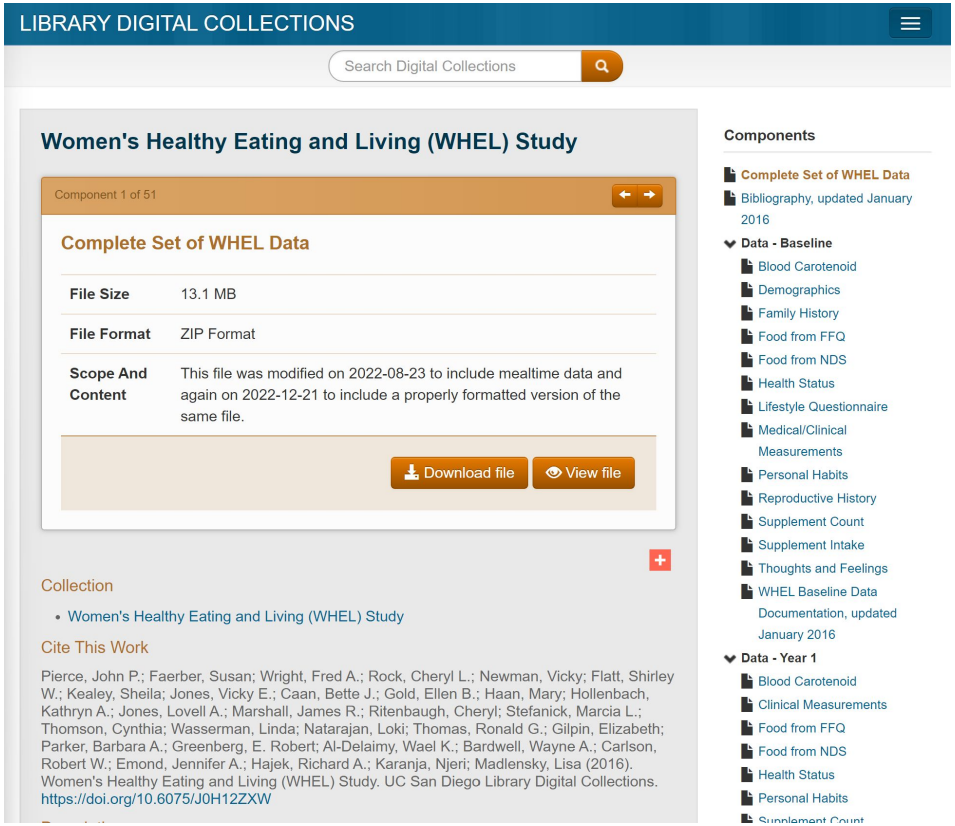
https://library.ucsd.edu/dc/object/bb2493244b



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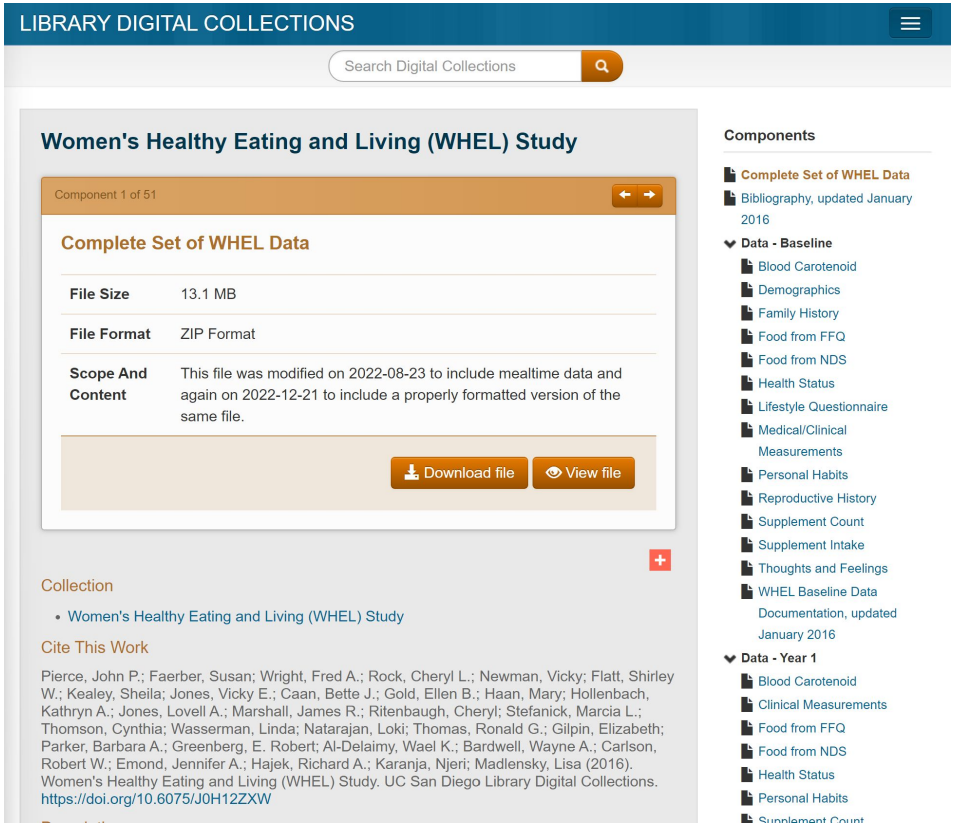
“Precision medicine…is an innovative approach to tailoring disease prevention and treatment that takes into account differences in people's genes, environments, and lifestyles.” - *FDA*



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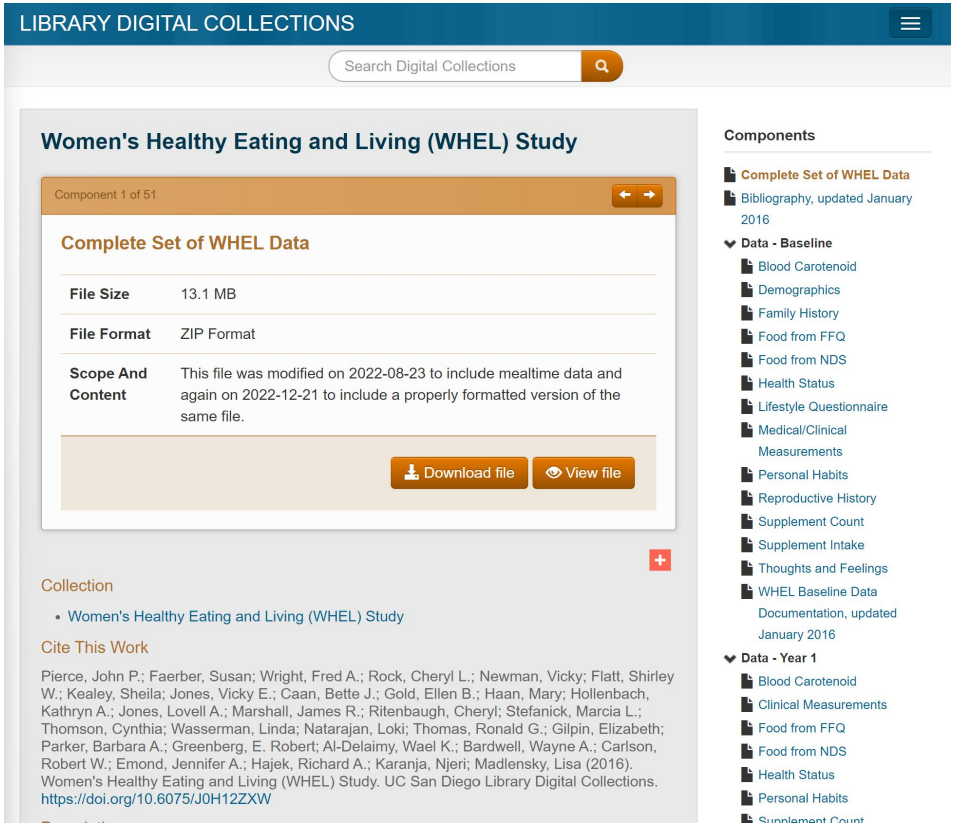

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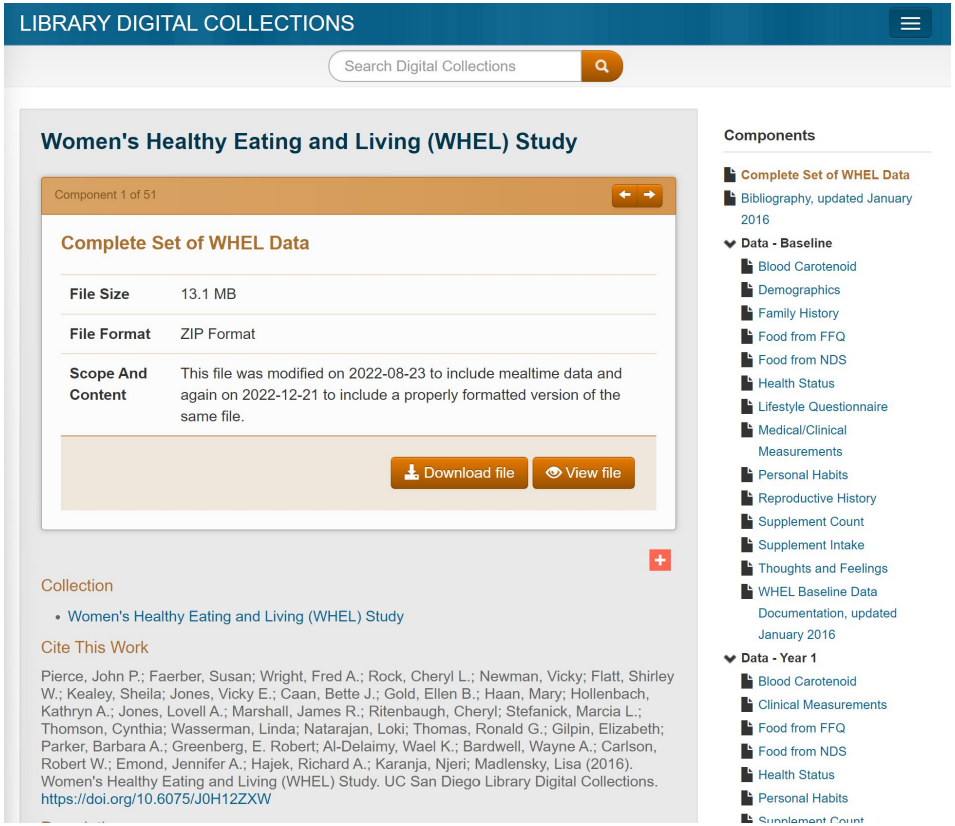

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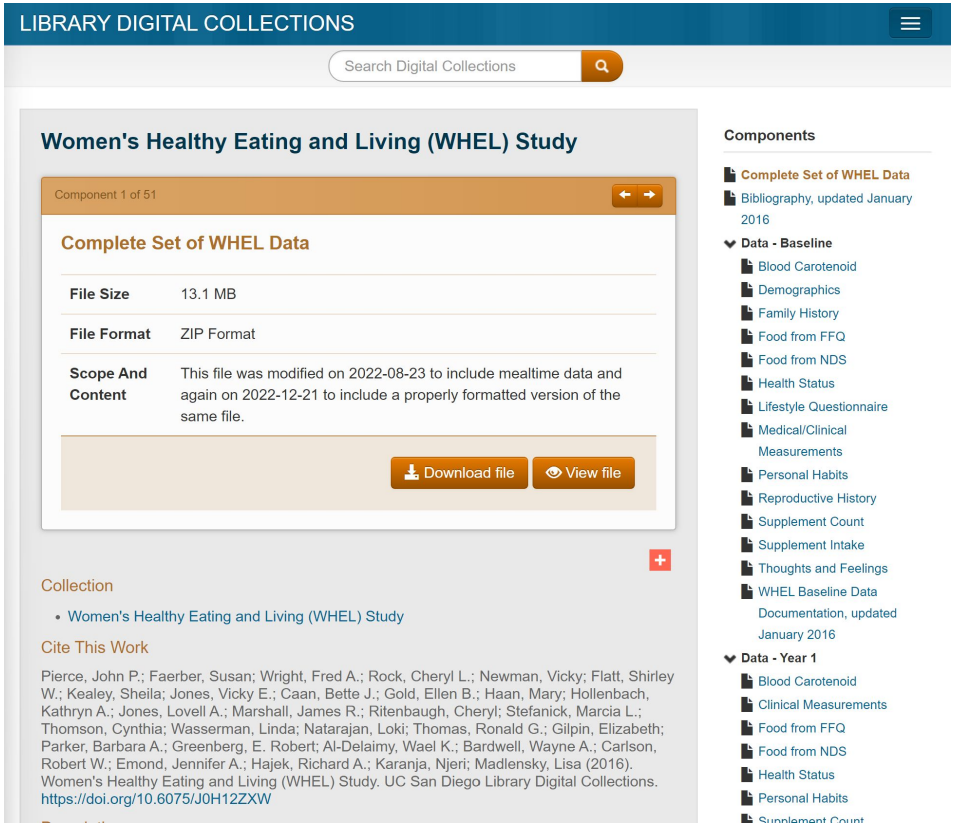
Assess impact on the likelihood of additional breast cancer events



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30 Datasets with **~3000** observations (rows) and **~27** variables (columns) each

The Dataset: Baseline Medical/Clinical Measurements

```
In [21]: base_measure.head(10)
```

Out[21]:

	ID	Lump/Mast	Radiation	Chemo	Tumor Type	Estr Recep	Prog Recep	Node Exam	Node Pos	Stage	...	Weight	BMI	Waist	Hip	Pulse	Bld Pres -Sys	Bld Pres - Dias	Menopause	An Es U
0	1002	1	2	2	3	1	1	18	1.0	II	...	65.50	23.0697	70.6	94.5	-9	-9	-9	1	
1	1003	1	2	2	3	1	1	14	0.0	I	...	60.00	23.4375	87.0	94.0	-9	-9	-9	2	
2	1005	2	1	1	3	3	3	29	0.0	II	...	68.63	32.4181	92.0	110.0	-9	-9	-9	2	
3	1007	2	1	2	4	0	0	21	1.0	II	...	55.45	23.3808	70.0	99.0	-9	-9	-9	2	
4	1008	2	1	1	3	1	1	16	0.0	I	...	64.40	25.4737	75.6	100.0	-9	-9	-9	2	
5	1009	2	1	1	3	1	1	6	1.0	II	...	81.90	31.5568	98.7	118.8	-9	-9	-9	3	
6	1010	2	1	2	3	1	1	23	4.0	II	...	72.27	31.4871	86.0	111.5	-9	-9	-9	2	
7	1011	1	2	2	1	0	1	8	6.0	II	...	59.00	23.0469	73.5	95.0	-9	-9	-9	3	
8	1012	1	2	1	3	1	1	9	0.0	I	...	62.50	27.2304	83.0	108.0	-9	-9	-9	2	
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10 rows × 22 columns

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Patient ID's - connected and included in ALL 30 datasets

Based on the WHEL's Study Dataset...

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Is there some **predictive power** in a patient's diet, clinical measurements, and lifestyle (over time) with their recurrence in their breast cancer condition?

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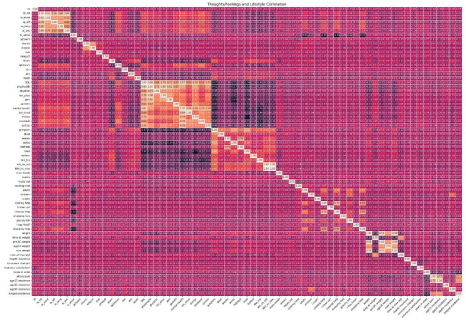

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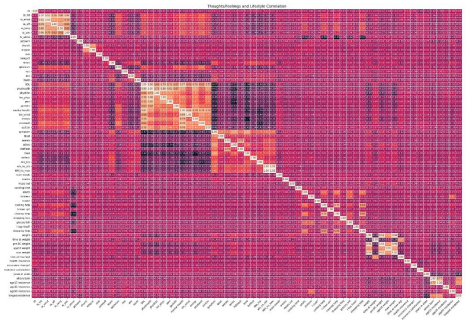

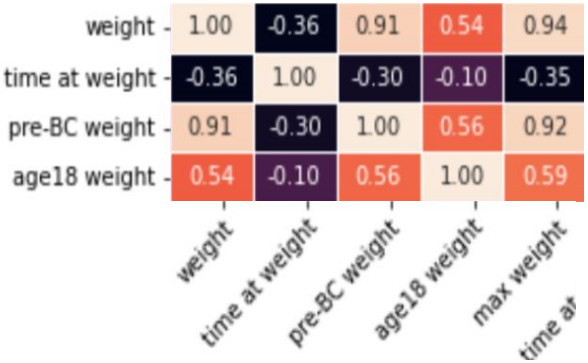

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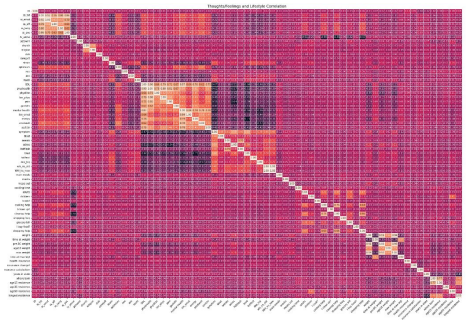

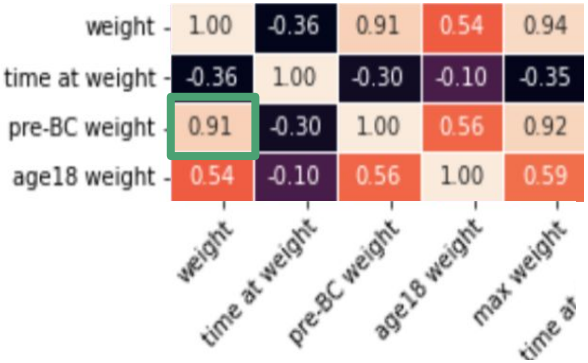

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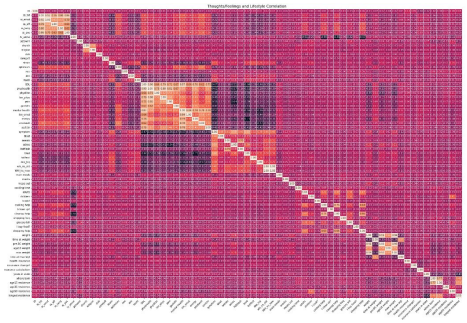

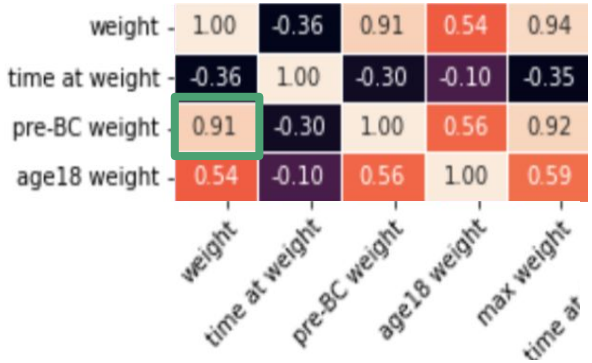

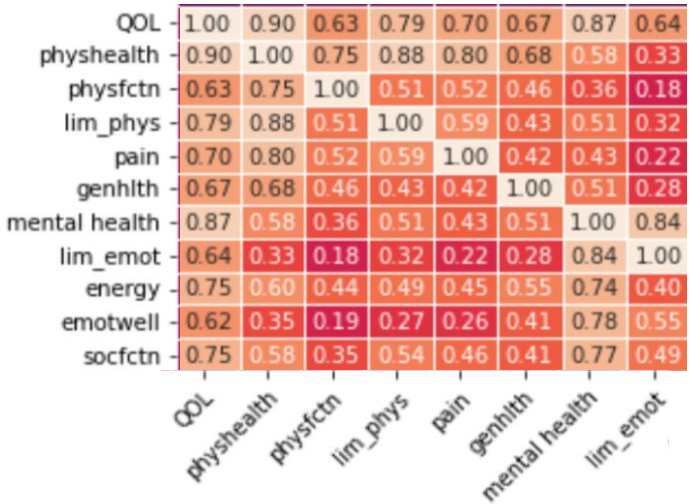

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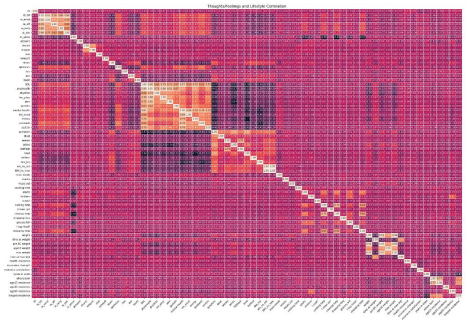

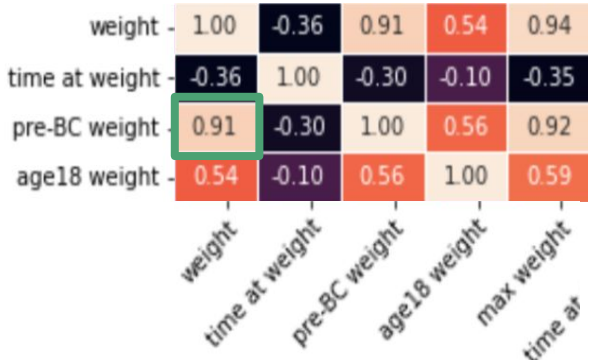

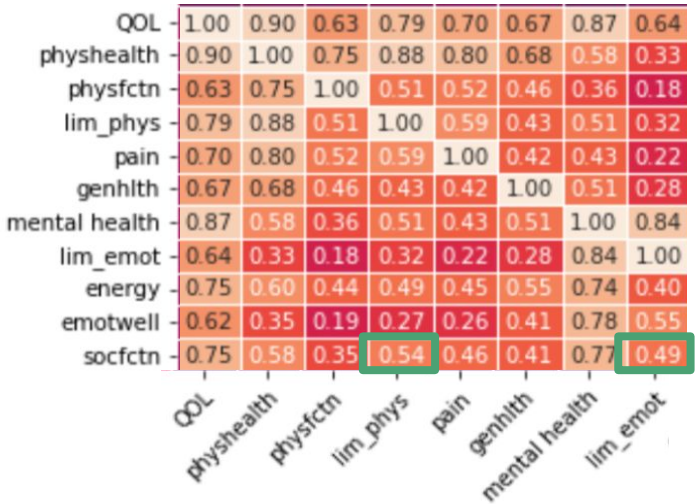

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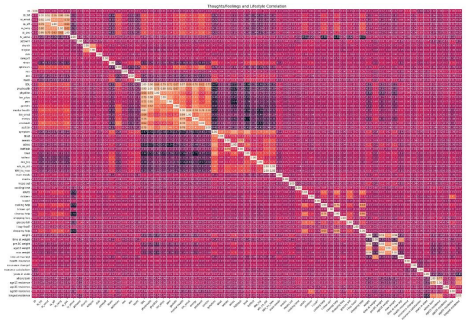

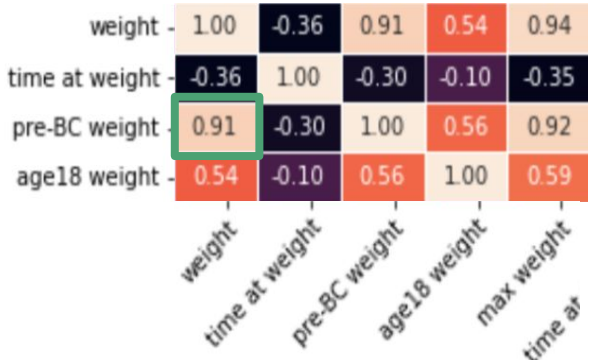

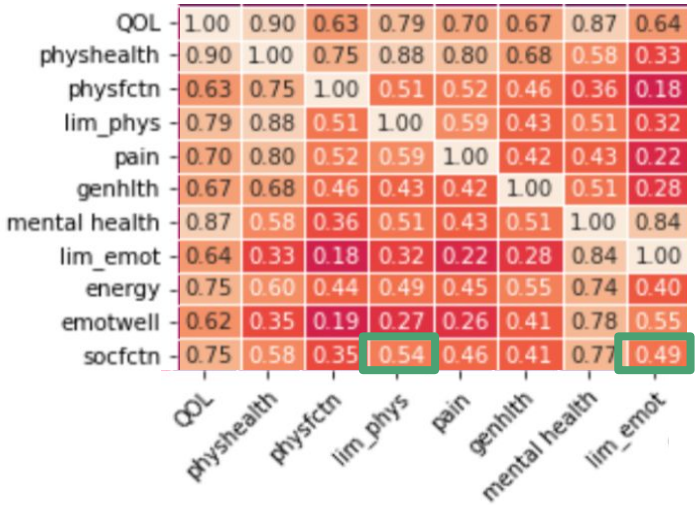

sanity checks

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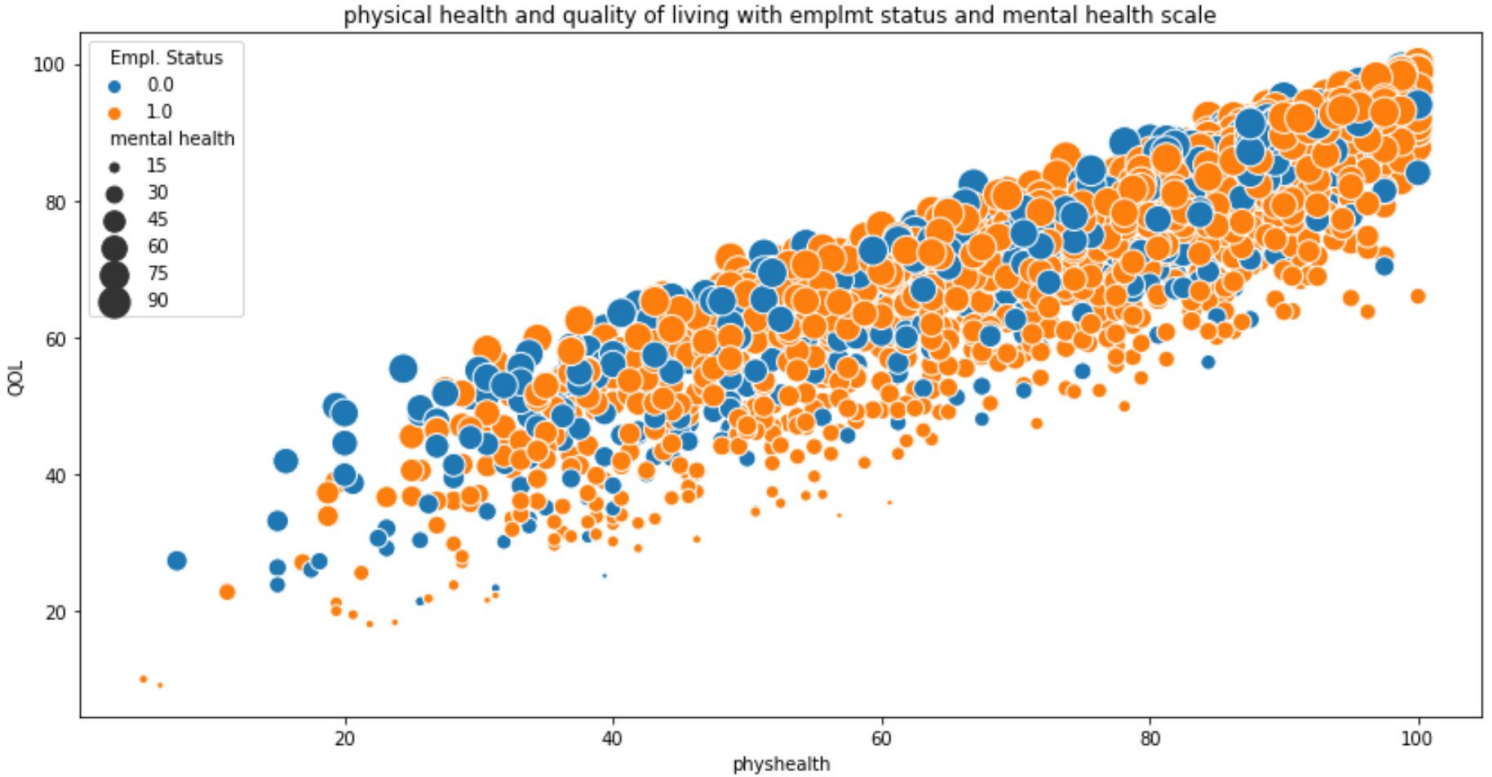

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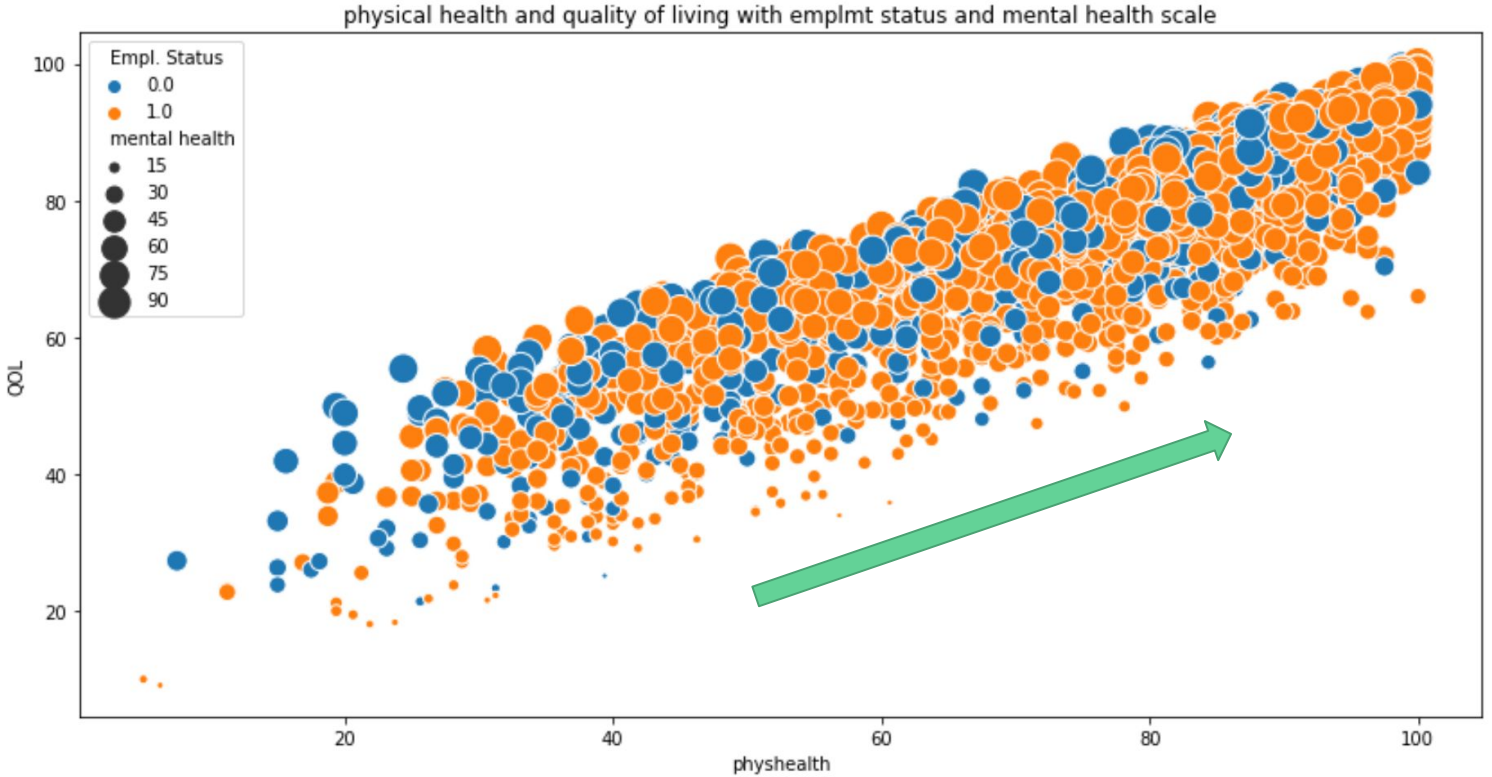

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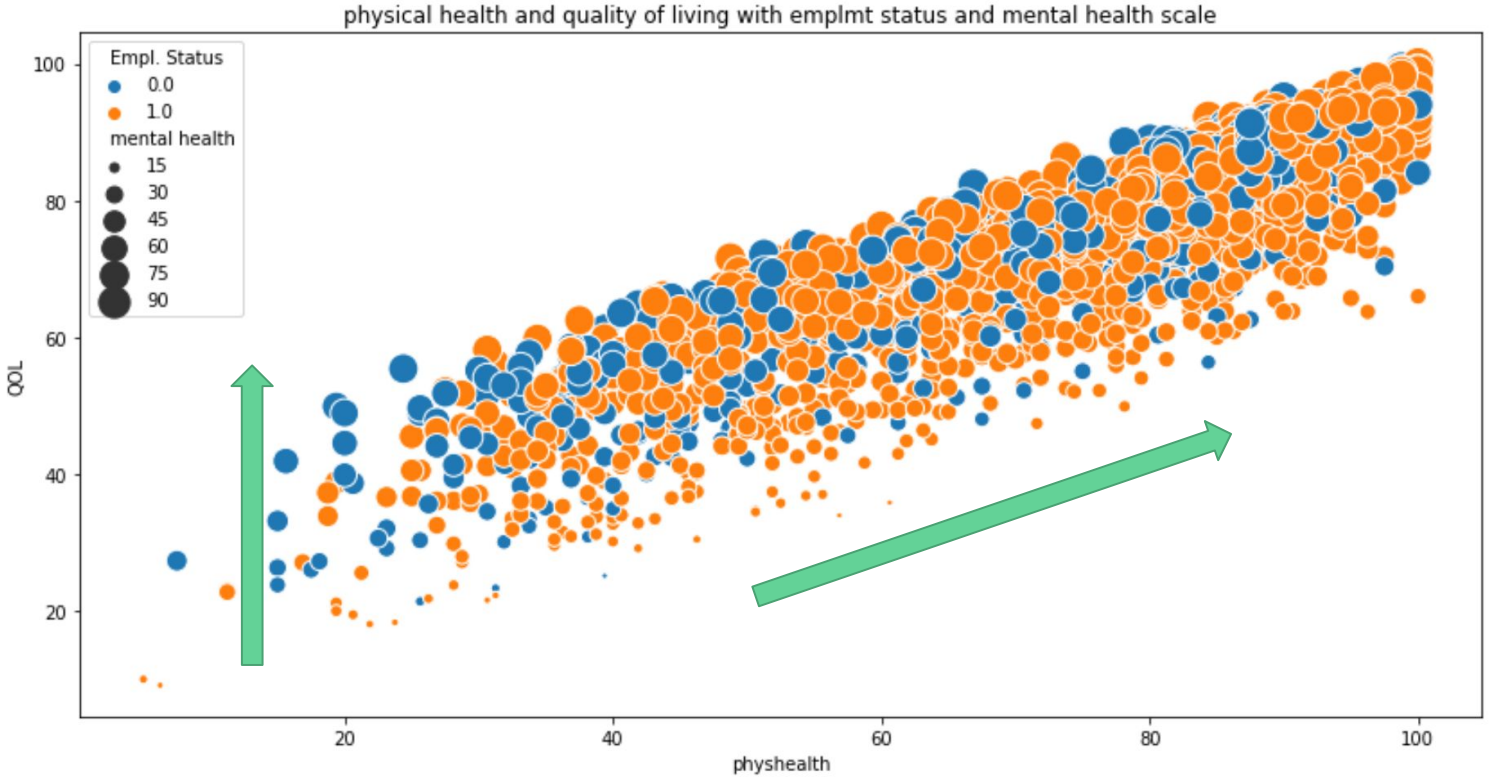

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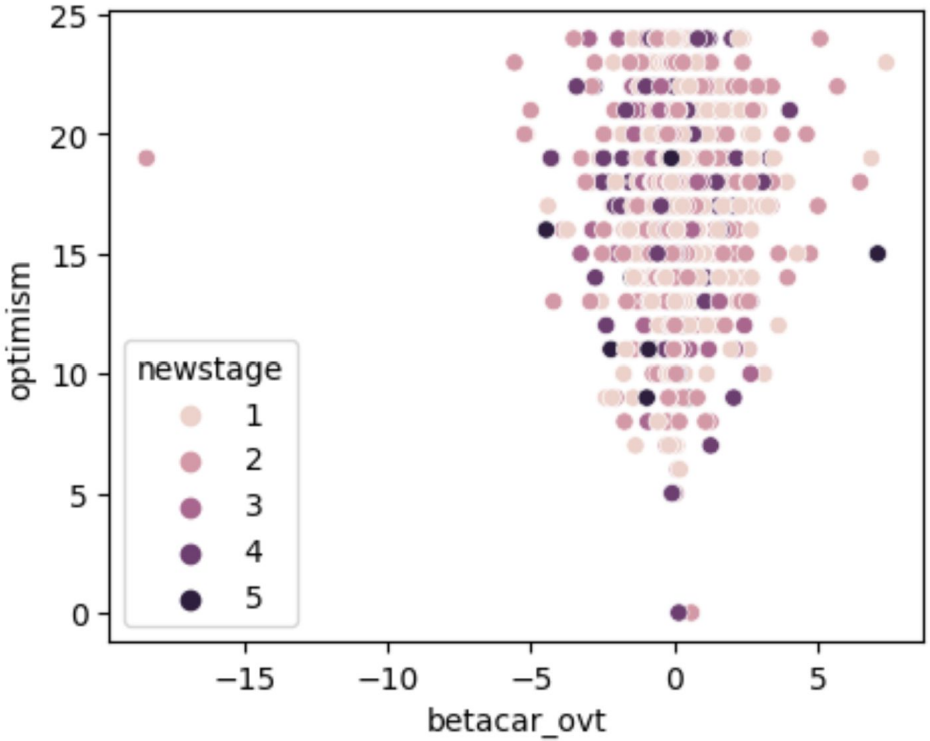

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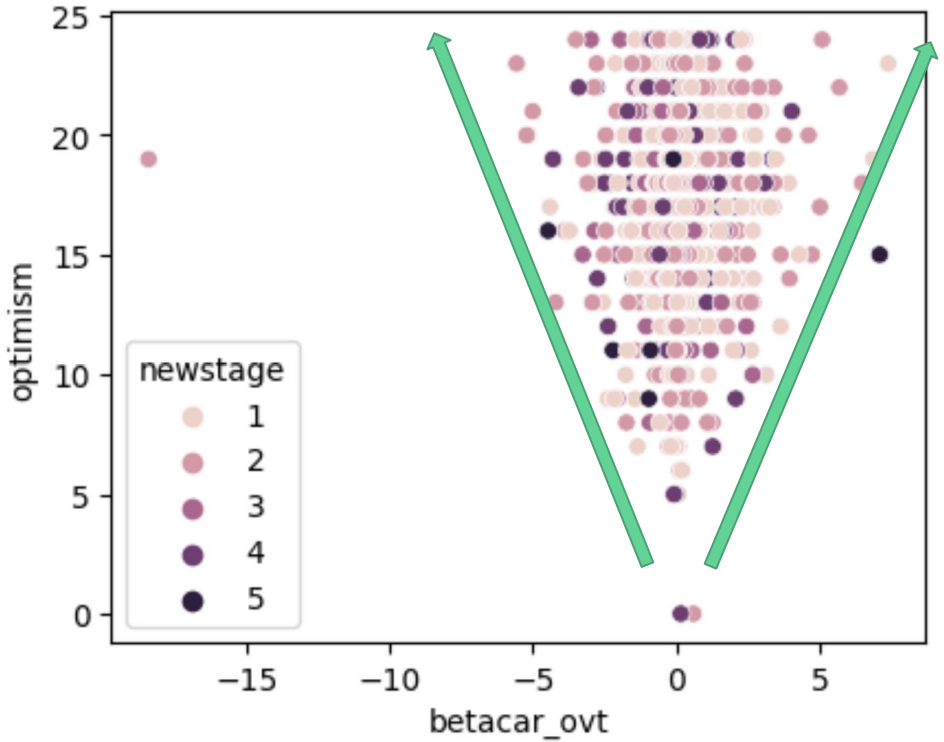

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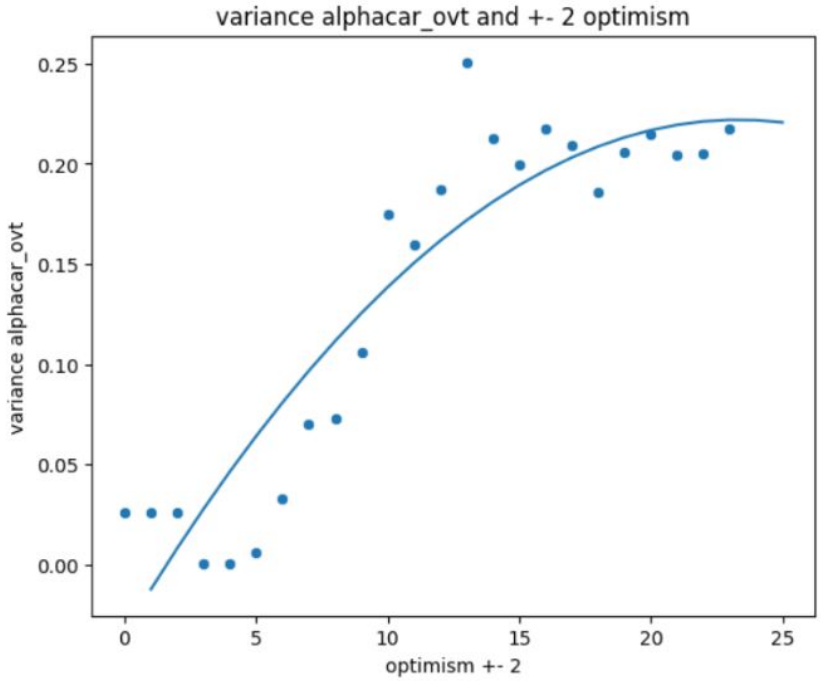

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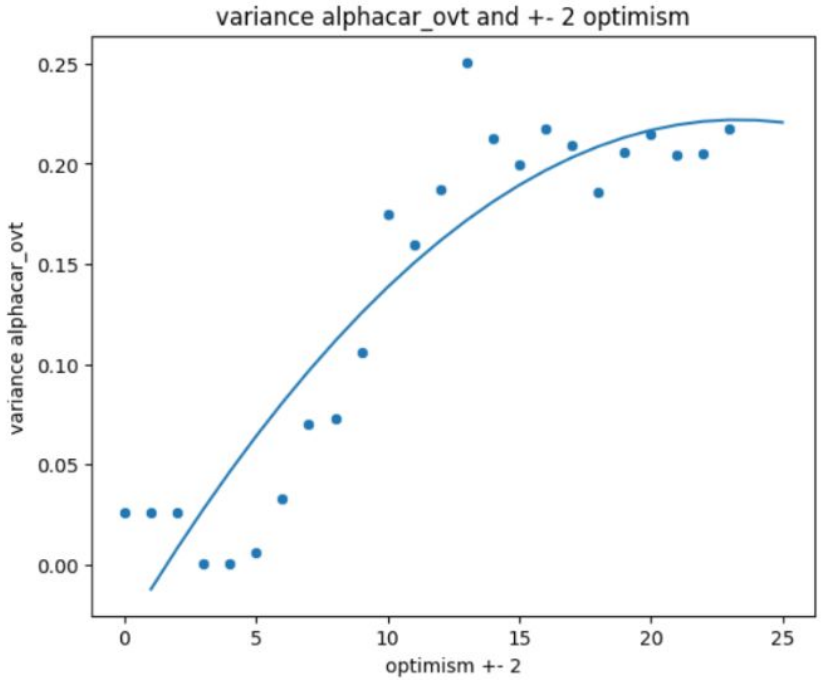

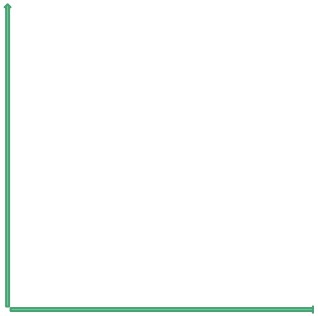

x-axis: optimism interval (+-2)

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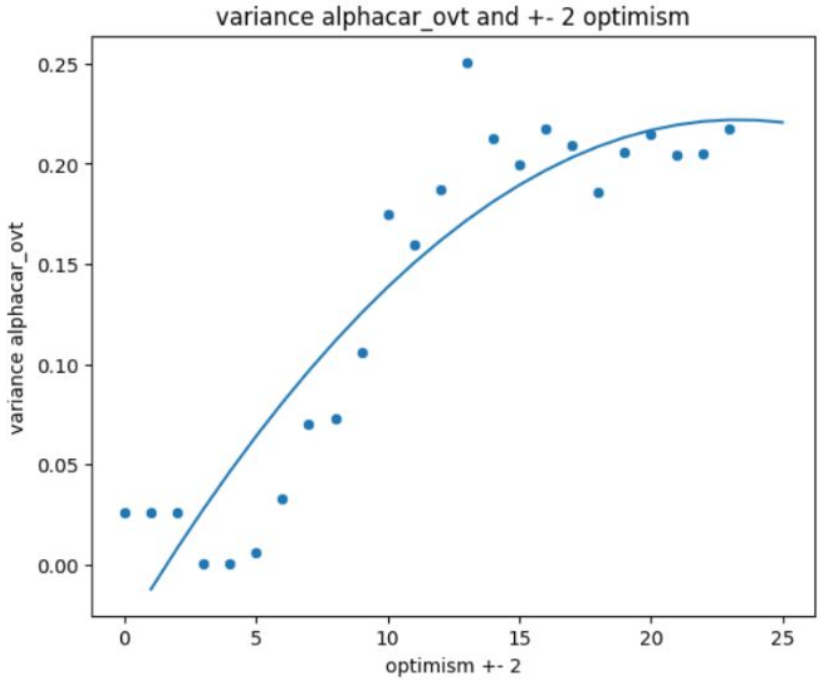

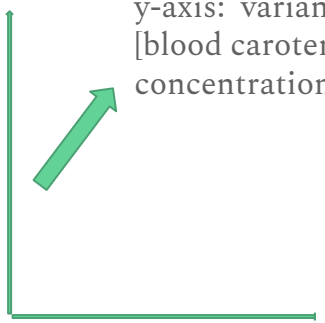

y-axis: variance of changes in [blood carotenoid] concentration over time

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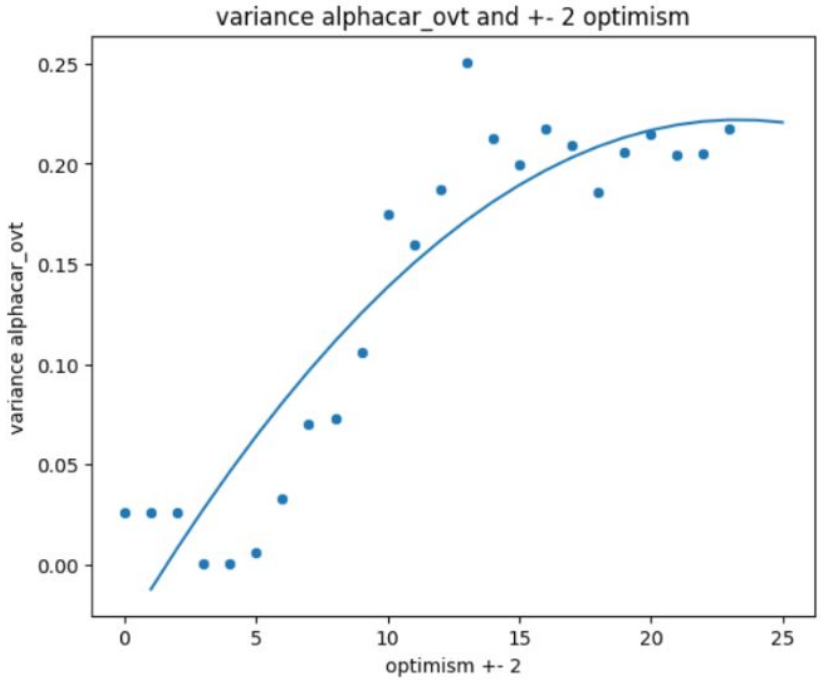
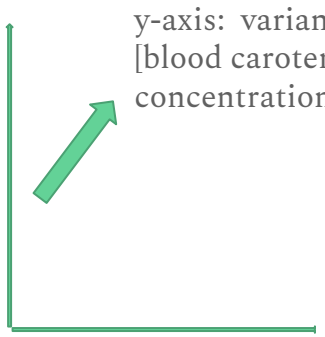
Uni-, Bi-, Multivariate Analyses





y-axis: variance of changes in [blood carotenoid] concentration over time

x-axis: optimism interval (+-2)

→ Variances of changes in alpha-carotene concentrations increases over increasing optimism intervals (+-2), then flatten out / slightly decrease

Outline

- Background & Data + Research Question
- Exploratory Analysis
  - Uni-, Bi-, Multivariate Analyses
- **Predictive Analysis**
  - **Machine Learning Models**
  - Solutions to Imbalanced Data
  - Performance Metrics & Assessment
- Limitations
- Closing & Acknowledgements

Binary Classification Model: Preprocessing

Binary Classification Model: Preprocessing

Target variable: breast cancer status

0 : No evidence of recurrence

> 0 : Local, Regional, Distant recurrence

```
[84]: endpoints_df.head(10)
```

Out[84]:

	id	intgrp	vitality	brcastatus	othcstatus
0	1002	3	1	0	0.0
1	1003	3	1	0	0.0
2	1005	4	1	0	0.0
3	1007	3	1	0	0.0
4	1008	4	1	0	0.0
5	1009	4	1	3	0.0
6	1010	3	0	4	0.0
7	1011	4	0	4	0.0
8	1012	4	1	0	0.0
9	1015	3	0	2	0.0

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Features: Year 4 - Baseline

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4	1008	4	1	0	0.0
5	1009	4	1	3	0.0
6	1010	3	0	4	0.0
7	1011	4	0	4	0.0
8	1012	4	1	0	0.0
9	1015	3	0	2	0.0

Features: Year 4 - Baseline

- *Metrics:* clinical measurements, blood carotenoids
- *Diet:* Food From NDS
- *Lifestyle:* personal habits, emotional health, quality of life (QOL)

Binary Classification Model: Preprocessing (Merging)

Binary Classification Model: Preprocessing (Merging)

	id	recurrence
0	1002	0
1	1003	0
2	1005	0
3	1007	0
4	1008	0
...	...	...
3083	13241	0
3084	13242	0
3085	13243	0
3086	13244	0
3087	13245	0

3088 rows × 2 columns

Binary Classification Model: Preprocessing (Merging)

	id	recurrence
0	1002	0
1	1003	0
2	1005	0
3	1007	0
4	1008	0
...	...	...
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3086	13244	0
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3088 rows × 2 columns

Target variable

Binary Classification Model: Preprocessing (Merging)

	id	recurrence
0	1002	0
1	1003	0
2	1005	0
3	1007	0
4	1008	0
...	...	...
3083	13241	0
3084	13242	0
3085	13243	0
3086	13244	0
3087	13245	0

3088 rows × 2 columns

Baseline *(Clinical measurements)*

ID	B_Height	B_Weight	B_BMI	B_Waist	B_Hip	B_Pulse
1245	159.00	61.6	24.3661	74.3	99.5	32
1248	171.46	61.2	20.8174	69.2	96.0	33
1249	161.50	60.4	23.1575	71.5	95.1	33
1250	168.40	45.3	15.9740	61.0	86.5	30
1253	161.20	78.6	30.2477	90.5	109.0	32

Year 4 *(Clinical measurements)*

ID	y4_Heightcm	y4_Weightkg	y4_BMI	y4_Waistcm	y4_Hipcm	y4_Pulse30
1002	166.50000	65.000000	23.446871	71.400002	97.900002	28
1007	153.39999	64.900002	27.579985	83.400002	105.600000	37
1010	154.30000	72.800003	30.577330	84.300003	104.000000	28
1012	151.50000	68.500000	29.844570	96.199997	110.000000	33
1018	162.89999	51.500000	19.407299	70.800003	88.599998	28

Binary Classification Model: Preprocessing (Merging)

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0	1002	0
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1018	162.89999	51.500000	19.407299	70.800003	88.599998	28

	id	recurrence	y4_Heightcm	y4_Weightkg
0	1245	0	-1.10001	2.800002
1	1249	0	-0.30000	7.600000
2	1250	0	-1.90000	-1.399998
3	1253	0	-0.20000	1.900000
4	1254	0	0.39999	-3.000002

Binary Classification Model: Preprocessing (Merging)

	id	recurrence
0	1002	0
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3083	13241	0
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3085	13243	0
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Baseline *(Clinical measurements)*

ID	B_Height	B_Weight	B_BMI	B_Waist	B_Hip	B_Pulse
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Merged based on ‘ID’

	id	recurrence	y4_Heightcm	y4_Weightkg
0	1245	0	-1.10001	2.800002
1	1249	0	-0.30000	7.600000
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(Year 4) - (Baseline)

Binary Classification Model: Preprocessing (Merging)

Repeat merging for
rest of dataframes ...

Binary Classification Model: Preprocessing (Merging)

Repeat merging for rest of dataframes ...

Shape: (655, 68) → *2433 rows lost !!*

	ID	QOL_ovt	energy_ovt	genhlth_ovt	optimism_ovt	pain_ovt	socfctn_ovt	lutein_ovt
0	1245	-32.312500	-20.0	-40.0	-2.0	-12.5	-50.0	-0.1697
1	1256	-36.687500	-5.0	10.0	-3.0	-50.0	-37.5	0.0980
2	1265	-6.312500	-5.0	-10.0	2.0	-12.5	0.0	0.0349
3	1266	0.437500	-10.0	0.0	2.0	25.0	-12.5	-0.1125
4	1276	30.646484	30.0	5.0	-1.0	25.0	37.5	0.0766

Binary Classification Model: Preprocessing (Merging)

Repeat merging for rest of dataframes ...

Shape: (655, 68) → *2433 rows lost !!*

	ID	QOL_ovt	energy_ovt	genhlth_ovt	optimism_ovt	pain_ovt	socfctn_ovt	lutein_ovt
0	1245	-32.312500	-20.0	-40.0	-2.0	-12.5	-50.0	-0.1697
1	1256	-36.687500	-5.0	10.0	-3.0	-50.0	-37.5	0.0980
2	1265	-6.312500	-5.0	-10.0	2.0	-12.5	0.0	0.0349
3	1266	0.437500	-10.0	0.0	2.0	25.0	-12.5	-0.1125
4	1276	30.646484	30.0	5.0	-1.0	25.0	37.5	0.0766

```
In [18]: ovt['recurrence_y'].value_counts()

Out[18]: 0    629
         1     26
         Name: recurrence_y, dtype: int64
```

629 (96%) had no recurrence
26 (4%) had recurrence

Outline

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Handling Imbalanced Data: Procedures

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Original, Preprocessed Data

	ID	QOL_ovt	energy_ovt	genhlth_ovt	optimism_ovt	pain_ovt	socfctn_ovt
0	1245	-32.312500	-20.0	-40.0	-2.0	-12.5	-50.0
1	1256	-36.687500	-5.0	10.0	-3.0	-50.0	-37.5
2	1265	-6.312500	-5.0	-10.0	2.0	-12.5	0.0
3	1266	0.437500	-10.0	0.0	2.0	25.0	-12.5
4	1276	30.646484	30.0	5.0	-1.0	25.0	37.5

Handling Imbalanced Data: Procedures

Original, Preprocessed Data

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Apply Resample Method

Handling Imbalanced Data: Procedures

Original, Preprocessed Data

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Apply Resample Method

New, Resampled Data

	ID	QOL_ovt	energy_ovt	genhlth_ovt	optimism_ovt	pain_ovt	socfctn_ovt
90	1563	-33.000000	-15.0	-20.0	-2.0	-50.0	-50.0
280	5569	23.187500	15.0	25.0	1.0	37.5	0.0
301	7249	13.312500	20.0	0.0	1.0	12.5	25.0
118	3299	7.292969	0.0	0.0	2.0	0.0	0.0
323	7305	-1.062500	0.0	5.0	4.0	-12.5	0.0

Handling Imbalanced Data: Procedures

Original, Preprocessed Data

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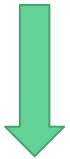

Train/Test Data

Handling Imbalanced Data: Procedures

Original, Preprocessed Data

	ID	QOL_ovt	energy_ovt	genhlth_ovt	optimism_ovt	pain_ovt	socfctn_ovt
0	1245	-32.312500	-20.0	-40.0	-2.0	-12.5	-50.0
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2	1265	-6.312500	-5.0	-10.0	2.0	-12.5	0.0
3	1266	0.437500	-10.0	0.0	2.0	25.0	-12.5
4	1276	30.646484	30.0	5.0	-1.0	25.0	37.5

Apply Resample Method

New, Resampled Data

	ID	QOL_ovt	energy_ovt	genhlth_ovt	optimism_ovt	pain_ovt	socfctn_ovt
90	1563	-33.000000	-15.0	-20.0	-2.0	-50.0	-50.0
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301	7249	13.312500	20.0	0.0	1.0	12.5	25.0
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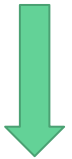

Train/Test Data

Classification Models

Linear regression
KNN
SVM (linear kernel)
Decision tree
Random forest

Handling Imbalanced Data: Procedures

Original, Preprocessed Data

	ID	QOL_ovt	energy_ovt	genhlth_ovt	optimism_ovt	pain_ovt	socfctn_ovt
0	1245	-32.312500	-20.0	-40.0	-2.0	-12.5	-50.0
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3	1266	0.437500	-10.0	0.0	2.0	25.0	-12.5
4	1276	30.646484	30.0	5.0	-1.0	25.0	37.5

Apply Resample Method

New, Resampled Data

	ID	QOL_ovt	energy_ovt	genhlth_ovt	optimism_ovt	pain_ovt	socfctn_ovt
90	1563	-33.000000	-15.0	-20.0	-2.0	-50.0	-50.0
280	5569	23.187500	15.0	25.0	1.0	37.5	0.0
301	7249	13.312500	20.0	0.0	1.0	12.5	25.0
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323	7305	-1.062500	0.0	5.0	4.0	-12.5	0.0

Train/Test Data

Classification Models

Compute Scores

Linear regression
KNN
SVM (linear kernel)
Decision tree
Random forest

Handling Imbalanced Data: Procedures

Original, Preprocessed Data

	ID	QOL_ovt	energy_ovt	genhlth_ovt	optimism_ovt	pain_ovt	socfctn_ovt
0	1245	-32.312500	-20.0	-40.0	-2.0	-12.5	-50.0
1	1256	-36.687500	-5.0	10.0	-3.0	-50.0	-37.5
2	1265	-6.312500	-5.0	-10.0	2.0	-12.5	0.0
3	1266	0.437500	-10.0	0.0	2.0	25.0	-12.5
4	1276	30.646484	30.0	5.0	-1.0	25.0	37.5

Apply Resample Method

New, Resampled Data

	ID	QOL_ovt	energy_ovt	genhlth_ovt	optimism_ovt	pain_ovt	socfctn_ovt
90	1563	-33.000000	-15.0	-20.0	-2.0	-50.0	-50.0
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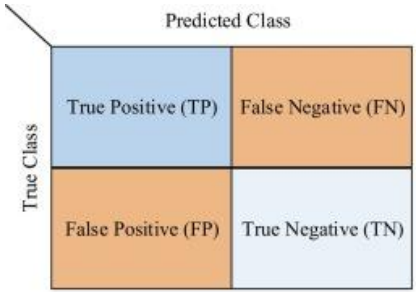
Train/Test Data

Classification Models

Linear regression
KNN
SVM (linear kernel)
Decision tree
Random forest

Compute Scores

Evaluate, Performance



TPR (recall)
TNR (specificity)
PPV (precision)
PNV
Accuracy
F1

Handling Imbalanced Data: Procedures

Original, Preprocessed Data

	ID	QOL_ovt	energy_ovt	genhlth_ovt	optimism_ovt	pain_ovt	socfctn_ovt
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1	1256	-36.687500	-5.0	10.0	-3.0	-50.0	-37.5
2	1265	-6.312500	-5.0	-10.0	2.0	-12.5	0.0
3	1266	0.437500	-10.0	0.0	2.0	25.0	-12.5
4	1276	30.646484	30.0	5.0	-1.0	25.0	37.5

Apply Resample Method

New, Resampled Data

	ID	QOL_ovt	energy_ovt	genhlth_ovt	optimism_ovt	pain_ovt	socfctn_ovt
90	1563	-33.000000	-15.0	-20.0	-2.0	-50.0	-50.0
280	5569	23.187500	15.0	25.0	1.0	37.5	0.0
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323	7305	-1.062500	0.0	5.0	4.0	-12.5	0.0

REPEAT PROCESS FOR EACH RESAMPLE METHOD

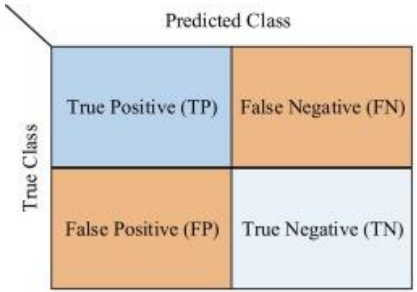
Train/Test Data

Classification Models

- *Linear regression*
- *KNN*
- *SVM (linear kernel)*
- *Decision tree*
- *Random forest*

Compute Scores

Evaluate, Performance



- *TPR (recall)*
- *TNR (specificity)*
- *PPV (precision)*
- *PNV*
- *Accuracy*
- *F1*

Outline

- Background & Data + Research Question
- Exploratory Analysis
  - Uni-, Bi-, Multivariate Analyses
- **Predictive Analysis**
  - Machine Learning Models
  - Solutions to Imbalanced Data
  - **Performance Metrics & Assessment**
- Limitations
- Closing & Acknowledgements

Our Best Model & Performance:
Up AND Downsampling on a Random Forest Classifier

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ROC AUC: 0.9436

Classification Report

	precision	recall	f1-score	support
no recurrence	0.87	0.85	0.86	46
recurrence	0.87	0.89	0.88	54

Confusion Matrix: True Negative: 39 False Positive: 7
False Negative: 6 True Positive: 48

Accuracy: 0.87
Precision: 0.873
Specificity: 0.848
Recall: 0.889
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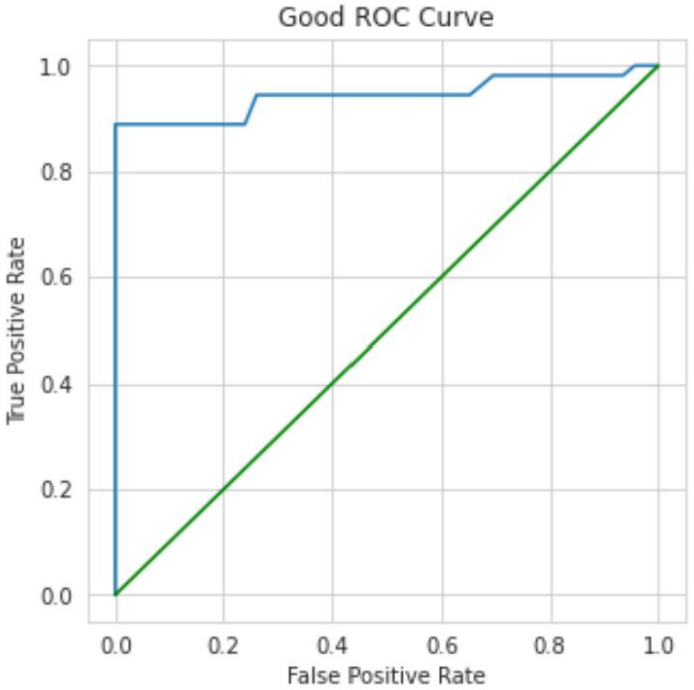

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Binary Classification Model: Preprocessing (Merging)

Repeat merging for rest of dataframes ...

Shape: (655, 68) → *2433 rows lost !!*

	ID	QOL_ovt	energy_ovt	genhlth_ovt	optimism_ovt	pain_ovt	socfctn_ovt	lutein_ovt
0	1245	-32.312500	-20.0	-40.0	-2.0	-12.5	-50.0	-0.1697
1	1256	-36.687500	-5.0	10.0	-3.0	-50.0	-37.5	0.0980
2	1265	-6.312500	-5.0	-10.0	2.0	-12.5	0.0	0.0349
3	1266	0.437500	-10.0	0.0	2.0	25.0	-12.5	-0.1125
4	1276	30.646484	30.0	5.0	-1.0	25.0	37.5	0.0766

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In [18]: ovt['recurrence_y'].value_counts()

Out[18]: 0    629
         1     26
         Name: recurrence_y, dtype: int64
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629 (96%) had no recurrence
26 (4%) had recurrence

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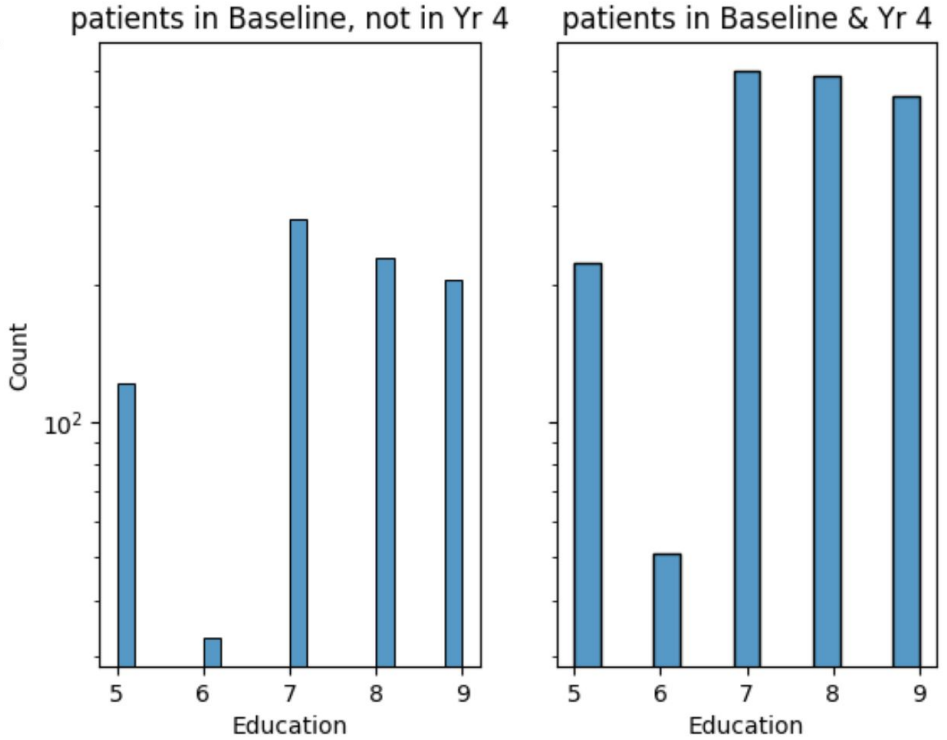

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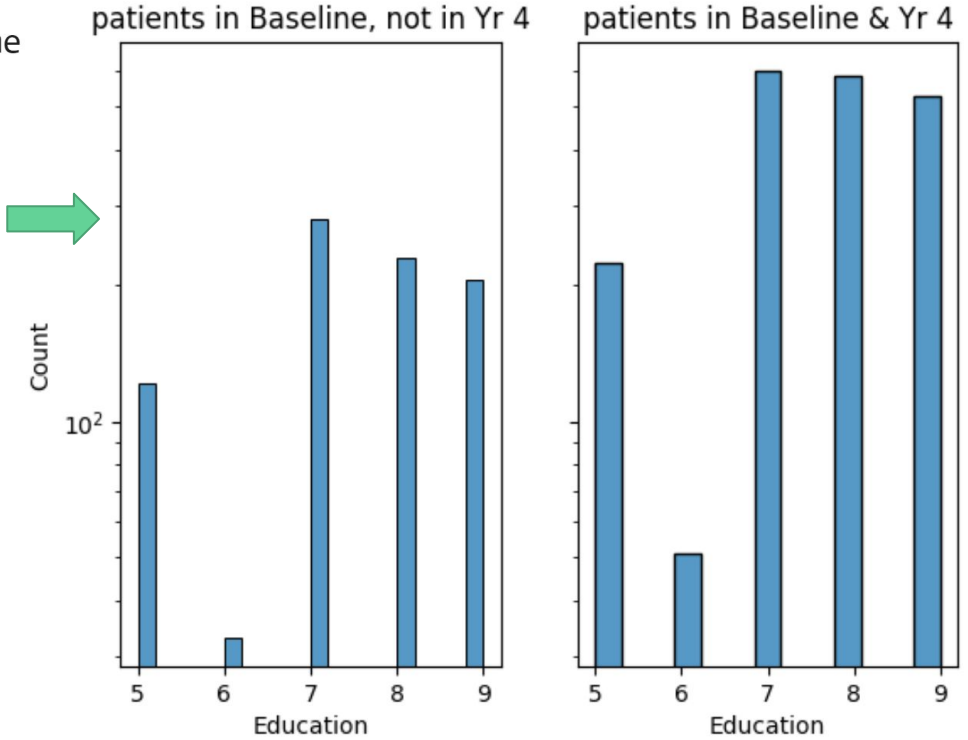

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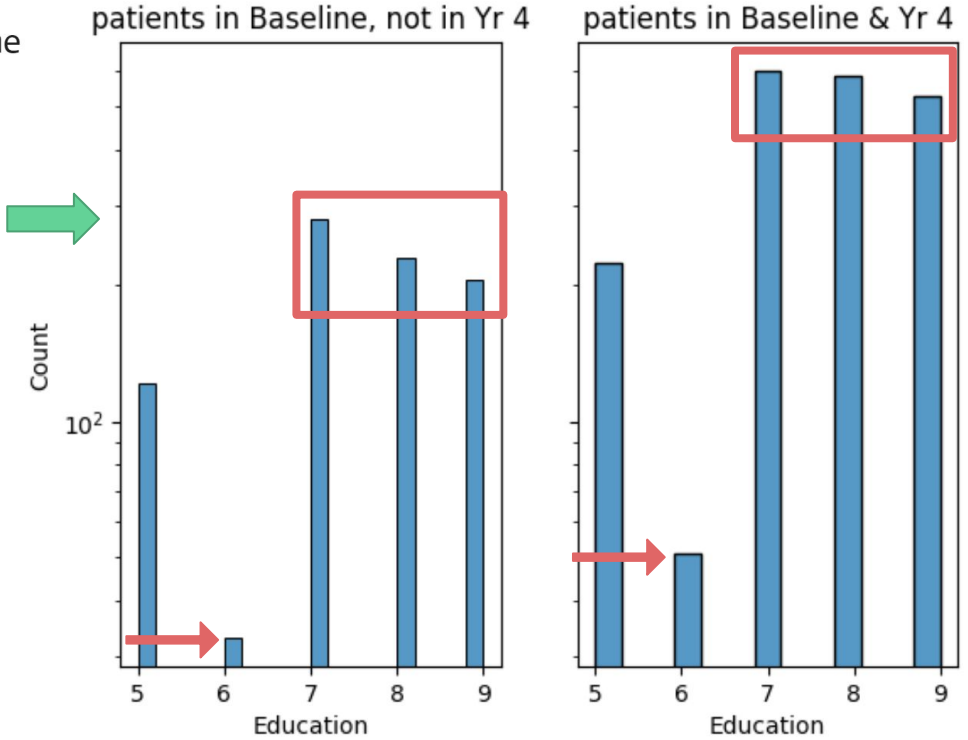

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https://github.com/pndang/Project_WHEL
https://github.com/leena-kang/WHEL_Study

Thank you!
Questions?

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pndang@ucsd.edu

Handling Imbalanced Data: Resample Methods

Original Data

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Upsample Minority Class (1:1)

```
print(upsampled['recurrence_y'].value_counts())
upsampled
```

```
1    472
0    472
Name: recurrence_y, dtype: int64
```

Downsample Majority Class (4:1)

```
downsampled = pd.concat([no_recur_downsampled, recur])
downsampled.recurrence_y.value_counts()
```

```
Out[51]: 0    76
         1    19
         Name: recurrence_y, dtype: int64
```

SMOTE (imblearn)

```
In [72]: X_train_smote.shape, y_train_smote.shape

Out[72]: ((944, 67), (944,))
```

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  - To improve our evaluation: ***cross validation***

Potential Applications