Journal of Informatics
Electrical and Electronics Engineering, 2024,
Vol. 05, Iss. 02, S. No. 112, pp. 1-12
ISSN (Online): 2582-7006

Refining Color Scheme Generation: Iterative K-Means Clustering and ARI Evaluation

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How to cite this paper: A. Yadav, P. Singh, "Refining Color Scheme Generation: Iterative K-Means Clustering and ARI Evaluation" *Journal of Informatics Electrical and Electronics Engineering* (*JIEEE*), Vol. 05, Iss. 02, S No. 001, pp. 1–12, 2024.

https://doi.org/10.54060/a2zjournals.jieee.112

Received: 08/01/2024
Accepted: 30/04/2024
Online First: 06/06/2024
Published: 31/12/2024

Abstract

Color goes beyond mere visual sensation, holding profound sway over emotions, thoughts, and perceptions. It communicates, evokes moods, and significantly influences judgments. Research underscores its importance, with up to 90% of product assessments being based solely on color, highlighting its pivotal role in crafting memorable experiences and defining brand identities. The fusion of art and technology presents a captivating synergy within the realm of image-derived color schemes. Color palette generation from images is pivotal in graphic design, interior decoration, and digital media. This study delves into methodologies for extracting dominant colors from images and generating cohesive color schemes. Leveraging K-Means clustering with the Within-Cluster Sum of Squares (WCSS) method, we showcase superior performance compared to traditional approaches. The evaluation of palette coherence using the Adjusted Rand Index (ARI) facilitates consistency within the generated color schemes. Integrating methodologies with design tools and advanced color harmonies opens avenues for further innovation and customization. This study underscores the transformative potential of image-based color scheme generation, bridging the gap between computational analysis and creative expression. Through the convergence of artistry and technological prowess, we aim to enhance the design landscape and enrich user experiences across various applications and industries.

Keywords

Adjusted Rand Index (ARI), Color Harmony, Color palette generation, K-Means clustering, Within-Cluster Sum of Squares (WCSS)

1. Introduction

Color is more than a visual sensation; it's a potent force that influences our emotions, thoughts, and perceptions. It communicates messages, evokes moods, and can even rally masses. Whether in digital experiences, products, or branding, color gives them a distinct voice, lifting them from the mundane to the extraordinary. Research shows that within 90 seconds of encountering a product, people form subconscious judgments, with up to 90% of that based on color alone. In design, especially in user interface (UI) design, integrating color is nuanced and challenging. UI designers must seamlessly blend color to communicate a brand's identity and elicit desired emotions from users. While clients may have personal preferences, designers rely on color theory, a structured framework that guides the strategic use of color. Color theory is the backbone of effective design, providing insights into color relationships, symbolism, and psychology. By understanding these principles, designers can create cohesive and impactful experiences. Extracting color palettes from images involves sophisticated algorithms that analyze pixel data to identify prominent colors. These palettes capture the essence of the original image and ensure consistency in design work. Color is dynamic and multifaceted, shaping perceptions and experiences. It serves as a powerful medium of communication, capable of eliciting emotions and leaving lasting impressions. By leveraging color theory and advanced techniques, designers create visually compelling designs.

Throughout history, color theory has evolved, from Sir Isaac Newton to modern computational tools. Image-Based Color Scheme generation represents a significant advancement, using machine learning and computer vision to extract, evaluate, and harmonize colors from images. This approach enhances visual aesthetics, adapts color schemes to context, boosts efficiency, ensures objective analysis, and drives innovation. Image-based color schemes enrich designs with captivating palettes, adapting to the subject matter and purpose of the design. Automated methods reduce manual effort while maintaining consistency and brand identity. This research promises innovation across various fields, democratizing expert-level color harmonization. In essence, this research merges artistic sensibilities with computational prowess to transform colors extracted from images into harmonious and context-aware color schemes. It bridges the gap between manual curation and automated methods, enriching designs with authenticity and depth. This fusion of art and technology fosters innovation in the digital landscape.

2. Literature Review

2.1. Origins and Evolution

The roots of color theory can be traced back to ancient civilizations, where early artists and philosophers pondered the nature of color and its role in perception. From Aristotle's exploration of primary colors to Leonardo da Vinci's studies of light and shadow, the quest to unravel the mysteries of color has spanned centuries. However, it was not until the 18th and 19th centuries that color theory began to coalesce into a systematic framework. Pioneers such as Isaac Newton and Johann Wolfgang von Goethe laid the groundwork for modern color theory, experimenting with prisms, color wheels, and spectral analysis to unlock the secrets of color.

2.2. Exploring the Vast Terrain of Color Theory

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Color theory centers on hue, value, and saturation. Hue represents the spectrum from red to violet, each with a unique

character. Value determines lightness or darkness on a grayscale. Saturation quantifies purity, from vibrant to subdued. Artists and designers manipulate these properties to evoke mood and symbolism in colors. Color theory emphasizes color harmonies, where complementary colors contrast sharply, while analogous colors blend harmoniously. Triadic and tetradic schemes offer balanced combinations. Understanding these harmonies enables artists and designers to evoke desired moods and narratives through precise color orchestration. [1]

Color theory finds application across a myriad of disciplines, from fine art and graphic design to interior decorating and fashion. In graphic design, for instance, color theory informs branding strategies, helping companies establish distinct identities and communicate their values effectively. In interior design, color theory guides the selection of palettes that enhance spatial perception, create focal points, and promote relaxation or stimulation, depending on the intended use of the space. Moreover, color theory plays a crucial role in digital design, where interfaces must balance aesthetics with usability, ensuring clear hierarchy, readability, and accessibility for users of all backgrounds.

2.3. Analyzing the Advantages and Limitations of Existing Color Extraction Tools

Automated color extraction tools have transformed the design industry, yet they come with their own set of limitations. Numerous commercial software applications now offer color extraction features, democratizing access for designers and creators alike. These tools typically feature user-friendly interfaces, allowing users to extract colors from images. Advantages of these tools include their efficiency, enabling quick color analysis and palette generation. Additionally, some tools offer color harmonization suggestions, aiding designers in creating visually pleasing and cohesive color schemes. [2]

Existing tools and methods often employ a straightforward K-means algorithm to extract cluster centers, representing the colors of the palette. However, they fall short in considering whether the generated palette is harmonized or contextually relevant. Additionally, their accuracy heavily relies on the quality and complexity of the analyzed image, making them susceptible to inaccuracies, particularly in cases with subtle variations in lighting and shadows. [3-4]

3. Color Analysis with Unsupervised Learning

Unsupervised learning autonomously discovers patterns in data, crucial for extracting colors and generating palettes from images. Techniques like K-means clustering group pixels based on color similarities, aiding palette creation by partitioning pixels into clusters representing dominant colors. This scalable and adaptable method analyzes large datasets, uncovering subtle color variations and refining palettes without manual labeling. K-means clustering, a popular technique, partitions data into K groups based on proximity to cluster centroids, iterating until convergence. It's widely used in image segmentation, market segmentation, and document clustering, providing detailed and cohesive color palettes. [5]

Below is an illustration (Figure 1) of how data points in a 2-dimensional space are grouped into four clusters after four iterations (as configured on the right-hand side).

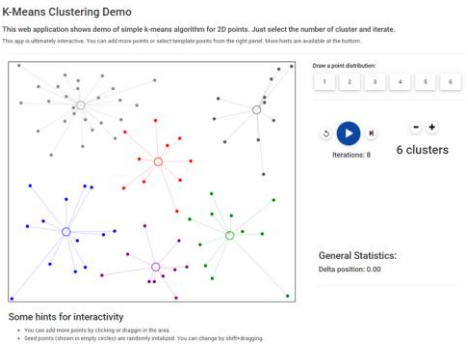

Figure 1. Working of K-Means Clustering

In K-Means clustering, each cluster is represented by a centroid, marked by larger circles. Data points are assigned to the nearest centroid, with the centroid calculated as the meaning of its cluster's points. [6-7] The algorithm iteratively minimizes the Euclidean distance between points and centroids until convergence. K-Means is sensitive to initial centroid placement, often leading to local optima. To address this, we run the algorithm multiple times with different initializations, selecting the result with the lowest Within-Cluster Sum of Squares (WCSS) or using advanced initialization techniques. [8]

3.1. Demystifying K-Means Clustering and Error Minimization

K-means clustering is a powerful algorithm widely used for partitioning a dataset into distinct clusters based on similarity. At the heart of this algorithm lies the concept of error minimization, specifically the minimization of the within-cluster sum of squares (WCSS). In this detailed exploration, we will unravel the intricacies of K-means clustering, delve into the computation of WCSS, and elucidate the process of selecting the optimal clustering solution. [9]

The K-means clustering algorithm operates based on the principle of minimizing the distance between data points and the centroids of their assigned clusters. At its core, K-means clustering seeks to achieve two primary objectives:

i. Minimize intra-cluster variance: By assigning each data point to the nearest centroid, the algorithm aims to minimize the variance within each cluster, ensuring tight cohesion and similarity among cluster members.

ii. Maximize inter-cluster variance: Simultaneously, the algorithm seeks to maximize the separation between clusters, ensuring distinctiveness and dissimilarity among different clusters.

3.1.1 Computing Within-Cluster Sum of Squares (WCSS)

The within-cluster sum of squares (WCSS) serves as a crucial metric for evaluating the quality of a clustering solution. WCSS quantifies the total squared distance between each data point and the centroid of its assigned cluster. Mathematically, WCSS for a given clustering configuration can be expressed as

$$WCSS = \sum_{i=1}^{K} \sum_{x \in C_i} \|x - c_i\|^2 \quad (1)$$

Where

- K is the number of clusters.
- C_i represents the set of data points assigned to cluster i.
- c_i is the centroid of cluster i.
- x denotes a data point within cluster Ci.
- $\|x - c_i\|^2$ calculates the squared Euclidean distance between x and c_i.

The objective of K-means clustering is to minimize this WCSS, thereby achieving a configuration of clusters that optimally captures the underlying structure of the data.

3.1.2 Selecting the Optimal Clustering Solution

Due to K-means' sensitivity to initialization and potential convergence to local minima, it is common practice to run the algorithm multiple times with different initializations. This ensures robustness and increases the likelihood of finding the global optimum. However, this approach yields multiple clustering solutions, each associated with its own WCSS value. To select the optimal clustering solution with the lowest error (WCSS), the following steps are typically followed:

i. Run K-means multiple times: Execute the K-means algorithm several times (e.g., 10 times) with the same dataset but

different random initializations of centroids. Each run produces a distinct set of cluster centroids and their corresponding WCSS.

ii. Calculate WCSS for each run: For each run of the algorithm, compute the WCSS value using the aforementioned formula. This involves summing the squared distances between each data point and its assigned centroid across all clusters.

iii. Compare WCSS values: After all runs are complete, compare the WCSS values obtained from each run. Identify the run with the lowest WCSS value, indicating the clustering configuration that minimizes the error or distortion in the data.

iv. Select the optimal solution: Choose the clustering result with the lowest WCSS value as the optimal solution. This configuration of cluster centroids represents the most cohesive and well-separated clustering solution, capturing the inherent structure of the dataset effectively.

3.1.3 Assessing Color Scheme Quality without Ground Truth: The Role of ARI

In The Adjusted Rand Index (ARI) is a statistical measure that evaluates the similarity between two sets of cluster assignments, accounting for chance agreement. It quantifies the agreement between the clustering results and a reference partition, such as ground truth labels, if available. However, ARI can also be applied in scenarios where ground truth is absent, making it particularly relevant for assessing clustering accuracy in the absence of external benchmarks. Mathematically, ARI computes the proportion of data point pairs that are either assigned to the same cluster in both the generated clustering and the reference partition or assigned to different clusters in both partitions, while adjusting for chance. [10] The formula for ARI is as follows:

$$ARI = (RI - E[RI])/(max\,(RI) - E[RI]\,) \tag{2}$$

Where

- RI (Rand Index) measures the similarity between two clustering solutions, considering both agreements and disagreements in cluster assignments.
- $E[RI]$ represents the expected value of the Rand Index under the assumption of independence between cluster assignments.
- $\max(RI)$ denotes the maximum possible value of the Rand Index, considering all possible pairs of data points.

A higher ARI score indicates greater agreement between the clustering results and the reference partition, with values close to 1 signifying perfect agreement and values around 0 indicating random clustering. To assess the effectiveness of color scheme generation without ground truth labels:

- Apply Clustering Algorithm: Use a clustering algorithm to partition extracted features (e.g., image colors) into distinct clusters.
- Calculate ARI: Compute the Adjusted Rand Index (ARI) to measure the agreement between clusters. A higher ARI indicates better internal consistency.
- Interpret ARI: A higher ARI suggests successful clustering, capturing the data's underlying structure for meaningful color schemes.
- Visual Inspection: Visually inspects the generated color scheme for coherence and aesthetic appeal, complementing ARI's quantitative measure with qualitative insights.

4. Methodology

In the pursuit of refining color scheme generation, the aim is to build upon the foundation laid by K-means clustering while exploring novel techniques to further improve efficacy and coherence. By leveraging advanced methodologies such as re-running clustering with varied parameters, the endeavor is to elevate the quality and versatility of the generated color schemes. [11-12]

4.1 Iterative Refinement with K-means Clustering

K-means clustering forms our color extraction methodology, iteratively rerunning the algorithm with varied initializations to ensure robustness. Randomness in centroid initialization mitigates convergence to suboptimal solutions. Within-Cluster Sum of Squares (WCSS) evaluates clustering quality, guiding parameter adjustments. Each iteration yields distinct centroids, aiding evaluation and comparison for quality assurance. [13]

4.2 Quantifying Coherence with Adjusted Rand Index (ARI)

To objectively assess clustering efficacy, we use the Adjusted Rand Index (ARI) to measure accuracy. ARI quantifies similarity between clustering solutions, standardizing evaluation of coherence and consistency. Calculated after each iteration, higher ARI scores indicate better alignment with data structure and cohesion within clusters, enhancing color scheme generation. [14-15]

4.3 Integration and Iteration for Optimal Results

Integration of methodologies yields a robust color scheme framework, combining clustering analysis, ARI assessment, and qualitative harmony evaluation. Iterative refinement ensures continuous enhancement, fine-tuning parameters for coherence and aesthetic appeal. This iterative approach reflects a commitment to innovation, maintaining high standards in color scheme generation. [16-17]

In conclusion, our multi-faceted approach to color scheme generation combines the power of K-means clustering with WCSS, quantitative assessment with ARI. By integrating these methodologies and iterating upon the process, we strive to push the boundaries of color scheme generation and elevate the design experience for users across various applications and industries. [18-19]

5. Implementation

5.1. Making necessary imports and Loading image

```
import pandas as pd
import numpy as np

from io import BytesIO
from PIL import Image, ImageColor
import colorsys

from sklearn.cluster import KMeans

import matplotlib.pyplot as plt
plt.style.use('ggplot')
import plotly.express as px
from mpl_toolkits.mplot3d import Axes3D
```

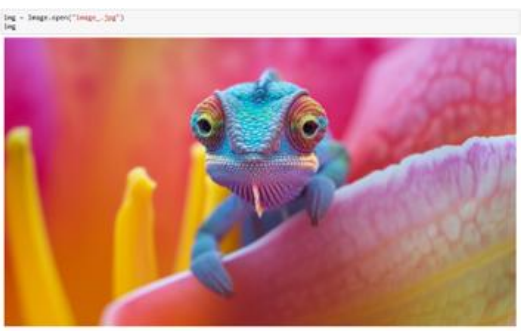

Figure 2. Making Imports and Loading Image

The script (Figure 2) utilizes pandas and numpy for data handling, BytesIO for binary data, PIL for image manipulation, colorsys for conversions, scikit-learn for KMeans clustering, matplotlib and plotly.express for visualization, and mpl_toolkits.mplot3d.Axes3D for 3D plotting. [20]

This code snippet (Figure 2) employs the Python Imaging Library (PIL) to load an image file titled "image_.jpg" and assigns it to the variable `img`. Essentially, it reads the image file, making it available for subsequent processing steps.

5.2. Fetching and Storing RGB colors

```
In [16]: n_dims = np.array(img).shape[-1]
         n_dims

Out[16]: 3

In [17]: if n_dims == 4:
             temp_img = Image.new("RGB", img.size, (255, 255, 255))
             temp_img.paste(img, mask=img.split()[3])
             img = temp_img

In [18]: r,g,b = np.array(img).reshape(-1,n_dims).T
```

Figure 3. Fetching RGB colors

Figure 3 ensures the image is in RGB format, converting RGBA if needed, and extracts RGB values into separate arrays for color analysis.

```
In [16]: df_rgb = pd.DataFrame({"R": r, "G": g, "B": b}).sample(n=1000)

In [17]: df_rgb

Out[17]:
```

	R	G	B
538679	186	123	166
907780	187	157	157
590811	156	72	108
812881	143	48	56
87788	205	121	180
...	...	...	...
478444	116	88	137
847471	189	145	136
809120	185	170	167
784481	229	164	0
828888	56	28	40

1000 rows × 3 columns

Figure 4. Storing RGB colors

```
# Create a 3D scatter plot
fig = plt.figure(figsize=(10, 8))
ax = fig.add_subplot(111, projection='3d')

# Plot the RGB values
ax.scatter(df_rgb['R'], df_rgb['G'], df_rgb['B'], c=df_rgb[['R', 'G', 'B']] / 255.0, alpha=0.5)

# Set labels and title
ax.set_xlabel('Red')
ax.set_ylabel('Green')
ax.set_zlabel('Blue')
ax.set_title('RGB Values Scatter Plot')

plt.show()
```

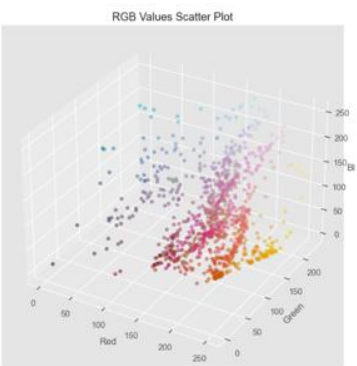

Figure 5. Plotting a 3D Scatter Plot

Figure 4 creates a DataFrame (df_rgb) for RGB color data, sampling 1000 points for efficiency. Figure 5 plots a 3D scatter plot using Matplotlib, with axes for red, green, and blue values, and colors normalized. Figure 9 shows color clusters, indicating dominant colors and their balance, with a diagonal line highlighting RGB value correlations. [21]

5.3. Generating a Color Palette Using Traditional K-Means Clustering Method

```
palette_size = 8
```

```
kmeans_model = KMeans(n_clusters=palette_size,
                      random_state=0,
                      init="k-means++",
                      n_init="auto").fit(df_rgb)

palette = kmeans_model.cluster_centers_.astype(int).tolist()

img_rgb = np.array([palette], dtype=np.uint8)
fig = px.imshow(img_rgb)
fig.update_xaxes(visible=False)
fig.update_yaxes(visible=False)
fig.show()
```

Figure 6. Color Palette Generation using K-Means

Figure 7. Color Palette using K-Means

Figure 6 generates a color palette using the K-Means clustering algorithm. First, the palette size is set to determine the number of colors. The K-Means model is then trained on RGB values from df_rgb, with parameters ensuring reproducibility and optimized convergence. Cluster centers' RGB values are extracted and converted to integers to represent dominant colors. Finally, the palette is visualized using Plotly's imshow as a single-row image (Figure 7) with hidden axes for clarity. [22]

5.4. Generating a Color Palette Using K-Means Clustering with WCSS

```
# Define the number of runs for K-means
num_runs = 10

# Initialize variables to store results
best_kmeans_model = None
min_wcss = float('inf')

# Iterate over multiple runs of K-means
for i in range(num_runs):
    # Run K-means clustering
    kmeans_model_wcss = KMeans(n_clusters=palette_size,
                               random_state=i,  # Use different random state for each run
                               init="k-means++",
                               n_init=1).fit(df_rgb)  # n_init=1 to only perform a single initialization

    # Calculate within-cluster sum of squares (WCSS)
    wcss = kmeans_model_wcss.inertia_

    # Update best model if this run has lower WCSS
    if wcss < min_wcss:
        min_wcss = wcss
        best_kmeans_model = kmeans_model_wcss

# Retrieve the cluster centers of the best model
best_cluster_centers = best_kmeans_model.cluster_centers_.astype(int).tolist()

# Print the best cluster centers
print("Best cluster centers:")
print(best_cluster_centers)

img_rgb = np.array([best_cluster_centers], dtype=np.uint8)
fig = px.imshow(img_rgb)
fig.update_xaxes(visible=False)
fig.update_yaxes(visible=False)
fig.show()
```

Figure 8. Color Palette Generation using K-Means with WCSS

Figure 9. Color Palette using K-Means with WCSS

Figure 8 implements the K-Means algorithm with multiple runs to find the optimal clustering solution. Here's a breakdown:

i. Define Number of Runs: num_runs = 10 specifies the number of K-Means iterations, each with different random initializations, to increase the likelihood of finding the best clustering solution. [23]

ii. Initialize Variables: best_kmeans_model = None: Stores the best K-Means model.
min_wcss = float('inf'): Tracks the minimum within-cluster sum of squares (WCSS).

iii. Iterate Over K-Means Runs: A for loop iterates num_runs times, each run initializing the K-Means algorithm differently. [24]

iv. Run K-Means Clustering: kmeans_model_wcss = KMeans(n_clusters=palette_size, random_state=i, init="k-means++", n_init=1).fit(df_rgb): Fits the model to RGB data, using a different random state (i) each time.

v. Calculate WCSS: wcss = kmeans_model_wcss.inertia_: Calculates WCSS for the current iteration.

vi. Update Best Model: If the current WCSS is lower than min_wcss, update min_wcss and best_kmeans_model.

vii. Retrieve Best Cluster Centers: best_cluster_centers = best_kmeans_model.cluster_centers_.astype(int).tolist(): Converts cluster centers to a list of integers.

viii. Print Best Cluster Centers: Outputs the RGB values of the best centroids found.

ix. Visualize Best Cluster Centers: Uses Plotly's imshow to display the best cluster centers as an image (Figure 9) with hidden axes.

5.5. ARI Calculation and Comparison

```
In [21]: from sklearn.metrics import adjusted_rand_score
         from skimage import io

         ari = adjusted_rand_score(best_kmeans_model.labels_, kmeans_model.labels_)
         print("Adjusted Rand Index (ARI):", ari)

         Adjusted Rand Index (ARI): 0.5106750316977775
```

Figure 10. ARI Calculation

This code segment (Figure 10) computes the Adjusted Rand Index (ARI) to evaluate the similarity between two clustering solutions obtained from different K-Means clustering methods. Here, the computed ARI value of approximately 0.511 indicates moderate agreement between the cluster assignments obtained from the K-Means clustering model trained using the WCSS method (best_kmeans_model.labels_) and those from the traditional K-Means clustering method (kmeans_model.labels_). This suggests that the two clustering solutions are somewhat similar, but there is room for improvement.

Now, discussing the reasons why K-Means clustering with the Within-Cluster Sum of Squares (WCSS) method is better than the traditional K-Means clustering method:

i. WCSS-based Initialization
K-Means clustering with WCSS method initializes cluster centroids using the "k-means++" method, which selects initial centroids that are well spread out and distant from each other. This initialization strategy helps to avoid convergence to suboptimal solutions and accelerates convergence towards the global optimum. In contrast, the traditional

K-Means method typically uses random initialization, which may lead to convergence to suboptimal solutions or slow convergence. [25]

ii. Automatic Adjustment of Initializations

In the WCSS method, the n_init parameter is set to "auto," allowing automatic adjustment of the number of initializations based on the number of clusters specified (palette_size). This adaptive approach ensures that an appropriate number of initializations are performed to find the best clustering solution efficiently. On the other hand, the traditional K-Means method often requires manual tuning of initialization parameters, which can be time-consuming and less effective in finding the optimal solution.

iii. Improved Reproducibility

K-Means clustering with the WCSS method sets the random_state parameter for reproducibility across multiple runs, ensuring consistent results for the same input data. This is particularly beneficial for experimental reproducibility and comparison of results. In contrast, the traditional K-Means method relies solely on random initialization, making it more prone to variability between runs. [26-28]

iv. Enhanced Performance

The WCSS method, by utilizing smart initialization and automatic adjustment of initializations, tends to converge faster and more reliably to better clustering solutions. This can result in improved performance in terms of convergence speed, clustering quality, and robustness to initialization variations compared to the traditional K-Means method. [29-30]

In summary, K-Means clustering with the Within-Cluster Sum of Squares (WCSS) method offers several advantages over the traditional K-Means clustering method, including improved initialization, automatic adjustment of initializations, enhanced reproducibility, and potentially better performance in terms of convergence and clustering quality. These advantages contribute to the effectiveness and reliability of the WCSS-based approach for clustering tasks.

6. Conclusion

The color palette generation process employed two distinct methods, each providing unique insights and optimizations. Utilizing K-Means clustering with the Within-Cluster Sum of Squares (WCSS) method proved superior to traditional K-Means. This approach strategically places centroids for faster convergence and better clustering results, enhancing performance through automatic adjustments and improved reproducibility across multiple runs. Evaluating palette coherence using the Adjusted Rand Index (ARI) yielded a score of 0.511, indicating moderate agreement between clustering solutions. This score highlights a moderate level of consistency and alignment with the underlying data structure, ensuring the generated palettes are reliable and visually appealing. In the pursuit of advancing color palette generation through image analysis, the study meticulously explored methodologies to extract meaningful insights from visual data. The WCSS-based K-Means clustering emerged as a standout approach, showcasing superior performance by facilitating faster convergence and improved clustering results. Automatic adjustments ensured consistency and reliability, reinforcing the algorithm's effectiveness. The integration of these methodologies with design tools and advanced color harmonies opens avenues for further innovation and customization. This study underscores the transformative potential of image-based color scheme generation, bridging the gap between computational analysis and creative expression. By combining these methods, the research advances the field, offering reliable and aesthetically pleasing color palettes suitable for diverse applications. In conclusion, the study demonstrates the significant potential of image-based color scheme generation, driven by a commitment to excellence and a passion for visual aesthetics. This innovative approach promises to enhance precision and efficiency in the colorful world of image analysis, paving the way for future exploration and creation.

Acknowledgement

I have made a lot of effort in completion of this project report. It would have been impossible without the kind and generous support of some individuals and organizations. First, I would like to thank the organization, Amity University, Lucknow, Uttar Pradesh, for providing such a platform to complete this project. I would then like to express my sincere gratitude towards Dr. Pawan Singh, for providing all the necessary information and constantly guiding me till the commencement of my report. I would also like to thank my colleagues for helping me and people who have willingly helped me out with their abilities.

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