ESG-Aware Portfolio Optimization using Regularization and Clustering

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Abstract

This study investigates environment-aware portfolio optimization by integrating green factors into systematic investment strategies using S&P 500 stocks from 2019 to 2024. Starting from a Sharpe ratio-maximizing framework, we progressively incorporate constraints on ESG scores and carbon emissions to evaluate the trade-offs between financial performance and sustainability. To improve robustness, we explore regularization and clustering-based approaches. Clustering is performed using combinations of ESG scores with Sharpe ratios and Scope 3 emissions to better segment the investment universe. The optimization framework includes constraints enforcing a minimum ESG score and limiting average emissions (Scope 1 + Scope 2), while aiming to maximize risk-adjusted returns. Through out-of-sample analysis, we assess the impact of ESG thresholds and regularization parameters on portfolio performance, and present a methodology that balances return maximization with environmental responsibility.

1 Introduction

Environmental, Social, and Governance (ESG) investing has gained prominence as investors increasingly seek to integrate ethical, sustainable, and risk-aware considerations into their investment decisions. ESG data provides valuable insights into a firm's environmental footprint, social responsibility, and corporate governance practices, making it an essential input for constructing responsible investment portfolios.

In recent years, the demand for environmentally conscious or "green" portfolios has intensified, driven by growing awareness of climate change, regulatory pressure, and evolving investor preferences. Asset managers are now aligning portfolios not only with financial objectives but also with global sustainability goals and climate risk mitigation frameworks. Industry benchmarks and agreements—such as the United Nations Sustainable Development Goals (SDGs) and global emissions reduction targets—have further amplified the importance of integrating environmental metrics, like greenhouse gas emissions, into portfolio construction.

This study leverages ESG scores and scope-wise carbon emissions along with historical returns data for S&P 500 stocks to explore a variety of portfolio optimization strategies. We assess the impact of incorporating environmental constraints, such as minimum ESG score thresholds and carbon emissions caps, on portfolio performance. In addition, we examine the effectiveness of regularization and clustering on ESG metrics, Sharpe ratios, and Scope 3 emissions—to enhance robustness. We aim to develop a portfolio construction methodology that balances financial performance with environmental responsibility under various investment scenarios using ML and statistical techniques.

2 Data Description

We utilize ESG data provided by WRDS (Wharton Research Data Services) database, focusing on four key components:

1. Overall ESG Score: this is a standardized score between 0 to 100. This score is a numerical measure of a company's performance in environmental, social, and governance (ESG) areas. These scores are provided by various data vendors, such as Sustainalytics, Refinitiv, S&P Global, and MSCI. They help investors and researchers assess a company's sustainability practices and their potential impact on financial performance and risk.

2. Direct Greenhouse Gas Emissions (Scope 1): this denotes direct GHG emissions that occur from sources that are owned or controlled by the company.

3. Indirect Greenhouse Gas Emissions (Scope 2): this corresponds to the indirect greenhouse gas emissions from the consumption of purchased electricity, heat or steam. Scope 2 emissions can be computed using the energy mix of the country (location-based) or the energy mix of the utility company supplying the electricity.

4. Indirect Greenhouse Gas Emissions (Scope 3): scope 3 are other indirect emissions, such as the extraction and production of purchased materials and fuels, transport-related activities in vehicles not owned or controlled by the reporting entity, electricity-related activities not covered in Scope 2. Scope 3 upstream emissions include the indirect emissions that come from the supply side, while scope 3 downstream emissions are mostly associated with the product sold by the entity.

This data is complemented by daily closing prices of S&P 500 stocks spanning from 2019 to 2024, which we use to compute monthly returns for portfolio optimization. To ensure consistency and comparability across securities, all ESG scores and emissions metrics are standardized. Close price data was taken from Bloomberg.

To maintain data quality and avoid bias in optimization, we exclude tickers with missing ESG or emission values from our analysis.

3 Data Analysis

To gain preliminary insights into the relationship between ESG characteristics and financial performance, we conducted an exploratory data analysis using S&P 500 stocks from 2019 to 2024. Daily price data was used to compute annualized returns, volatility, and Sharpe ratios, while ESG scores and carbon emission metrics (Scope 1, 2, and 3) were standardized for cross-stock compatibility.

We created a series of year-wise scatter plots to examine how ESG scores relate to return, risk, and return-to-risk ratios. These visualizations allowed us to explore whether higher

ESG performance correlates with improved financial outcomes. The plots for 2020, a year heavily impacted by the COVID-19 pandemic, show increased dispersion in both returns and risk across companies, a sign of heightened market volatility. Notably, some stocks with high ESG scores exhibited better resilience during this period, maintaining relatively favorable Sharpe-like ratios despite the broader market stress.

Across all years, we observed no strong linear relationship between ESG scores and either returns or risk individually. However, the Sharpe ratio plots revealed certain outlier firms that combined high ESG scores with superior risk-adjusted performance, reinforcing the possibility of constructing ESG-conscious portfolios without sacrificing financial efficiency. These findings justified our focus on enhanced optimization techniques, such as regularization and clustering. that can integrate ESG and carbon emission constraints while striving for strong performance.

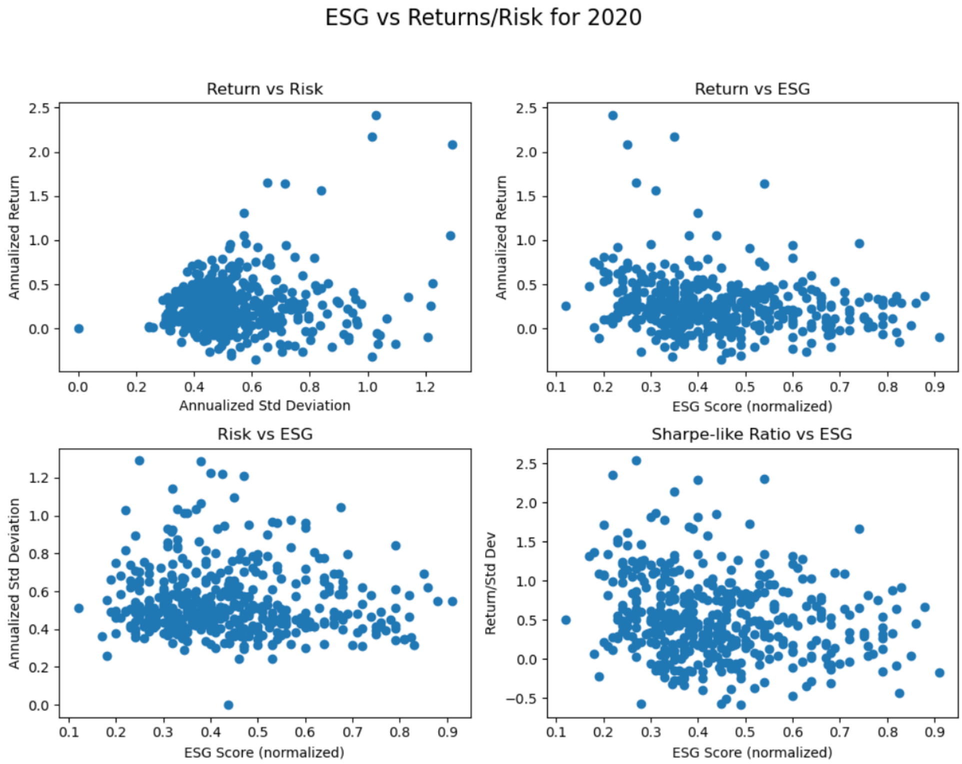


Figure 1: ESG vs Returns/Risk Scatter Plots for 2020

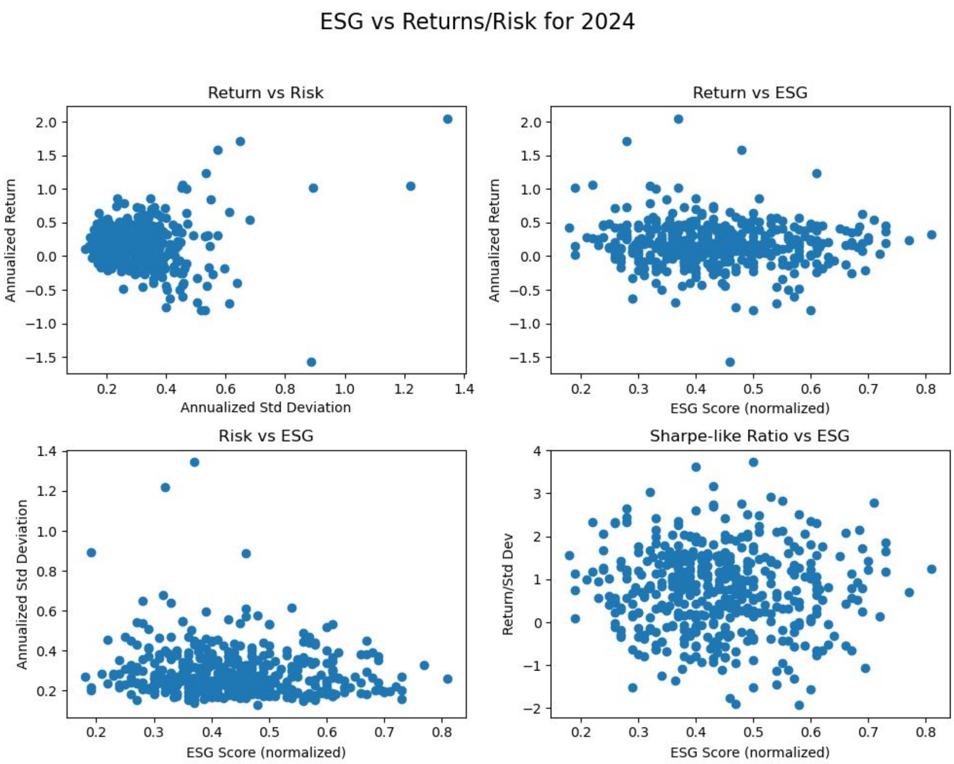


Figure 2: ESG vs Returns/Risk Scatter Plots for 2024

4 Methodology

4.1 Sharpe Ratio Maximization

The Sharpe ratio is defined as:

$$SR = \frac{\mathbb{E}[R_p - R_f]}{\sigma_p}$$

where R_p represents the portfolio return, R_f is the risk-free rate, and σ_p is the portfolio standard deviation. The goal of the portfolio optimization is to maximize this ratio by adjusting the weights of the assets. The optimization problem can be expressed as:

$$\max_w \frac{w^T \mu - R_f}{\sqrt{w^T \Sigma w}}$$

subject to $\sum_i w_i = 1$ and $w_i \geq 0$.
where w is the vector of asset weights, μ is the expected log-returns of the assets, and Σ is the covariance matrix of returns.

4.2 ESG and Emission-Constrained Portfolio Optimization

To incorporate ESG constraints, we impose a minimum weighted ESG score requirement for the portfolio. This constraint is formulated as:

$$\sum_i w_i \times ESG_i \geq \text{ESG Threshold}$$

where ESG_i is the ESG score for asset i the threshold is the minimum acceptable weighted ESG score for the portfolio. The optimization problem now includes this additional constraint while maintaining the objective of maximizing the Sharpe ratio.

In addition to ESG constraints, we also consider limiting the carbon emissions of the portfolio. The total emissions for each asset are represented by Scope 1 and Scope 2 emissions (Scope 3 emissions are harder to estimate and hence, we included these in the clustering analysis to get a rough idea without imposing a strict constraint), which can be combined as:

$$\sum_i w_i \times Scope1_i + Scope2_i \leq \text{Emission Threshold}$$

where $Scope1_i$ and $Scope2_i$ are the Scope 1 and Scope 2 emissions of asset i, and the emissions threshold sets the maximum allowed emissions for the portfolio. The objective function remains the same, but the portfolio optimization must now also satisfy this emissions constraint.

4.3 Regularization in Portfolio Optimization

Regularization is employed to limit the portfolio variance and reduce the risk of large fluctuations in portfolio returns. The portfolio variance is constrained as follows:

$$\text{Variance Constraint:} \quad w^T \Sigma w \leq \text{Variance Limit (U)}$$

This helps mitigate the impact of outliers and high-risk assets.
where Σ is the covariance matrix and U is the upper bound on portfolio variance. This regularization ensures thar the portfolio is diversified while controlling the risk at the same time.

4.4 ESG-Constrained and Regularized Optimization

Combining both environmental constraints and variance regularization, the objective becomes:

$$\max_w \frac{w^T \mu - R_f}{\sqrt{w^T \Sigma w}}$$

subject to the following constraints:

$$\sum_i w_i = 1, \quad w_i \geq 0, \quad \sum_i w_i \times ESG_i \geq \text{ESG Threshold},$$

$$\sum_i w_i \times Scope1_i + Scope2_i \leq \text{Emission Threshold}, \quad w^T \Sigma w \leq \text{Variance Limit}$$

This optimization problem ensures that the portfolio is well-balanced in terms of risk, return, ESG scores, and emissions.

4.5 Constructing Different Optimization Portfolios

Using the constraints defined above, we created baseline portfolios and then supplemented them with additional constraints to understand how each led to an improvement (if any) in the outcome. The outcome was judged based on average ESG score, average carbon emissions, and Sharpe ratio.

The following comparative portfolios were created, all with the common objective of maximizing the Sharpe Ratio, albeit with different constraints:

1. Baseline portfolio only focused on Sharpe-maximization, without any environmental constraints or regularization, i.e. the base portfolio.

2. Base portfolio with regularization, i.e. the regularized base portfolio.

3. Regularized base portfolio with ESG constraints.

4. Regularized base portfolio with ESG and emission constraints.

4.6 Portfolio Optimization with Rebalancing

In our approach, we optimize the portfolio periodically using a rebalancing period of T days (typically 21 trading days - one month). For each rebalancing period, we use historical data up to the current date to compute the log-returns and covariance matrix. The portfolio optimization is then performed with the constraints (varying depending on the portfolios defined above) applied to ensure the desired Sharpe ratio, ESG score, and emission limits.

Results are collected for each rebalancing period and the performance is evaluated in terms of realized Sharpe ratio, portfolio returns, and the weighted ESG and emissions scores.

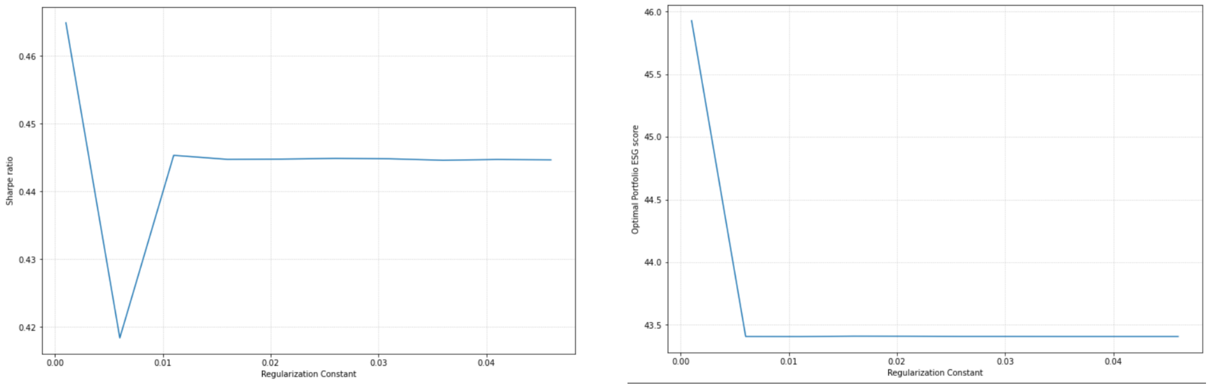
4.7 Threshold Selection via Iterative Regularization

In order to determine appropriate thresholds for variance regularization, ESG score constraints, and carbon emissions limits, we employed a systematic search over a predefined grid of threshold values, assessing the performance of each configuration through back-tested Sharpe ratios and sustainability metrics. This empirical, data-driven threshold selection process ensured that the constraints imposed were not arbitrarily chosen, but grounded in an informed trade-off analysis between performance and sustainability goals.

4.7.1 Variance Regularization Thresholds

To control portfolio volatility, we introduced a constraint on the portfolio variance using an upper bound U. To select a suitable value for U, we iteratively tested the optimization algorithm across a range of thresholds:

$$U \in \{0.001, 0.006, \ldots 0.0046\}$$



(a) Regularization Constant vs. Sharpe Ratio (b) Regularization Constant vs. ESG Score

Figure 3: Impact of Regularization Threshold on Sharpe Ratio and ESG Score

For each value of U, the portfolio was re-optimized and backtested over multiple rebalancing periods. The realized Sharpe ratio and the stability of portfolio weights were recorded to evaluate the trade-off between risk and return. This process helped identify values of U that provided improved Sharpe ratios and better overall ESG scores, as seen in the plots above.

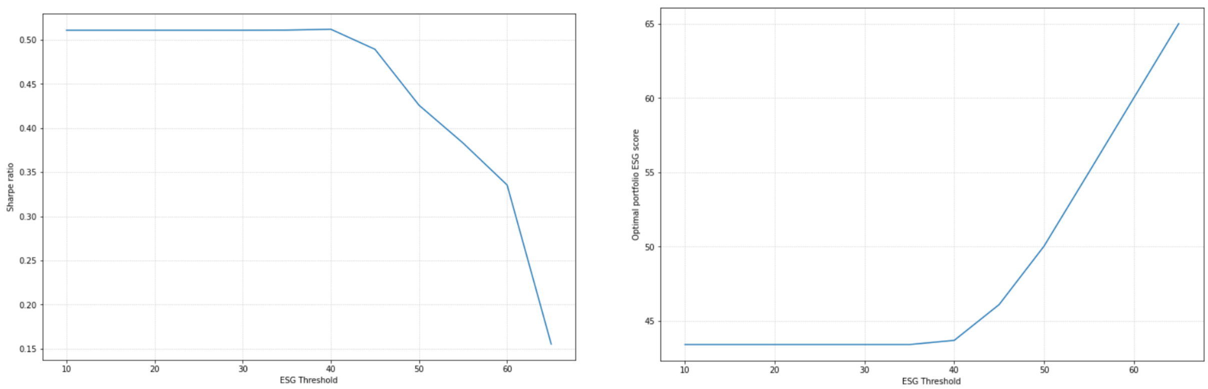
Based on these plots, we set the regularization constant as 0.003.

4.7.2 ESG Score Thresholds

The ESG constraint ensures the portfolio maintains a minimum acceptable sustainability profile. To determine an appropriate ESG threshold, we tested values in the range:

$$\text{ESG Threshold} \in \{10, 15, 20, \ldots, 65\}$$

Each threshold was evaluated by optimizing the portfolio while enforcing the minimum weighted ESG score. The realized Sharpe ratios and the actual portfolio ESG scores were recorded. This enabled us to observe the trade-off between financial performance and sustainability, identifying thresholds where ESG performance could be improved with minimal sacrifice to returns.



(a) ESG Threshold vs. Sharpe Ratio (b) ESG Threshold vs. ESG Score

Figure 4: Impact of ESG Threshold on Sharpe Ratio and ESG Score

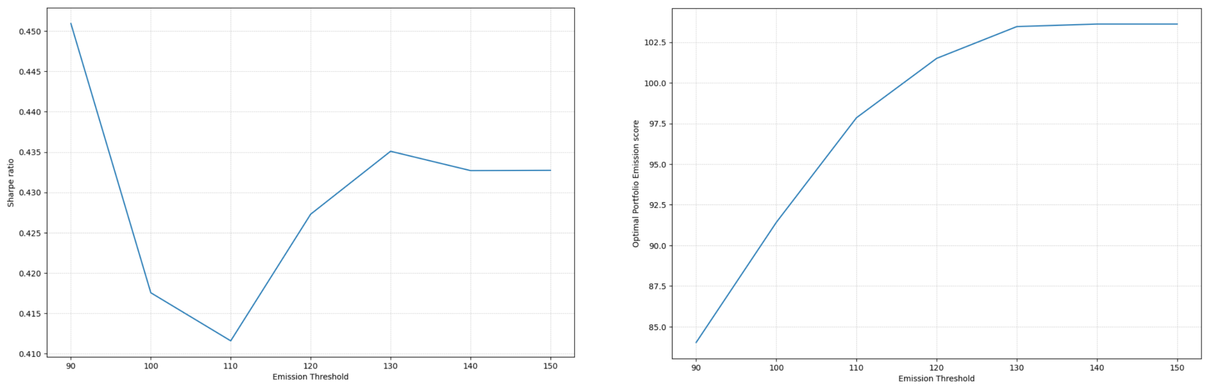
Based on these plots, we set the ESG threshold at 45.

4.7.3 Emissions Thresholds (Scope 1 + Scope 2)

For the emissions constraint, which aims to reduce the carbon footprint of the portfolio, we imposed an upper limit on the weighted sum of Scope 1 and Scope 2 emissions (the range of values selected was based on the median emission score across stocks)

$$\text{Emission Threshold} \in \{90, 100, \ldots, 150\}$$

As with the ESG thresholds, each emissions threshold was tested independently by rebalancing portfolios under the constraint and recording the realized Sharpe ratios, emissions scores, and returns. The results provided insight into how stricter emissions constraints affected performance, enabling a balance between environmental impact and portfolio efficiency.



(a) Emission Threshold vs. Sharpe Ratio

(b) Emission Threshold vs. ESG Score

Figure 5: Impact of Emission Threshold on Sharpe Ratio and ESG Score

Based on these plots, we set the Emissions Threshold at 90. However, we note that the emissions threshold can also be set by the user taking into account their sustainability goals and achievable emission limits, since carbon emissions vary drastically based on the company, product, and manufacturing processes involved.

5 Filtering the Investment Universe via Clustering

To enhance portfolio construction by strategically targeting a refined set of favorable risk-adjusted returns and sustainability characteristics, we employed clustering. We started with clustering the data by using all 3 features - ESG, Sharpe ratio and Scope 3 Emissions to see the overall clusters in the dataset. The following 3D plot summarizes the different clusters we saw in the data.

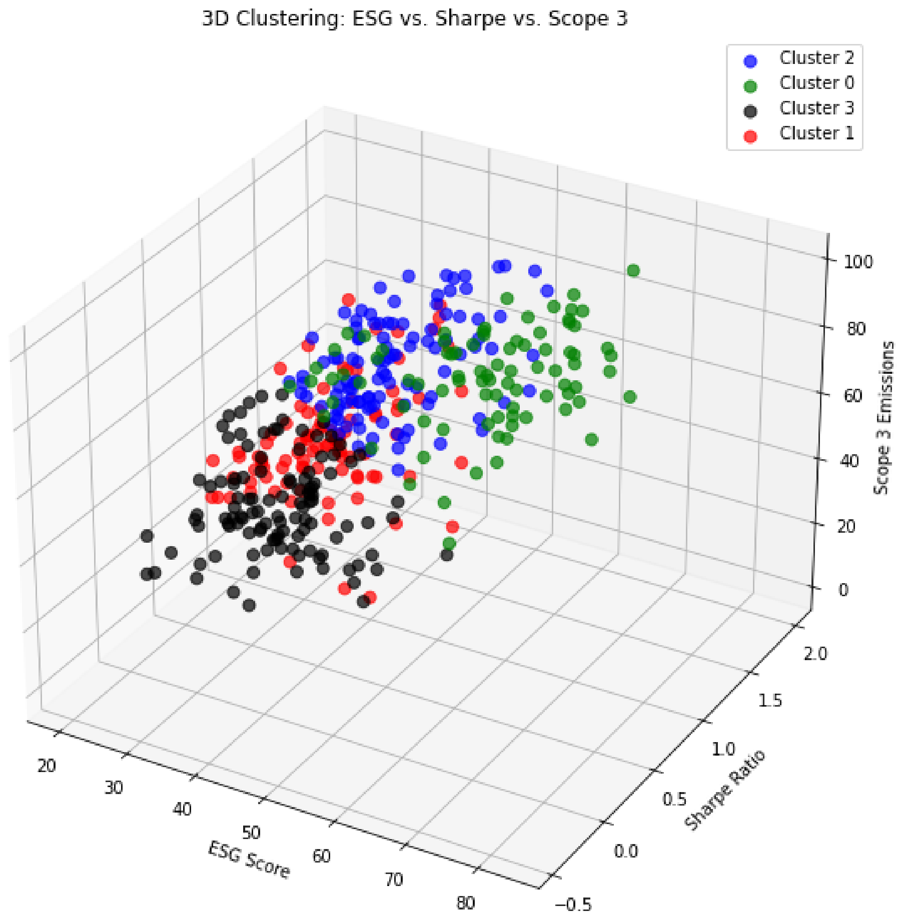


Figure 6: Clustering results using ESG, Sharpe ratio and emissions

Since no clear demarcation was observed between the clusters, we decided to follow two clustering approaches using KMeans which focused on only 2 of the 3 features at a time, which simplified the process and made it easier to choose the best cluster.

5.1 Clustering Based on ESG and Sharpe Ratio

The first method clustered stocks based on their realized Sharpe ratios and ESG scores, leveraging historical return data to compute Sharpe ratios and combining this with average ESG scores per stock.

The clustering process involves:

1. Computing Sharpe ratios and standardizing ESG scores.
2. Applying K-means with $k = 3$, with clusters representing high, medium, and low Sharpe-ESG combinations
3. Selecting the cluster with the highest mean Sharpe ratio and ESG score for portfolio formation.

This clustering revealed a distinct group (Cluster 3) characterized by moderate Sharpe ratios and high ESG scores, suggesting an attractive subset of stocks with desirable financial and environmental performance.

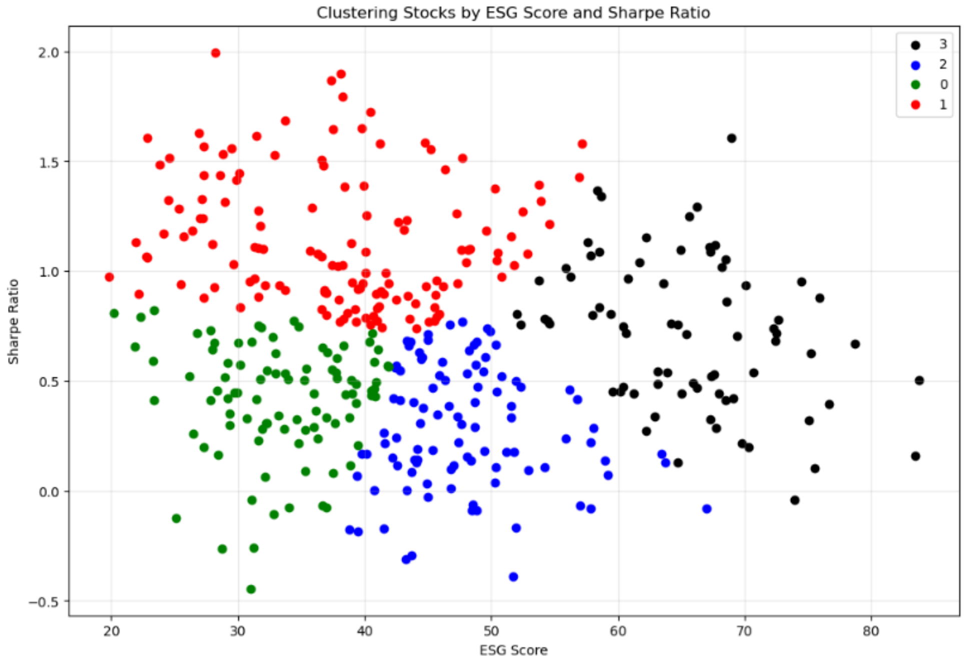


Figure 7: Clustering based on ESG Scores and Sharpe

5.2 Clustering Based on ESG and Scope 3 Carbon Emissions

The second approach clustered stocks based on ESG score and Scope 3 greenhouse gas emissions. Scope 3 emissions refer to indirect emissions in a company's value chain, such as those from suppliers or customers. Unlike Scope 1 and 2 emissions, Scope 3 values are harder to estimate, subject to greater variability, and more prone to under-reporting or inconsistent methodologies across companies and sectors. Due to this measurement uncertainty and potential bias, using Scope 3 emissions as a hard constraint in the optimization process could lead to misleading or unfair penalization of certain companies.

Instead, we leverage clustering to identify and focus on groups of stocks that naturally combine high ESG scores with relatively low Scope 3 emissions, thereby achieving the same sustainability goals in a softer and more data-aware manner. This approach allows us to filter the investment universe toward companies that are not only high-performing but also exhibit credible sustainability practices without over-relying on potentially noisy emissions data.

Similar clustering steps were followed, except with ESG scores and Scope 3 emissions as the parameters.

This method identified clusters that trade off between high ESG scores and high emissions, with one cluster again (Cluster 2) combining relatively low emissions and moderate to high ESG scores.

5.3 Portfolio Optimization with clustering

Before clustering, we had four portfolio optimization problems with different sets of constraints as formulated in Section 4.5. We then restricted the optimization process to only include stocks within the most favorable cluster obtained from both clustering techniques,

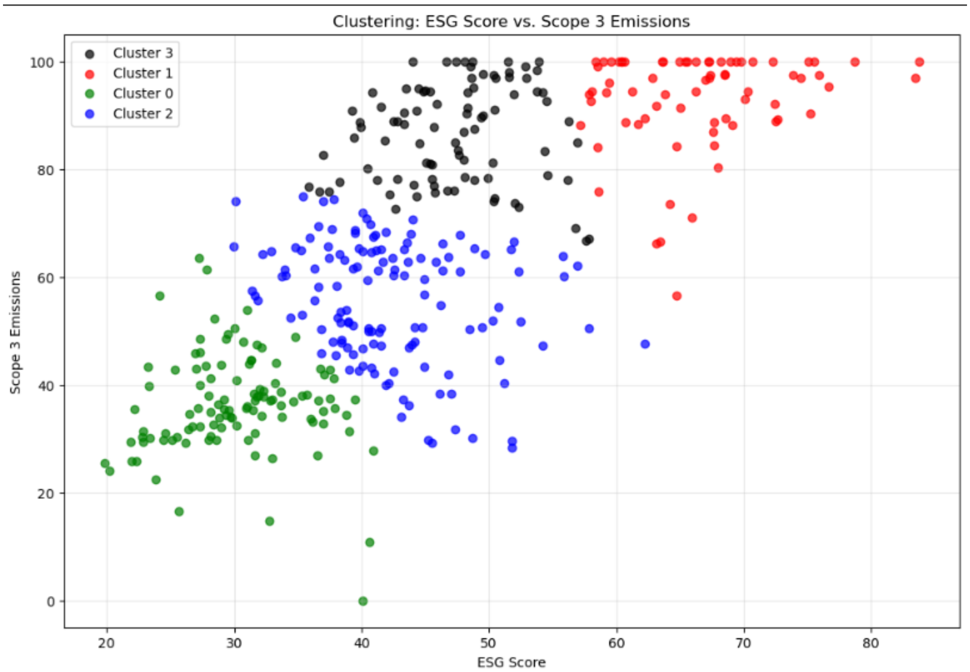


Figure 8: Clustering based on ESG Scores and Scope-3 Emissions

and compared the performance of these post-clustering portfolios to the original set of pre-clustering portfolios.

This comparative analysis helps assess whether clustering improves the trade-off between sustainability and performance, and whether it provides a more reliable way to integrate environmental factors, particularly noisy variables like Scope 3 emissions, into portfolio selection.

Detailed summary of the results (pre- and post-clustering) provided in Section 6.

6 Results and Analysis

In this section, we present the performance of the optimized portfolios under various configurations:

- Portfolio 1: Sharpe ratio maximization without constraints, a.k.a the Base
- Portfolio 2: Base with regularization.
- Portfolio 3: Base with regularization, and ESG constraints.
- Portfolio 4: Base with regularization, ESG constraints, and emission constraints.
- Portfolio 5: Base with regularization, ESG constraints, and emission constraints, along with clustering based on ESG scores and Sharpe ratios.
- Portfolio 6: Base with regularization, ESG constraints, and emission constraints, along with clustering based on ESG scores and Scope 3 emissions.

Method	Sharpe Ratio	ESG Score	Emission Score	Weights Count	Turnover
Portfolio 1	1.086	42.52	103.61	14	0.255
Portfolio 2	1.181	45.73	115.83	17	0.218
Portfolio 3	1.162	46.86	117.86	17	0.220
Portfolio 4	1.303	45.22	90.00	17	0.207
Portfolio 5	0.573	60.42	90.00	7	0.125
Portfolio 6	1.456	45.04	90.00	16	0.163

Table 1: Portfolio Metrics Across Optimization Strategies

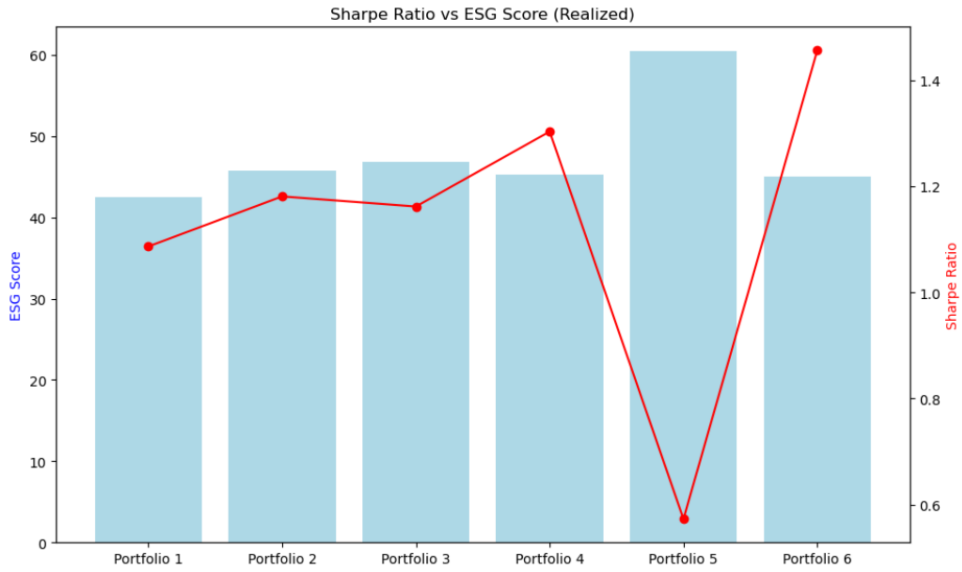


Figure 9: Sharpe Ratio v/s ESG Score across Portfolios

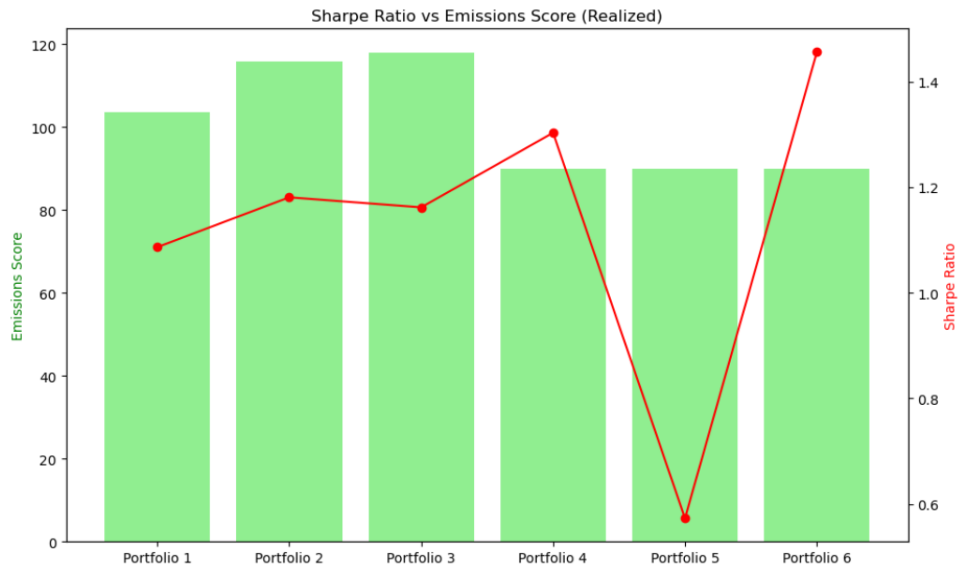


Figure 10: Sharpe Ratio v/s Emission Scores across Portfolios

The following are our key observations and analysis:

- Regularization slightly improves out-of-sample performance as can be seen in the results and plots. It increases the out-of-sample sharpe ratio achieved by the portfolio by 0.095.
- Adding the ESG constraint to the portfolio increases the ESG score achieved by the portfolio which is in line with the purpose of the constraint.
- Adding the emission constraint to the portfolio reduces the emissions achieved by the portfolio and also causes an increase in the out-of-sample sharpe ratio to a value of 1.303. We suspect this is due to the randomness in sampling of the out-of-sample points since we did not do anything which would cause an increase in the sharpe ratio.
- Clustering improves performance on both fronts - sharpe ratio and emissions which is a strong case for using clustering to identify stocks which give good returns and are ESG-friendly. We achieve a maximum sharpe ratio with ESG constraints, regularization and emission constraints along with clustering based on ESG scores and scope 3 emissions. We also see less emissions and an ESG score of 45.04 which is above our constraint threshold.
- All portfolios also achieve a low turnover rate of $\leq 26\%$ which is preferable. We also see that out of all the stocks, there are only about 10-20 stocks which have a significant (≥ 0.01) weight in the portfolio. Thus, only a fraction of all the stocks are driving the performance in every investment horizon.

7 Conclusion

This study illustrates the trade-offs and synergies between financial performance and ESG integration in portfolio optimization.

While the unconstrained base portfolio offers decent returns, enhancements such as regularization and environmental constraints contribute to more stable, sustainable portfolios. Notably, the inclusion of emission limits significantly reduces carbon exposure with minimal impact on the Sharpe ratio. Clustering based on ESG and Sharpe ratios, however, leads to overly sparse portfolios and diminished returns, underscoring the risks of over-filtering. In contrast, clustering using ESG and Scope 3 emissions achieves the best balance—delivering the highest Sharpe ratio, controlled emissions, and healthy diversification.

Overall, the findings underscore the importance of carefully designed constraints and clustering approaches in building portfolios that effectively balance financial performance with sustainability goals—demonstrating that responsible investing need not come at the expense of returns.

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