Statistical Study of Fruit-Infused Chocolate Science, Process and Product

Mason Chen[1], Kaitlyn Zhang[1], Charles Chen[2]
[1]Stanford University OHS, Palo Alto, CA, USA, mason05@ohs.stanford.edu
[2]Applied Materials, Sunnyvale CA, USA, charles.chen.training@gmail.com

Abstract
This paper will apply "STEAMS" methodology on Chocolate Science. The science will mainly address how the antioxidants in chocolate help reduce free radical formation and increase production of nitric oxide. Free radicals, atoms with an odd number of electrons, damage blood vessels when oxidized by LDL which consequently increases the risk of heart disease (Technology and Engineering). Nitric oxide relaxes blood vessels which increases blood flow. Data was collected on 20+ chocolate ingredient nutrition factors from 60+ different types of chocolate but were missing the Cocoa%. AI Neural Network algorithm was utilized to impute the missing Cocoa%. The hyperbolic tangent activation function was used to create the hidden layer. In order to overcome the Neural over-fit issue, definitive screening design (DSD) DOE technique was used to optimize the AI Neural algorithm. The optimal Neural setting can improve validation fitness R-Square by more than 20%. Based on the optimized neural model, Chocolate Type and Vitamin C are the highest predictors of estimating Cocoa%. Because fruit is high in Vitamin C, there could be further health benefits from dark fruit chocolate. This may indicate the potential to evaluate a 4th Chocolate Type: Fruit Chocolate – which may be healthier than Dark Chocolate. Several Fruit Chocolate Process are compared on the challenges of making Fruit Chocolate product.

Key Words: Flavonoids, Fruit Chocolate, Antioxidant, Neural, Clustering

1. Introduction

Many people like eating chocolate but have concerns that chocolate is unhealthy. Are they sure whether eating chocolate is unhealthy? The objectives of this paper are to find out if eating chocolate is unhealthy, what diseases can be prevented by chocolate, why can chocolate prevent those diseases, what chocolate nutrition help prevent those diseases, how to select the best chocolate for preventing those diseases, and how the Fruit-Infused chocolate can lower the sugar amount?

1.1 Atrial Fibrillation Literature Research

Some literature research has studied the benefit of eating chocolate can lower the relative risk of CVD (cardiovascular disease). Research shows that individuals consuming chocolate > once per week have a lower risk of AF (Atrial Fibrillation: a type of common cardiovascular heart disease) than individuals consuming chocolate regularly. In Figure 1, the x-axis is the chocolate consumption (30 g / week) while the y-axis is the risk of CVD. There was little further reduction in the risk of heart disease greater than 3 servings per week. This proves that chocolate, especially dark [1], may be inversely associated with AF and a healthy snacking option. A lot of time was taken to find this chart that showed chocolate does help prevent heart disease [2].

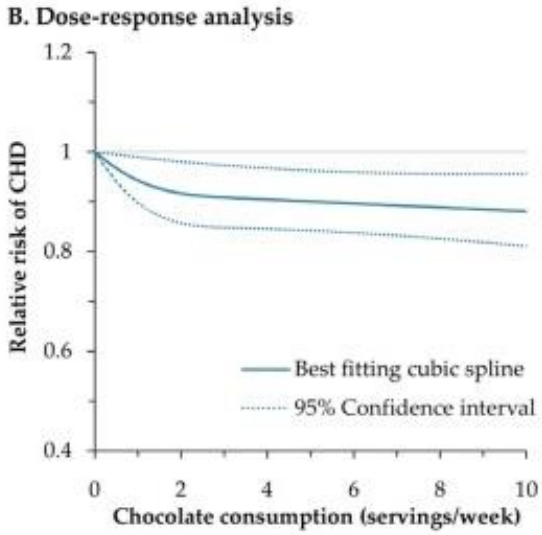

Figure 1: Chocolate Consumption vs Risk of Cardiovascular Heart Disease [3] (1 serving = 30 g)

In Figure 2 Scatterplot, the median life expectancy has been correlated to the mean chocolate consumption across major countries. No correlation was indicated by random scattering pattern. There is no strong and direct evidence to demonstrate eating chocolate is detrimental to human health.

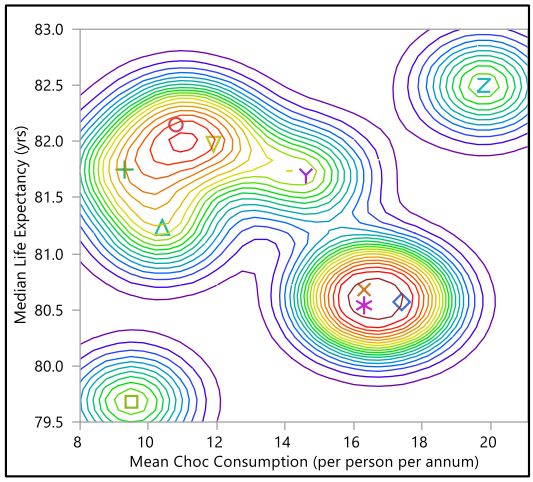

Figure 2: Life Expectancy vs. Chocolate Consumption

1.2 Study Chocolate Ingredients

Most chocolates are made from milk powder, sugar, cocoa butter (butter extraction from liquor), and cocoa liquor. Dark chocolate has more contents of cocoa liquor, cocoa butter and less of sugar. White chocolate has the opposite quantities. Milk chocolate composition is in the between Dark Chocolate and White Chocolate. Will these composition patterns indicate which chocolate type is healthier? Authors will like to study Chocolate Technology and Science in the following section.

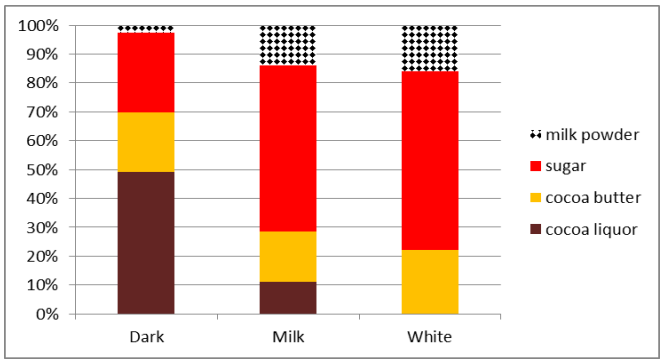

Figure 3. Chocolate Ingredients

1.3 Flavonoids Science and Structure

Now that chocolate is proven to help prevent against heart disease, what is the critical ingredient in chocolate that prevents against heart disease? Flavonoids are the most abundant polyphenols in the human diet [4], representing 2/3 of those digested [5]. Polyphenols are compounds found abundantly in natural food sources that have antioxidant properties. Flavonoids have the general structure of a 15- carbon skeleton as shown in Figure 4. The structure is abbreviated as C6-C3-C6 and consists of two phenyl rings (A and B) and a heterocyclic ring (C). There are seven different types of flavonoids (classified based on its chemical structure): flavones, flavanol, flavanones, isoflavones, anthocyanidins, chalcones, and catechins. Chocolate flavonoids are flavanols. Antioxidants are the critical ingredient that prevents against heart disease. The higher the antioxidant, the higher the cocoa percent. Dark chocolate has the highest cocoa percent, so it should be the healthiest chocolate [6].

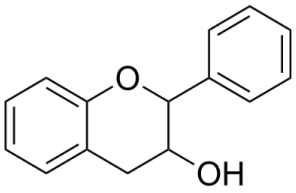

Figure 4: Flavonoids Structure

Why do antioxidants prevent heart disease? Cocoa flavanols which contain antioxidants promote healthy blood flow from head to toe [7]. Flavonols are known to increase blood flow and revive your body, slowing aging. They do this by triggering the natural production of a compound - nitric oxide. Nitric oxide relaxes blood vessels, keeping them open, allowing blood to distribute nutrients and oxygen all around. Therefore, by boosting nitric oxide levels, the body becomes more nourished, strong, and consequently youthful. The heart, brain, and muscle depend on a healthy circulatory system [8]. Supporting healthy blood flow is essential to helping maintain exceptional health throughout life [9]. Flavanol benefits include a longer life, weight control, and prevention of cardiovascular disease, cancer, diabetes, and neurodegenerative disease [10]. People with heart diseases should eat less saturated fat, trans fat, sodium, and cholesterol [11]. They should eat more dietary fiber [12]. We know that chocolate contains antioxidants which are the key ingredient that prevents heart disease [13]; however, is chocolate the only food that prevents heart disease? Antioxidants can prevent heart disease is because it reduces free radical formation. Free radicals are atoms with an odd number of electrons. When radicals form, they become highly reactive which causes cells to function poorly or die [14]. As shown in Figure 5, excess free radicals initiate Cardiovascular disease **(**CVD**)** by damaging blood vessel. Bad

cholesterol, Low-Density Lipoproteins (LDL), can also and only cause CVD after the oxidation of free radicals [15]. The oxidized components attract macrophages which absorb & deposit cholesterol [16].

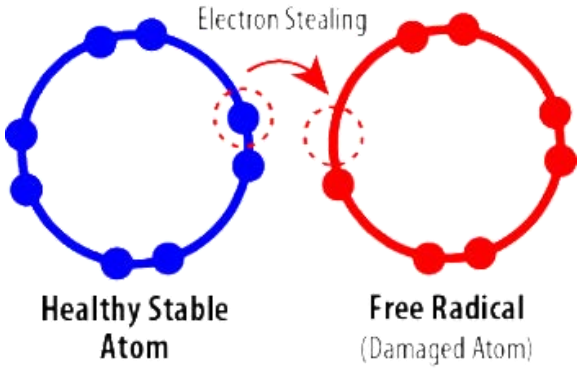

Figure 5: healthy stable atom and free radical

Chocolate is actually a powerful source of antioxidant. Antioxidant prevents aging which is healthy for human body. Antioxidants are also essential to preventing heart disease since it increases blood flow. Apple and Blueberry are well known fruits with excellent antioxidant functions. In Fig.6, if chocolate's serving size is equal to apple, it has the most antioxidant amount among all the foods listed. The next objected interested is why Chocolate can have such rich antioxidant effects?

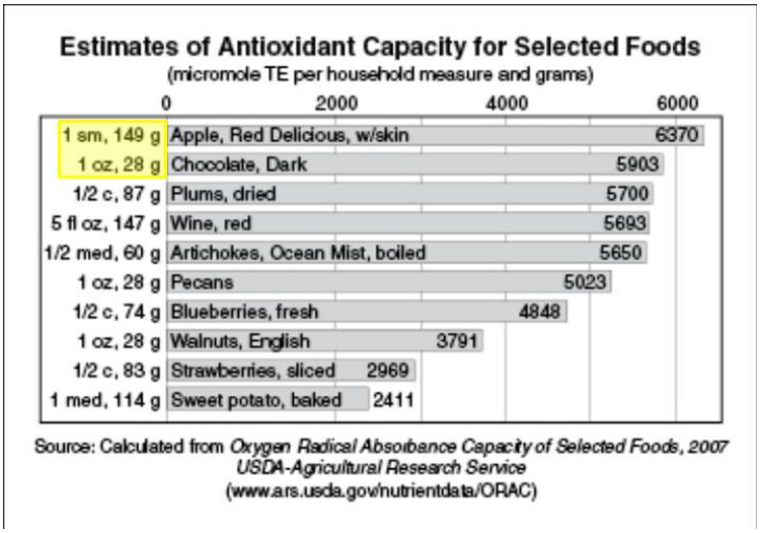

Figure 6: Estimates of Antioxidant Capacity

2. Chocolate Process, Technology and Fruit Chocolate

Chocolate's high fat and sugar content is a downside, compared to its high levels of healthful plant-based substances termed antioxidants or flavonoids. A 2-ounce serving of premium dark chocolate may contain 13 grams of fat — 20 percent of the total daily fat recommended for a person who eats 2,000 calories per day. Much of that fat is the unhealthy saturated variety. Since the juice is spread out in the chocolate, it doesn't overpower the taste of the chocolate. The opportunity to replace part of the fat matrix with

water-based juice droplets allows for greater flexibility and tailoring of both the overall fat and sugar content. Pickering discovered a new way to stabilize emulsions — combinations of liquids like the egg yolk and oil in mayonnaise that normally would not mix together [17].

2.1 Chocolate Manufacturing Process and Technology

What chocolate manufacturing process is critical to determine which chocolate is healthy. In Fig. 7 chocolate process flow chart, Cacao pods are first collected from cacao trees. Then, cacao beans are eliminated of its pods and dried under the hot sun. Different type of cacao beans will decide what chocolate ingredient in rich. The dried beans are shipped to chocolate makers and washed thoroughly. Cacao beans are cooked in a certain high temperature and roasted to control certain chocolate attributes. Nibs, or the "fruit" of the cacao bean, are grinded into cocoa liquor. Cocoa butter is extracted from cocoa liquor. The remaining cocoa cake is grinded into cocoa powder. The cocoa liquor is added with cocoa butter, sugar, and other ingredients depending on the manufacturer and the chocolate type. The mixture is soothed under heating (conching) before put in molds, cooled, and shipped. Understand this chocolate manufacturing process will help us categorize chocolate types and their major ingredients as well as process control.

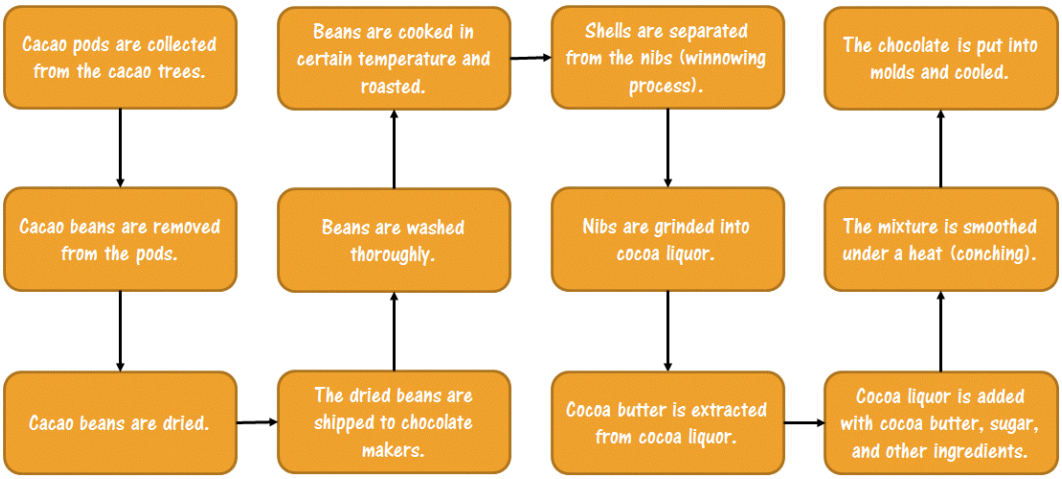

Figure 7: Chocolate Manufacturing Process [18]

2.2 Fruit Chocolate Process Challenges

Infusing products with fresh herbs or fruit rinds, involves chocolate, which is highly sensitive to heat and never should be boiled. A host substance must be used apart from the chocolate for the infusion to work and then the infused liquid can be added to the carefully melted chocolate [19]. Chocolate is an emulsion of cocoa butter and water or milk combined with cocoa powder. Lecithin appears on the ingredient label in many chocolates because it is an emulsifier that fosters the process. Pickering's method used solid particles rather than an emulsifier. Fumed silica particles are used in combination with chitosan under acidic conditions (pH 3.2–3.8) to prepare water-in-oil emulsions, the oil phase being sunflower oil, molten cocoa butter, and ultimately white, milk, and dark chocolate [20].

2.3 Freeze Dried Fruit in Chocolate

Freeze drying could unlock the potential of red berries and citrus fruits as decorations and inclusions in chocolate while preserving the color and nutrients of the fruit [21]. Many

fruits such as strawberries and oranges were not previously suitable in chocolate confectionary due to a high water content that reduces shelf life. Freeze drying extracts almost all of the water content and preserves the color and nature of the fruits opening up fresh possibilities for manufacturers. Fruit is typically added to chocolate as an air dried product such as the dried raisins and banana chips. Nutrients are also maintained after freeze drying. Vitamin content, phenolic content and antioxidant activity were all preserved after the low temperature process. Freeze dried fruits maintain a fresh flavor and bright color. It won't fell like a fruit. It will be dry and slightly crispy. Freeze dried powders such as raspberry, strawberry, orange and blackcurrant can be used to make these fruit infused chocolate truffles. The options for freeze dried fruits in confectionary range from enrobing whole or large pieces to using small fruit pieces or powders as inclusions inside chocolate like adding nuts. The typical shelf-life for a freeze-dried fruit is around 12 months. The strawberry was proving as most popular offering.

2.4 Fruit-Infused Chocolate

Infusion is the process of transferring the flavor of one product into another. A new technology [22] would infuse chocolate with fruit juice (Apple, Orange Cranberry), vitamin C water or diet soda, lowering the fat by 50 percent, according to research shared at 2013 American Chemical Society. Although chocolate, particularly the dark variety, offers cancer-fighting agents such as antioxidants, its high fat and sugar content lessens these benefit. Replacing sugar with fruit juice or soda reduces the overall sugar content. How to Flavor Chocolate. Chocolate goes well with almost any fruit flavor. Citrus flavors, like orange and lemon, grapefruit and lime, tart fruits like cranberries, pomegranates, and even pineapple also pair nicely with chocolate [23]. The taste and "mouth feel" leaves much to be desired. Using a technique known as a Pickering emulsion [24], filler liquid is added to the chocolate in the form of micro-bubbles, which help it retain its lush, velvety texture. Plus, it will also prevent "sugar bloom" -- the unappetizing white film that coats the surface of chocolate that's been on the shelf for a while.

3. Graphical and Statistical Analysis of Chocolate Science and Product Type

Section 1 explained the Chocolate scientific research and Section 2 explained the traditional Chocolate Process, and the modern Fruit Chocolate Technology. This section will conduct statistical modeling to demonstrate the trending of Fruit Chocolate.

3.1 Raw Data Collection

It's critical to collect the right chocolate data. Target was chosen since it had plenty of chocolate products (enough sample size) and was extremely convenient for collecting data. 60+ different types of chocolates were collected, and each had 20 variables. Ensuring good data quality is critical to screen out noise data. Not all 20 variables were used; instead, only 8 variables that were crucial to heart disease based on Define Phase were used as shown in Figure 8.

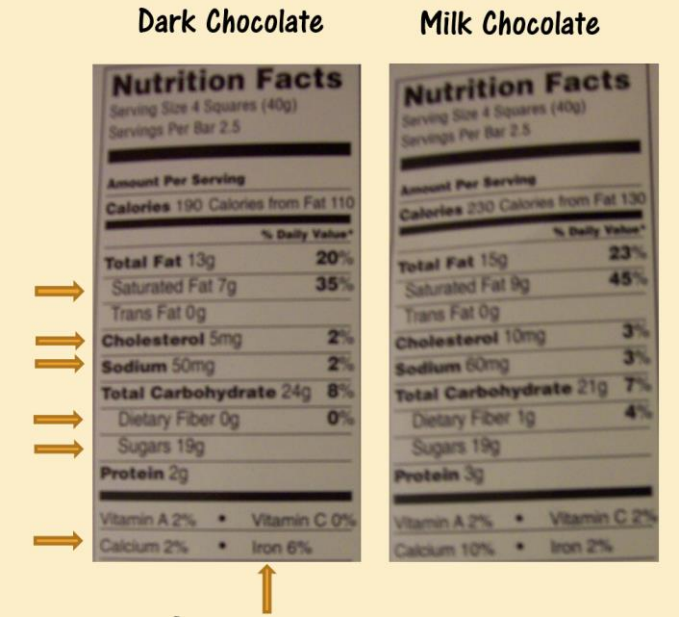

Figure 8: 8 chocolate nutrition variables chosen

3.2 Variable Clustering of Chocolate Nutritions Science

Variable clustering (Figure 9) was conducted to find out and analyze the correlations between the ingredients within the cluster. The red squares near each form different clusters. There is one large red group on the top left, two medium groups in the middle, and another large one located in the bottom right. The top 2-3 highest correlations, based on highest r-squares (Figure 10), were analyzed. The 8 variables chosen by scientific research were saturated fat, cholesterol, iron, dietary fiber, sugar, calcium, cocoa percent, and sodium. Will the top 8 variables chosen by JMP clustering match the 8 variables chosen by science? The first cluster was grouped because the higher the saturated fat, the higher the total, and therefore, the higher the calories. Saturated fat was chosen since it had a high r-square which matches one of the 8 variables chosen by research. The second cluster justified that calcium and cocoa percent should have a negative correlation since dark chocolate contains the most cocoa and should have the least amount of milk. The lower the cocoa percentage, the higher the milk since white chocolate contains the most milk but the least amount of cocoa. The three highest r-squares from the second cluster were cocoa-percent, cholesterol, and calcium which all match the 8 variables chosen by science. For the third cluster, sugar and carbohydrates have the highest r-square and sugar matches with the top 8 variables. For the last cluster, dietary fiber and iron had the highest r-square and also matches with the 8 variables. In conclusion, the 8 variables chosen by statistics do match the 8 variables chosen by science. Statistics can back up Chocolate science. Question here is how can we differentiate Fruit Chocolate Product from traditional Chocolate Products (Dark, Milk, White). Can we claim Fruit Chocolate as 4th Chocolate Product Type today.

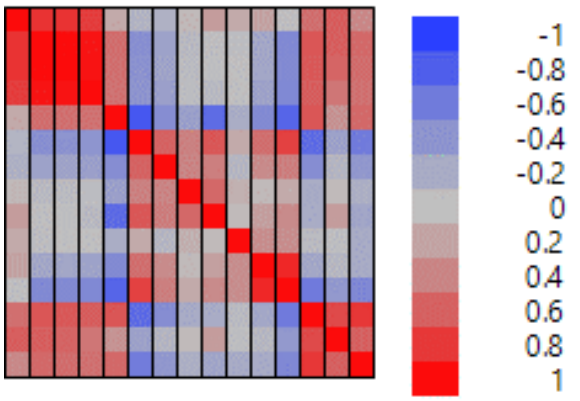

Figure 9: Correlations Color Map

Cluster	Members	RSquare with Own Cluster
1	Calories (g)	0.789
1	Calories_from_Fat (g)	0.976
1	Total_Fat (g)	0.977
1	Saturated_Fat (g)	0.935
2	Cocoa_Percent	0.742
2	Cholesterol (mg)	0.811
2	Vitamin_A	0.505
2	Vitamin_C	0.412
2	Calcium	0.726
3	Sodium (mg)	0.345
3	Carbs (g)	0.876
3	Sugar (g)	0.874
4	Dietary_Fiber (g)	0.888
4	Protein (g)	0.73
4	Iron	0.803

Figure 10: Cluster Members and R-Square

3.3 Modern Neural Network Algorithm

Due to missing values of Cocoa% in most Chocolate Product, in order to differentiate Fruit Chocolate Product, the modern Neural Network [25-27] (known as Artificial Intelligence) was conducted to find the patterns of different product types. Neural Network implements a fully connected perceptron (hidden nodes) with one or two layers. The functions applied at the nodes of the hidden layers are called activation functions. In this Neural Algorithm, only three product types (Dark, Milk, and White) are listed in the Predictive Model, which on purposely exclude the Fruit Chocolate as 4th Chocolate Type.

In Figure 11, the optimal neural setting was further validated based on the available chocolate products. Both the R-Square of Training and Validation are beyond 0.99. The optimal neural setting has significantly improved the validation goodness fit R-Square by more than 0.2 (20%) while sustaining the very perfect training R-Square. Based on the sensitivity ranking of predicting the Cocoa%, Chocolate Type is still the top factor but not a dominant one. Vitamin_C has surprisingly emerged as the second top predictor. It may suggest that, in addition to dark, milk, white chocolates, the fourth "fruit" chocolate should be added. The optimal Neural Algorithm only enhances the modeling goodness fit, but also reveals the hidden Chocolate Science and Product in the Profiler Sensitivity Analysis. Neural Network algorithm has been repeatedly criticized on its "Black Box"

transformation as it is unclear how the data is transformed. However, most data scientists should dig deeper on the modeling sensitivity and map these patterns to the real "science and engineering" world.

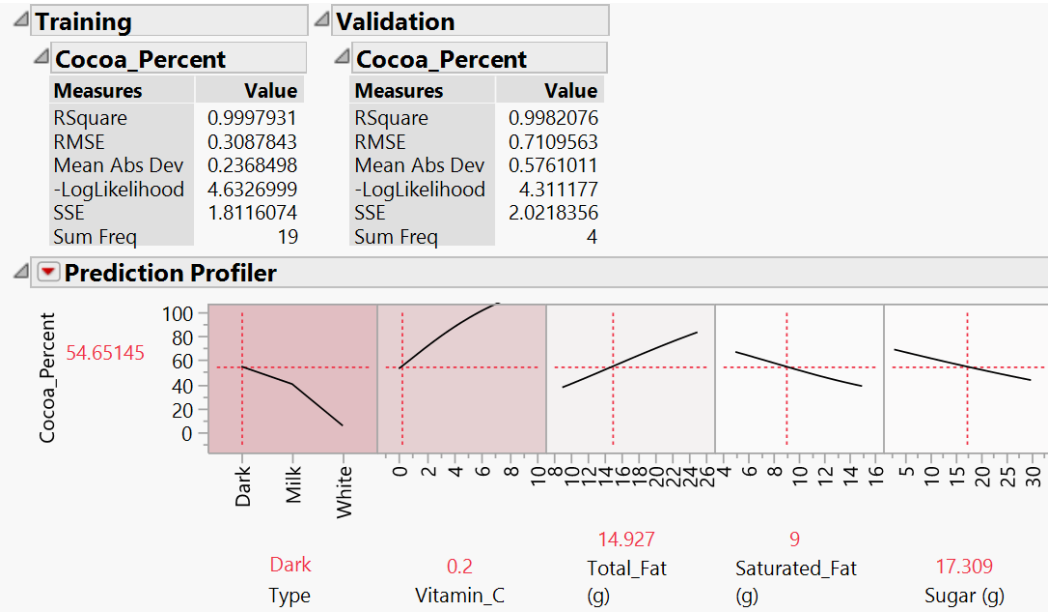

Figure 11: Neural Analysis of Chocolate Product Type

4. Conclusions

This paper has studied the Chocolate Science and Anti-Oxidant CVD prevention mechanism. Fruit Chocolate is a healthy trend to make Chocolate Product less-sugar and more-vitamin C. Several Chocolate process techniques have been introduced to overcome the Chocolate-Infused heating challenges. Both JMP Cluster Variable and Neural Algorithms have further explored the Chocolate Science and demonstrated the Fruit-Chocolate potential to become the 4th Chocolate Product Type. Statistical modeling approach is powerful to conduct scientific research on Food Nutrition Science. The same Data Mining approach can be extended to most Scientific Research fields which can shorten the Research and Development learning curve and product development cycle.

Acknowledgments

I would like to thank my biology advisor Mr. Patrick Giuliano for helping and supporting me throughout this project.

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