Identification of Adaptive Thermogenesis in Humans Using Machine Learning from CALERIE Dataset

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Abstract: In recent years, weight loss has become a serious concern in humans due to a rise in obesity rates. Different solutions have been developed for different body types. Nonetheless, maintaining a weight loss is a challenge since most people end up regaining the lost weight. The phenomenon is known as adaptive thermogenesis (AT). Using the CALERIE study dataset, the article proposes to use machine learning to estimate the chance of adaptive thermogenesis. Adaptive thermogenesis is determined by the difference between predicted and measured Resting metabolic rates as provided by the CALERIE study dataset. Depending on whether or not AT is below 5 percent of RMR, AT is scaled into binary form. Three state-of-the-art machine learning algorithms were then applied to the dataset, namely logistic regression, decision tree classifiers, and explainable boosting machines. These models explain AT in humans in the simplest form possible. Different training rates led to different results for each algorithm. Despite the explainable boosting machines' higher accuracy when given more data for training, the logistic regression classifier provided better generalization as training data reduced from 80% to 60%. Several modelling approaches provided results that underlined that body temperature, BMI, alcohol intake, and waist to height ratio (WhtR) were more relevant with AT. This explains why thermogenesis is observed in warm-blooded animals, an occurrence that is primarily determined by body temperature. AT is increased in humans with a poor body type and excessive alcohol consumption. In other words, a poor lifestyle promotes AT in humans.

Keywords: Adaptive thermogenesis, machine learning, resting metabolic rate, classification, explainable boosting machines, CALERIE study

1. INTRODUCTION

Early detection of weight gain could prevent many future problems in humans. Despite this, the growing obesity rate in the world drives researchers to identify the reasons for weight gain. There are many strategies to shed excess body weight, but very few to sustain the weight loss after weight loss. In humans, adaptive thermogenesis (AT) is one such factor that discourages weight loss. The current work is about the detection of this phenomenon in humans using the CALERIE study dataset from Duke School of medical sciences. The next topic is thermogenesis and adaptive thermogenesis (AT).

1.1. Thermogenesis and Adaptive Thermogenesis

In humans, thermogenesis allows the body to maintain its optimum temperature by burning energy. Adaptive thermogenesis refers to the human body's choice to burn either stored energy (fat) or readily available energy (glucose). When the body prefers to burn stored fat then it's functioning at its best, if it doesn't then it's a problem. An individual with this problem is incapable of using the stored fat on their body. The excess energy from consumed food, also known as food consumption, keeps adding to fat reserves if it is not completely burned. This phenomenon also disagrees with starvation or any other weight loss technique, as the body remembers the earlier weight and tries to compensate for the loss of weight. Adaptive thermogenesis is hard to detect as it involves actual metabolic rate as opposed to ideal metabolic rate. AT can be explained by the residual of the metabolic rates, resting metabolic rate (RMR) in particular. RMR is the basic energy requirement for a human body at rest to perform all involuntary bodily essential actions such as respiration, organ function, digestion, etc. Speaking about RMR there are many energy expenditure models as shown in figure 1 which explains the daily energy expenditure need for a body called Total Daily Energy Expenditure (TDEE). Basal metabolic rate (BMR) is the rate of energy expenditure of a person at rest; it eliminates the variable effect of physical activity. BMR accounts for approximately 60% of daily energy expenditure. As such, it includes the energy needed for normal body cellular homeostasis, cardiac function, brain and nerve function, and so on. Numerous formulas exist to calculate RMR/BMR based on inputs such as age, gender, weight, height, and another based on gender and fat-free mass (FFM). As figure 1 show the energy expenditure for a day TDEE is the summation of Resting Energy Expenditure (REE) and non-Resting energy expenditure (nREE). Each form of the word is self-explanatory as REE accounts for energy expenditure at rest whereas nREE accounts for a non-resting state of the body like any physical activity, chewing and grinding of food, etc.

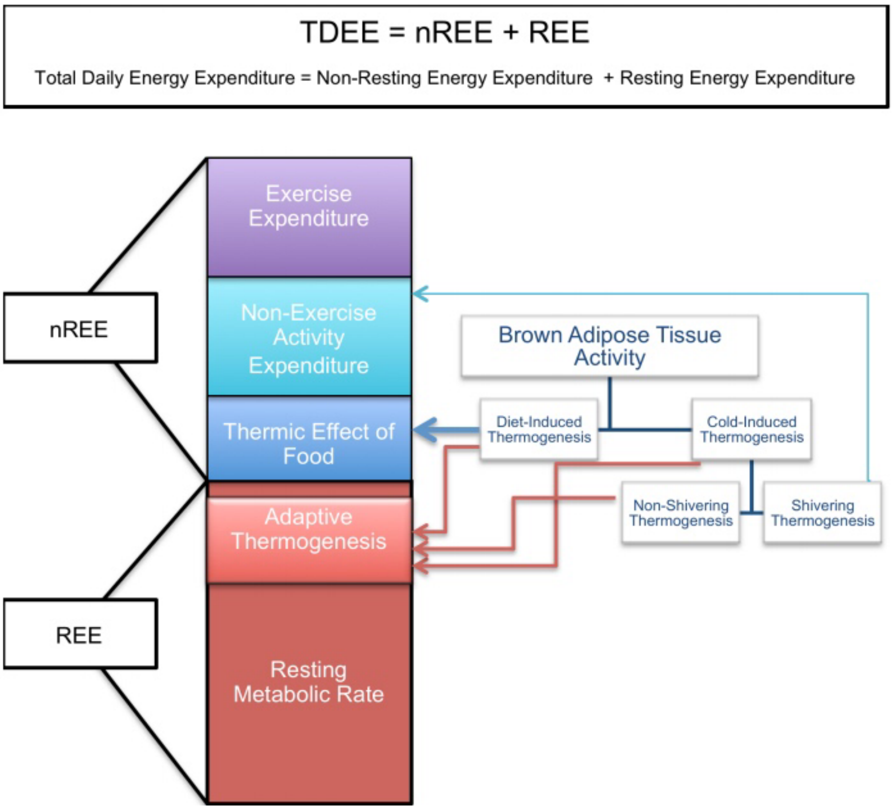

Figure 1: Total Daily Energy Expenditure (TDEE)

Under conditions of standardized physical activity, adaptive thermogenesis occurs when body weight or its components (fat-free mass and fat mass) show a decrease in energy expenditure beyond what would be predicted from body weight or its components. Diet-induced thermogenesis (DIT), cold-induced thermogenesis (CIT), shivering and non-shivering thermogenesis are the mechanisms used by the brain to achieve a healthy body weight by responding to hormonal inputs given by the organs with a normal metabolic rate, Non-Resting Energy Expenditures (nREE) also play a crucial role in this. To maintain reduced body weight, different models have been proposed for energy homeostasis.

EE changes during weight loss are modelled in the following ways:

A. Mechanical Model: According to a mechanical model, EE decreases with weight loss as energy stores are lost.

B. Threshold Model: Based on the threshold model, weight loss below a threshold decreases EE but there is no further increase in EE after losing more weight.

C. Spring loading Model: Adaptive thermogenesis is directly proportional to the amount of weight loss maintained in the spring loading model. It can be compared to Hooke's law that suggests that tension (T) on a spring is equal to a constant (k) multiplied by the change in length of the spring (x) in the spring-loading model. We consider "T" to be adaptive thermogenesis, "k" to differ between individuals but not to be affected by weight loss, and "x" to be the amount lost. To understand AT, all the variables (inputs) responsible would need to be understood since k is different for every individual.

$$T = k*x \Rightarrow (k = ?) \text{---------------------} (1)$$

1.2. Problems Associated with weight loss sustainability

In addition to affecting mental health, obesity reduces the quality of life and reduces life expectancy [15]. As a result of obesity, there has also been an increase in diabetes, heart disease, stroke, and some types of cancer in the United States and worldwide. Weight gain is often accompanied by metabolic syndrome -- an array of conditions that causes high blood sugar, abnormal cholesterol, and triglycerides levels, and high blood pressure which raises the risk for diabetes, heart attacks, and strokes.

Often, visceral fat builds up around the heart, inside the liver, and in other organs. Cirrhosis and liver cancer can develop from liver fat, resulting in the need for a liver transplant. There are now some expert groups that refer to metabolic-associated fatty liver disease (MAFLD) as an alternative term for non-alcoholic fatty liver disease (NAFLD). In addition to some types of cancer, weight gain contributes to others. At least 13 types of cancer are associated with overweight or obesity, including breast cancer, colon cancer, kidney cancer, and pancreatic cancer, notes the Centers for Disease Control and Prevention. Pregnancy complications may also occur as a result of being overweight and obese.

1.3. CALERIE study dataset

Concerning the human body metabolic rates and weight loss, there was one study which is highlighted the most which is the CALERIE study. An association was identified between a dataset from a clinical Trial by Duke University, the school of medical sciences in association with the National Institute on Aging (NIA), and the National Institute on Diabetes, Digestive, and Kidney Diseases. As the CALERIE study is a huge study covering the majority of the medical tests and observations a few parameters were identified based on the keywords identified so far which can be seen in table 1. This data covers all the energy consumption, expenditure, and anthropometric measurements whereas AT is measured using equation 2 where the predicted and measured RMR are extracted from the CALERIE study dataset.

$$AT = \text{Predicted RMR} - \text{Measured RMR} \text{-------------} (2)$$

2. LITERATURE REVIEW

2.1. Correlation between weight loss and adaptive thermogenesis

Individuals lose weight to varying degrees during calorie restriction [1]. It would be helpful to identify determinants of weight loss to formulate new interventions to improve individual outcomes in treating obesity [2- 4]. In metabolic adaptation, the calorie restriction can alter the energy requirement of the body, thereby altering the intensity and duration of weight loss [3-7].

Table 1: Input parameters identified for Adaptive Thermogenesis

Terms	Parameter
WhtR	Waist to height ratio
meanumb	Mean waist size over umbilical cord
BMI	Body Mass Index
clinwt	Body weight
GENDER	sex
height	Body Height
TEE	Total Energy Expenditure
RMR	Resting metabolic rate
PA	Physical activity level
AT	Residual RMR (Adaptive Thermogenesis)
EI	Energy Index
tgrams	Food consumption in grams
tfat	Fat consumption in grams
tcarb	Carbohydrates in grams
tprot	Protein in grams
aniprot	Animal protein in grams
vegprot	Vegetable protein in grams
alcohol	Alcohol quantity
fma	Fat mass based on DXA
ffma	Fat free mass

The metabolically active mass declines more readily when the energy deficit continues [3, 4, 8] than would otherwise be predicted. This may also counteract body weight loss [5]. During various weight loss phases, there may be changes in body composition that affect adaptive thermogenesis [7, 9-11]. The initial weight loss during calorie restriction appears to be caused more by a reduction in the body's muscle, a skeletal mass so-called fat-free mass (FFM) than in fat mass (FM) [7, 9]. FFM is the most responsive determinant of EE distribution [12], when FFM drops during early phases of caloric restriction, EE declines (i.e. adaptive thermogenesis) which can be tracked by altered insulin, sympathoadrenergic, thyroid, and adipokine signalling [4]. In these circumstances, adaptive thermogenesis can be identified during caloric restriction and may predict long-term energy deficiency [3, 4, 13, 14]. The range of adaptive thermogenesis has a range of 1% of measured RMR value to a maximum of 50% of RMR. Beyond that it could be life threating and increase in body weight ratios in record levels. This phenomenon can also be observed in patient undergoing hypo-thyrodism which results in quick weight gain. Usually, a healthy individual would gain weight instantly, it may happen over a prolonged period of time. But an overweight individual who loses a lot of weight could result in massive adaptive thermogenesis in their body resulting in weight regains and endocrine disorders.

2.2. Earlier findings on machine learning in successful weight-loss

Weight loss can be achieved with pharmacotherapy (e.g., orlistat) or surgical interventions (e.g., bariatric surgery), but weight regain is often the result of unsustainable lifestyle habits [16]. Up to 55% of participants in weight loss programs can lose up to 5% of their original body weight within a year through diet and exercise programs, which are cheaper and safer than surgery [17]. However, studies have shown that weight loss leads to regaining up to 100 percent of the weight lost after 6 months [18,19]. In addition to adherence problems [18], motivation problems [20], knowledge problems [21], coping skills, and ineffective self-regulation management [22], the key component of weight loss failure is self-regulation problems [23,25].

The application of artificial intelligence (AI) could be an emerging strategy for combating this issue of poor self-regulation. Artificial intelligence is a technique used to apply knowledge and skills derived from machine learning to process elements such as pattern recognition and decision-making. AI is popular because of its potential for solving real-world problems rationally, efficiently, and effectively. As a result of AI, obesity research can examine aetiologies, profile risk, standardize diagnosis (decision support system), tailor weight loss programs, conduct remote monitoring, and estimate prognoses [26-31]. The ratio of obese middle-aged and older adults, as well as younger adults, was around 45 % for 2017-2018 [32]. According to this study, weight management should begin at a young age to prevent chronic diseases such as obesity and diabetes, which often occur as people reach middle age due to a slower metabolism, more food consumption, and a more sedentary lifestyle [33-35, 41, 44].

2.3. Similar modelling techniques using AI Techniques for medical problems

The advent of AI and machine learning in the current day is extremely rapidly spreading into multiple fields. One of the most important field which deserved a lot more attention due to lack of expertise and availability is medical fields. Predicting human fall detection using ensemble-based machine learning technique using health-based data from blood pressure, heart rate, and sugar level [39]. Identify malarial parasite from microscopic images using ensemble modelling through MIoT data [40]. deep learning technique to identify histopathology images from invasive breast sample and CNN technique with deep learning provided better insights into the sample [42]. using Transfer learning on labelled data skin sample images a model is built using transfer learning via deep learning and CNN techniques [43]. An accuracy 99.13% is achieved to detect the presence of lung cancer in humans using CNN and ensemble of machine learning techniques [45]. Numerous viruses labelled imagery were used to trained a model to classify multiple viruses using logistic regression, Neural networks, KNN and naïve bayes techniques [46].

3. METHODOLOGY

Based on the parameters identified from table no. 1 an inter-relationship study is drawn against the AT, which is the derived element from equation no. 2. Then based on the nature of the data of AT it is decided whether to perform classification or regression study. Observations provide from techniques to fit the output from the input variables help further decide whether further data cleansing is a necessity. In the current scenario, feature scaling was performed to get better results also converting the nature of problem type from regression to classification.

3.1. Failure of regression models

The correlation heatmap in figure 2 is plotted against the features and includes a potential outlier test parameter called score as well. It is clear from the correlation heatmap that BMI, along with waist-to-height ratio (WthR), is highly correlated with adaptive thermogenesis outcomes. In addition, to mean waist size, measured over the umbilical cord, body weight and sex of the individual also showed some correlation compared to the other parameters. Overall protein consumption also showed an inverse relationship, which is also consistent with Pearson's correlation.

Based on these parameters, regression-based machine learning algorithms were applied to fit a model for adaptive thermogenesis. In table no. 2, the results of this implementation are nowhere near usable, therefore, a feature scaling would be suggested based on the nature of the AT, which is a continuous variable. At the end of this section, following the results table and highlights for AT, we will explain the feature scaling method.

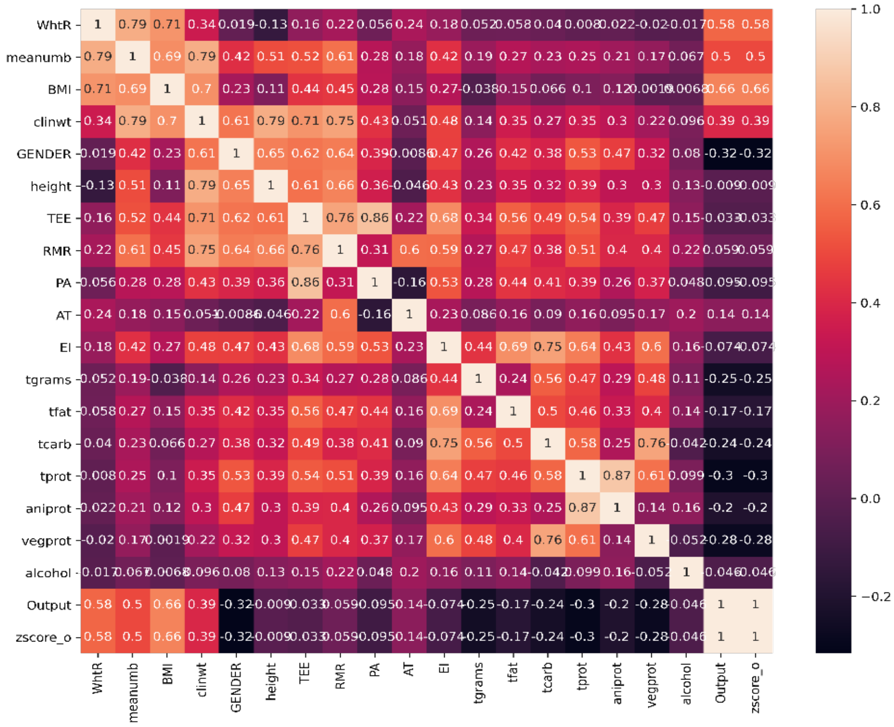

Figure 2: Correlational heatmap of features for Identification of AT

Table 2: Results of the regression analysis for AT

Model	MAE	MSE	RMSE	R2	RMSLE	MAPE
Bayesian Ridge	88.1712	12699.8	110.6832	0.134	1.4561	2.8351
Elastic Net	87.5445	12716.17	111.2128	0.1136	1.4243	3.0603
Lasso Least Angle Regression	90.5831	13313.11	113.37	0.0995	1.63	1.8465
Lasso Regression	88.2838	12923.29	112.2009	0.0965	1.4249	3.0592
CatBoost Regressor	89.0506	13139.01	112.9782	0.0962	1.6327	3.0472
Extra Trees Regressor	90.1231	12914.26	112.3331	0.0962	1.6209	2.1601
Random Forest Regressor	89.7273	12913.15	112.4162	0.0956	1.5109	2.5539
AdaBoost Regressor	90.2995	13422.48	113.9426	0.0852	1.3387	2.575
Ridge Regression	89.1727	13113.72	113.055	0.0804	1.4539	3.0411
Linear Regression	89.8385	13336.11	113.9859	0.0635	1.4769	3.0427
Huber Regressor	94.4714	13819.4	116.1046	0.0239	1.416	3.2058
Least Angle Regression	91.962	13734.05	116.0432	0.0161	1.4799	3.4825
Orthogonal Matching Pursuit	96.274	14945.84	120.5176	-0.0268	1.5384	2.2719
Gradient Boosting Regressor	97.6204	14832.91	120.5589	-0.0425	1.472	3.1256
Light Gradient Boosting Machine	95.8494	15088.7	121.5515	-0.058	1.3896	3.4977
K Neighbors Regressor	99.6361	15017.46	120.7594	-0.059	1.6036	3.3874

Due to low variance and high biases in the data during testing, high underfitting has been observed. The model is too simple to learn from too few parameters, thereby fitting the dataset into a mathematical model. Consequently, a change is introduced in the form of the selection of features for the AT variable.

3.2. Feature Scaling

AT variable is converted to a binary output based on the RMR values of the individual. If the AT is less than or equal to -5% of the RMR variable then the output is set AT = 1 else set AT = 0. Now this problem has become a classification problem which is explained below.

IF AT <= -5% of RMR

THEN AT == 1

ELSE AT == 0

Now, this becomes a Binary classification problem either 0 or 1. Therefore, a classifier is proposed to predict whether the individual is undergoing AT or not.

4. RESULTS AND DISCUSSION

A large number of machine learning-based classification algorithms were run on the newly scaled variable of the Adaptive Thermogenesis parameter, which is the parameter of interest. Due to the nature of the problem, logistic regression (LR) is the first and foremost algorithm to use. As an alternative to decision trees (DT), an algorithm called the decision tree classifier is considered. [37,38] The Explainable Boosting Machine (EBM) is currently the state-of-the-art machine learning algorithm. This algorithm demystifies the black box of machine learning as well as the no-free lunch theorem. With more data provided for learning purposes, EBM produced a better result than linear regression, which could generalize the solution with fewer data. The following figures 3-5 are used to display metrics such as accuracy and F1-score for algorithms used for building models using data 80% for training and 20% for testing. Based on the results, EBM produced significantly better results than others with 78.4% accuracy and a 73.9% F1 score. In figure 6 overall importance scores were across the model built using EBM. In this figure, it can be observed that unlike other machine learning techniques EBM models do check for combinational inputs. Where animal protein and alcohol consumption provided the highest weightage to the model followed by pulse, blood pressure, and body anthropometric measurements like waist size, waist to height ratio, etc, and its combinations. EBM removes the vulnerability of black-box modelling using ensemble learning techniques for better accuracy and creates the factor of greater explainability.

According to Figure 4, the train and test dataset sizes varied from 70% training to 30% testing and the EBM model dramatically degrades, because it is heavily dependent on more data. However, the LR model was superior to DT in that it was able to make better generalizations in the face of fewer data. In figure 5, the train and test sizes are shown to be 60% and 40% of the data respectively. All the models performed poorly but LR provided an F1-score and an accuracy that was decent enough.

Test size = 20%

	LR	DT	EBM
Accuracy	0.7076	0.6153	0.7846
F1 Score	0.6771	0.5966	0.7397
C.M	T 0: 33, 9 T 1: 10, 13 P: 0, 1	T 0: 27, 15 T 1: 10, 13 P: 0, 1	T 0: 39, 3 T 1: 11, 12 P: 0, 1

Figure 3: Metrics for 20% test size

Test size= 30%			
	LR	DT	EBM
Accuracy	0.7319	0.690	0.680
F1 Score	0.709	0.623	0.629
C.M	0 49 14 T 1 12 22 0 P 1	0 54 9 T 1 21 13 0 P 1	0 51 12 T 1 19 15 0 P 1

Figure.4 metrics for 30% test size

Test size = 40%			
	LR	DT	EBM
Accuracy	0.7131	0.6589	0.6976
F1 Score	0.6859	0.6116	0.6578
C.M	0 65 21 T 1 16 27 0 P 1	0 65 21 T 1 23 20 0 1 P	0 67 19 T 1 20 23 0 1 P

Figure.5 metrics for 40% test size

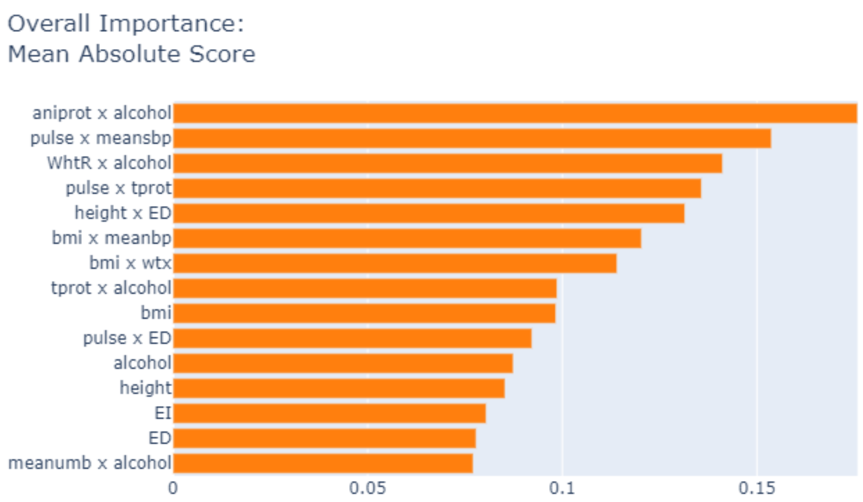

Figure 6: Feature importance for EBM model

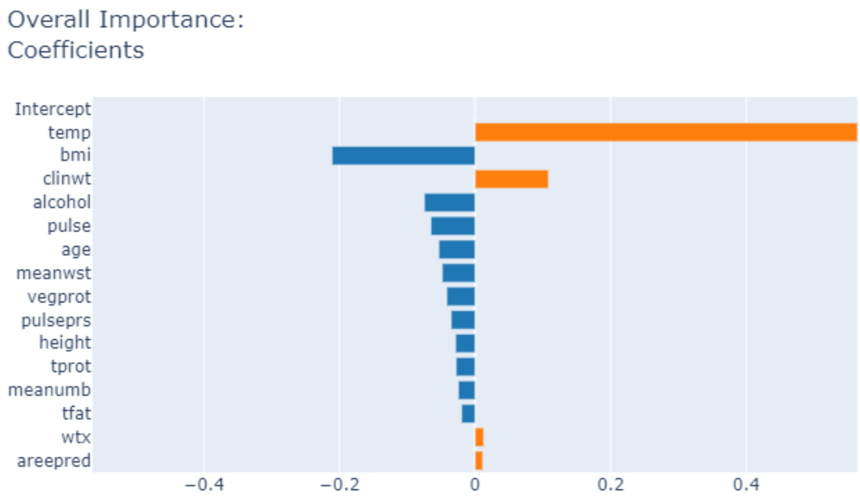

Figure 7: Feature importance for LR model

Using the correlation heatmap from figure 2, it is observed that body temperature has a significant dependence on other features. In addition to BMI, body weight is also a factor that can lead to multicollinearity since BMI has a relationship with body weight. Following pulse and age, the alcohol showed another inverse relationship.

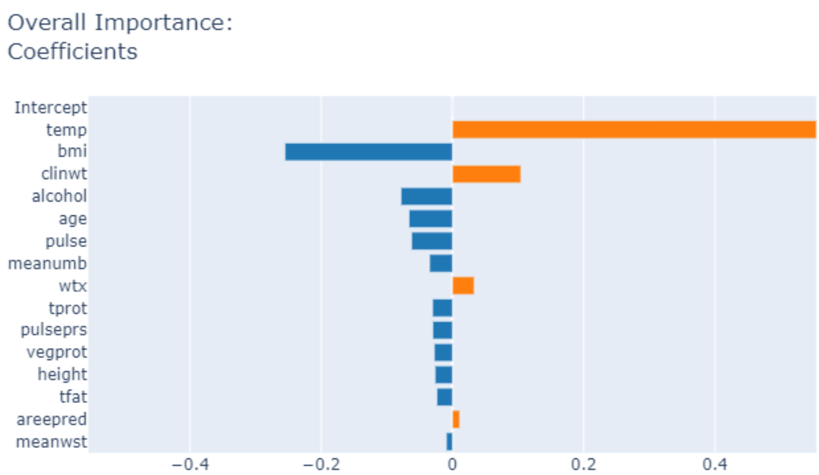

Figure 8: Feature importance for LR model

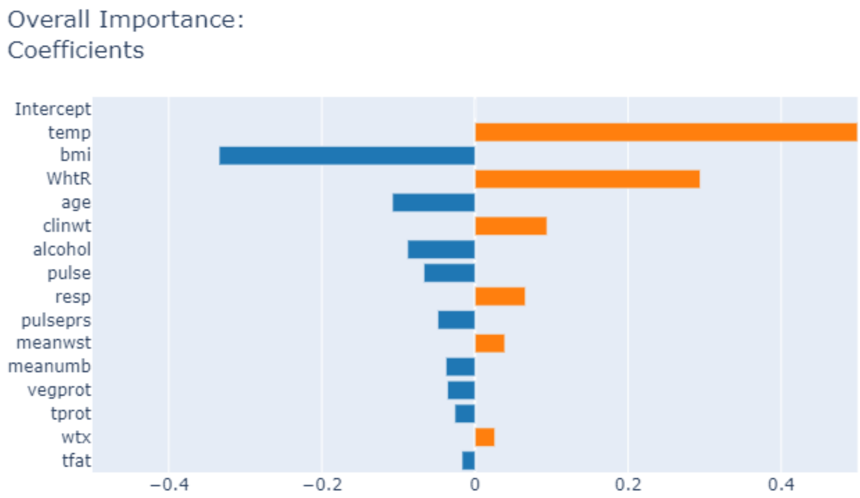

Figure 9: Feature importance for LR model

The overall feature importance graphs from figure 7-9 represent the models built using the logistic regression technique. Of which figure 7 represents the 20% test and figures 8,9 represent 30 and 40% test data respectively. In every model, temperature gave the highest importance followed by BMI and alcohol consumption rate. Interestingly, the graphs of feature importance for only LR models for both experiments for 30% and 40% test data reveal that Logistic Regression (LR) is by far the most probable choice. In all cases, body temperature, BMI, Alcohol, pulse, and waist to height ratio (WhtR) showed up at the forefront of importance levels. The original dataset is used to create a synthetic dataset, which is used for the validation of different models. In addition, 30% of the test data model is used to validate the model using synthetically generated data based on the original CALERIE study dataset. Adaptive Thermogenesis (AT) in humans can be identified using these models and they provided satisfactory results.

5. CONCLUSION

With the development of these models, it can be a substitute for invasive techniques but still has its limitations in being correct all the time. Limitations such as 78.46% probability to identify an individual with Adaptive thermogenesis with all non-invasively trackable parameters. Where body temperature, alcohol, and protein consumption played a major role. When this model is tested with synthetically generated data which has a similarity index of 86.7% with original data, AT classification achieved an accuracy of 0.66372. The limitations of correctly classifying an individual with insulin resistance have a probability of 84.37% with an AUC score of 0.58 which can be further improved with more data. Adaptive thermogenesis is still more of a scientific term than a real-world term, generally termed as weight regains for some reason which is yet to be identified. If that reason is identified the problem can be directly pinpointed and resolved. In the proposed study using all non-invasive parameters, a machine learning model is generated, with this model it will be easier to identify whether the individual is undergoing AT. If identified which parameter is being influenced the most. Based on the influences one could target the remedy to reduce the particular influence on his/her body. This model is designed for the range of age groups between 20-53 years, both sexes, height between 147-204cms, weight between 43-99kgs. With the latest advancements in wearable technology, even temperature sensor is being observed as one of the features while being sold commercially, which ended up being one of the major features of the proposed work.

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