AI for Fragrance Design

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Abstract

AI for fragrance design builds on IBM's work on Chef Watson to create a system for designing new fragrances. Our system generates alternative fragrance formulations and selects the formulation that best optimizes design objectives. We use machine learning to predict both the technical performance of candidate fragrances (shelf stability and skin irritation) as well as the human response (pleasantness and gender appropriateness). We identify if a fragrance is novel by comparing its notes to a large set of commercially available fragrances. The end goal is to use artificial intelligence to design award winning new fragrances.

1 Introduction

Fragrances are designed by Master Perfumers who typically train for 10 years before they become proficient at their craft [1]. There are many technical aspects that must be mastered, such as how to formulate fragrances that won't irritate the skin and that won't turn cloudy or turn color when left on the shelf for months. Beyond the technical requirements, a perfumer must create a fragrance that smells good, triggers a desired emotional response and is unique.

The goal of our work is to help create new and novel fragrances that perform well technically, but more importantly, smell good and are unique. We are building on earlier work on computation creativity for food that used models of flavor pairing and psychological modes of olfactory pleasantness to identify recipes of dishes that would taste and smell good [2]. In the fragrance space, we don't have the equivalent of the flavor pairing hypothesis, we can't use a simple model of olfactory pleasantness, and surprise comes not in the combination of ingredients, but from the combination of fragrance notes for a perfume [3].

2 Fragrance Creation

Fragrance creation begins when a perfumer specifies a set of target notes, the technical requirements for the new fragrance, and the target market. We use a generate and evaluate architecture to create new fragrances. Each fragrance is evaluated and scored using a multi-attribute evaluation function that considers how well it hits the target notes, its overall pleasantness, its technical performance, and its uniqueness in the market.

To know whether a fragrance is unique, you need to know the set of existing fragrances. Fragrances are typically characterized by the set of fragrance notes exhibited in the top, middle and base of the fragrance. A unique combination of fragrance notes indicates a unique fragrance. Figure 1 shows a plot of 3319 commercially available perfumes we have collected from a publicly available web

31st Conference on Neural Information Processing Systems (NIPS 2017), Long Beach, CA, USA.

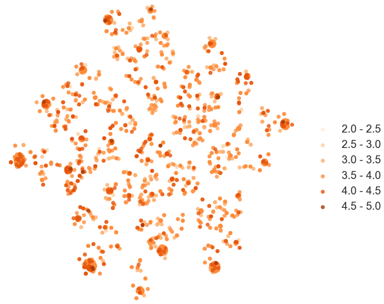

Figure 1: Commercially available perfumes, projected by fragrance categories and colored by success.

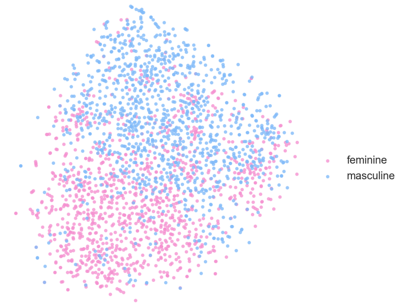

Figure 2: Commercially available perfumes, projected by notes and colored by target gender.

Table 1: Gender Confusion Matrix

Gender	Predicted Female	Predicted Male
Female	189	42
Male	43	202

Table 2: Rating Class Confusion Matrix.

Rating	Predicted High	Predicted Low
High	1021	716
Low	547	1019

site [4]. The plot is a t-SNE projection of the dominant odor characteristics of each perfume, colored by their average rating [5]. This non-linear dimensionality reduction method allows us to uncover cluster relationships in the high-dimensional data set and to project them in the 2D dimensional space with the intrinsic structure preserved. You can see that the perfumes tend to form clusters around some of the more highly rated ones, representing a "copy cat" effect. The white spaces in the diagram indicate combinations of fragrance notes that have not been explored commercially. Creating fragrances in these white spaces will create new and novel combinations of fragrance notes.

Just producing a unique fragrance is not enough. The fragrance needs to be appropriate for the intended consumer and highly rated. Figure 2 shows a t-SNE projection of the sub notes of the perfumes colored by intended gender. A dominant note might be citrus, while a sub-note might be mandarin orange or lemon zest, both types of citrus. Using the collected data, we train classifiers to predict target gender and average rating for unseen fragrances, characterized by their notes. The performance of the classifiers is shown in tables 1 and 2. We can see that gender prediction is relatively good at over 80%, while ratings prediction is only about 62%. From the diagrams, you can see that gender is fairly well separated. While for ratings, the clusters of copy cat formulas makes distinguishing highly rated formulas more difficult.

Any perfume that is not shelf stable, is flammable, or irritates the skin will be rejected both by regulators and the market. We use machine learning to predict the technical properties of fragrance formulas. These learned models are then used to filter prospective formulas to remove those that will not meet regulatory requirements.

3 Conclusions

Fragrance creation is an area that is ripe for the application of AI because it requires deep technical knowledge, the ability to predict human response to complex combinations of ingredients and the need for originality. Our work is aimed at helping Perfumers be more creative and productive.

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