Comparison of Raw and Corrected GC-IMS Data

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2025-11-13

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1. Introduction

This report compares the **raw** and **corrected** GC-IMS Peak Table using the same evaluation metrics presented in the Stability Analysis, namely **Relative Standard Deviation (RSD)** and **variance explained by external factors**.

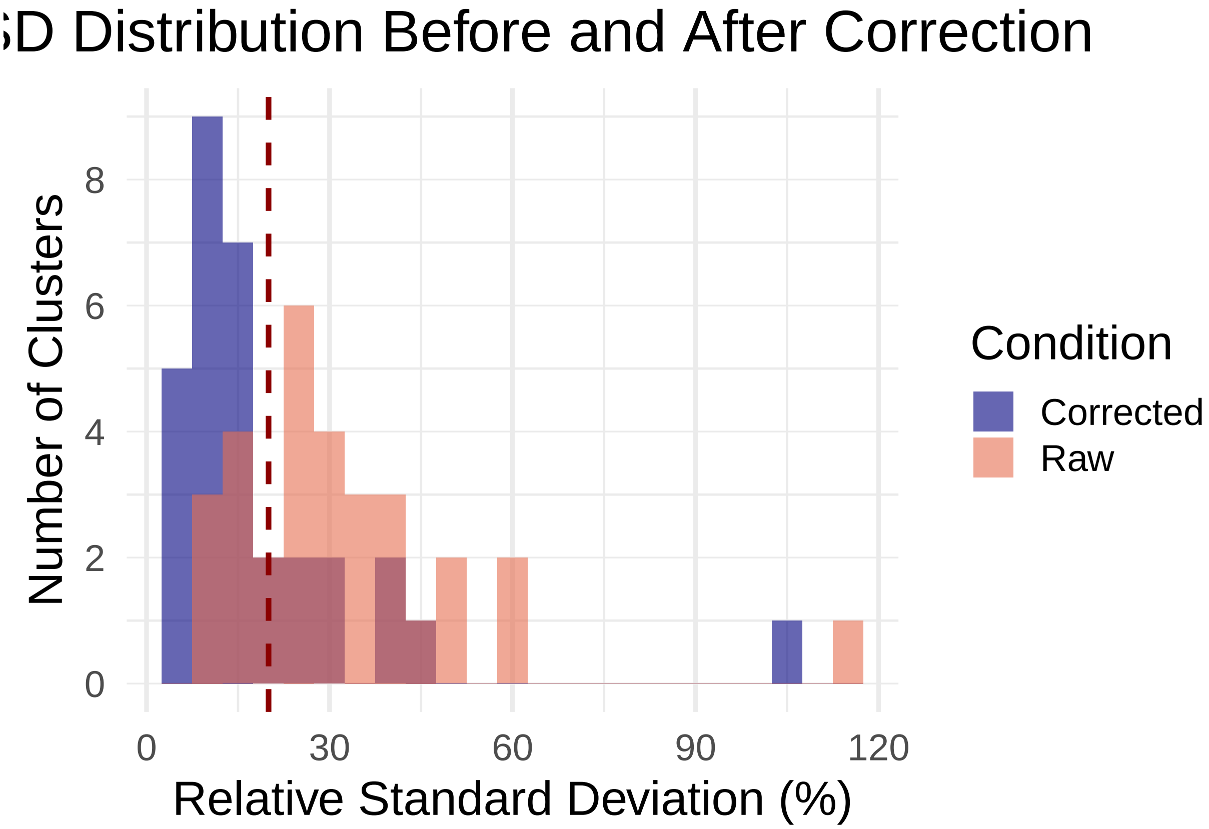
The correction applied is based on the orthogonalization procedure described in the EPO Correction Report. Rather than repeating theoretical explanations, this document focuses on quantifying the improvement in signal stability and reduction of unwanted variability after correction.

2. Apply Correction

```r
df <- read.csv("../../data/peak_table_var.csv")
intensities <- df %>% dplyr::select(starts_with("Cluster"))

intensities_final <- orthogonal_correction(
  intensities,
  df %>% dplyr::select(elapsed_time, batch)
)$corrected
intensities_final <- as.data.frame(intensities_final)
```

3. Relative Standard Deviation (RSD)



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4. Cluster Stability

To evaluate how much the correction improves the technical robustness of the dataset, we compute the number of clusters whose Relative Standard Deviation (RSD) falls below the 20% threshold, both **before** and **after** correction. This threshold is commonly used as an orientative benchmark in metabolomics quality control.

Condition	Stable_Clusters	Proportion
Raw Data	7	22.6 %
Corrected Data	22	71 %

Figure 1: Proportion of clusters with RSD below 20%, before and after correction

The correction process increases the proportion of stable clusters from **22.6%** to **71%**, confirming that the removal of variance associated with acquisition order and batch improves overall signal reliability.

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5. Explained Variance by External Factors

Condition	Elapsed_Time	Batch
Raw	29.73	34.82
Corrected	0.00	0.00

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6. Principal Component Analysis (PCA)

We now perform a new PCA on the corrected data to explore whether the dominant sources of variation are still aligned with external variables. The PCA on raw data already showed strong trends related to `elapsed_time` and `batch`, as shown in previous reports.

6.1 PCA of Raw Data

6.2. PCA of Corrected Data

Compared to the PCA of the raw data, the corrected data shows a more homogeneous distribution of variance across components, and no evident separation or gradient is observed when coloring by elapsed time or batch. This suggests that external influences no longer dominate the variance structure after correction.

```
library(patchwork)

# Data frames
var_df_corr <- data.frame(PC = paste0("PC", 1:6),
                          Variance = explained_corr[1:6])
var_df_raw <- data.frame(PC = paste0("PC", 1:6),
                         Variance = explained_var_raw[1:6])
```

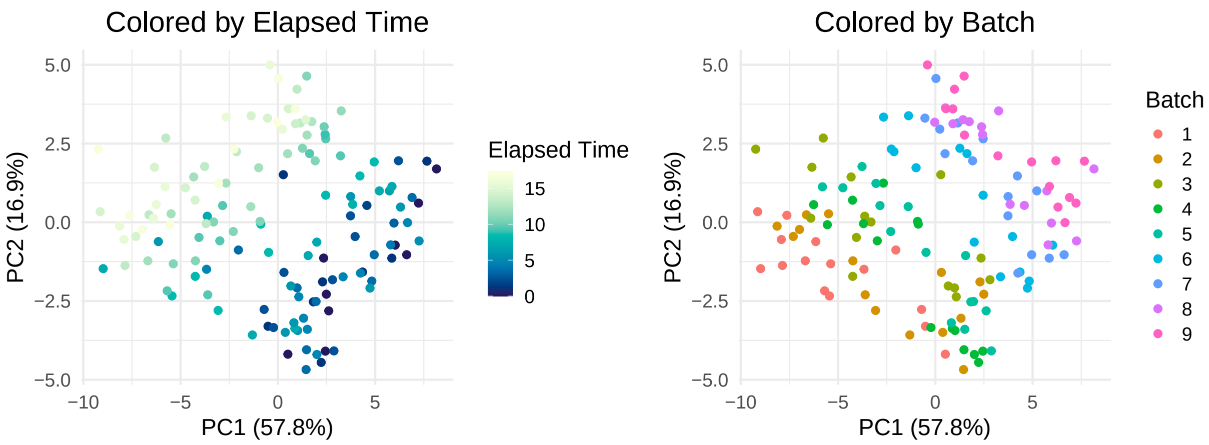


Figure 2: PCA of raw data colored by elapsed time (left) and by batch (right)

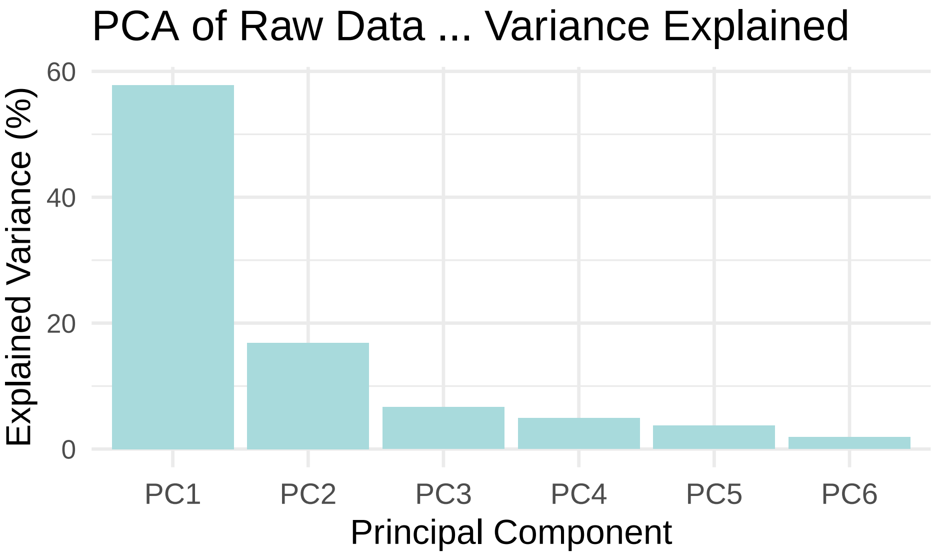


Figure 3: Explained variance by the first six PCA components (raw data)

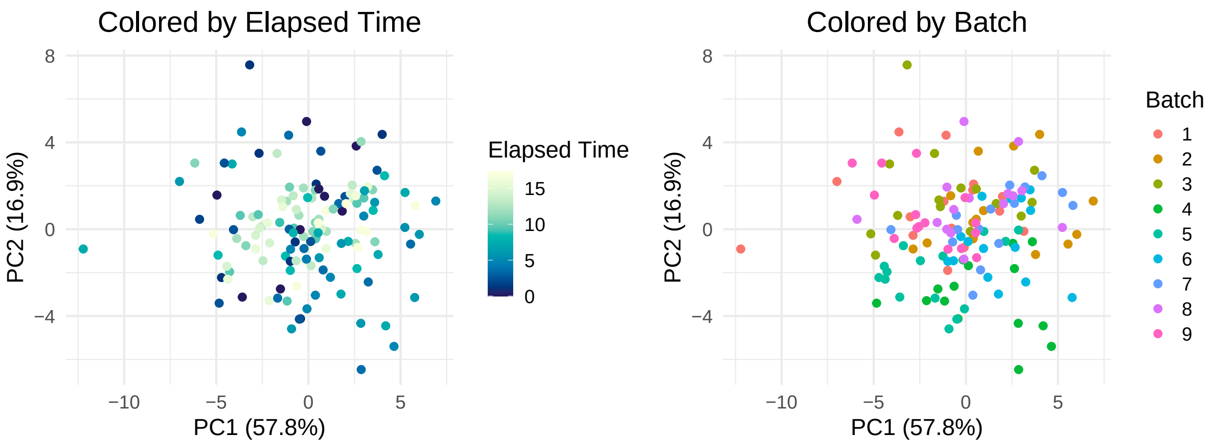


Figure 4: PCA of corrected data colored by elapsed time (left) and by batch (right)

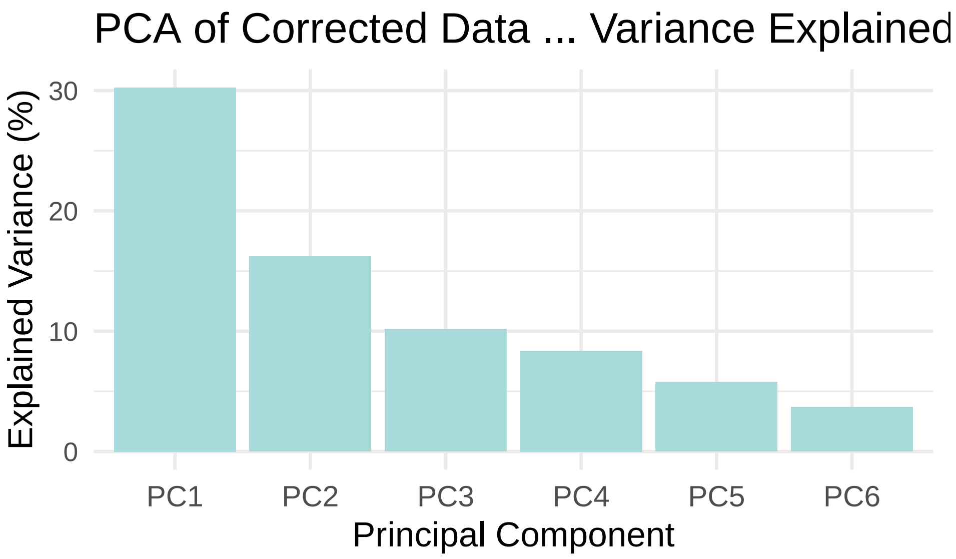


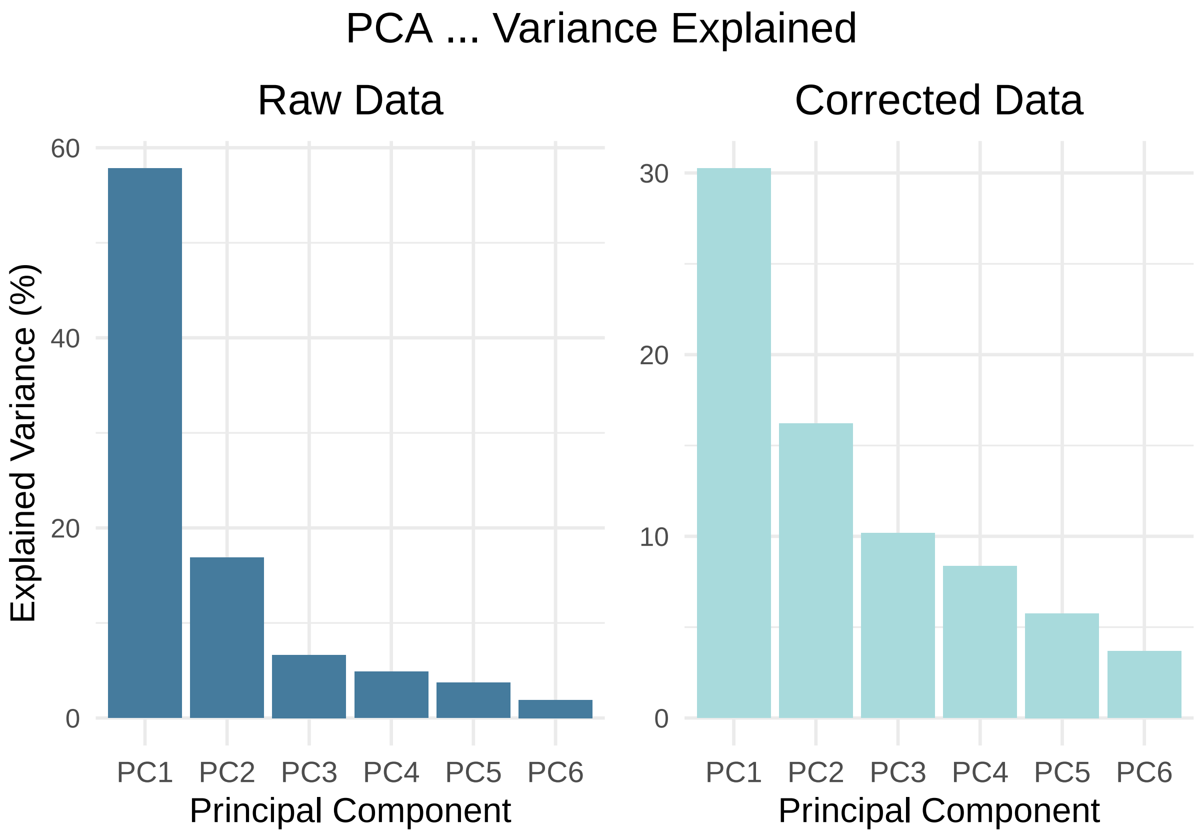
Figure 5: Variance explained by the first six PCA components (corrected data)

```r
# Plots
p_raw <- ggplot(var_df_raw, aes(x = PC, y = Variance)) +
  geom_col(fill = "#457B9D") +
  theme_minimal(base_size = 13) +
  labs(title = "Raw Data",
       x = "Principal Component", y = "Explained Variance (%)") +
  theme(axis.text.x = element_text(size = 11),
        plot.title = element_text(hjust = 0.5))

p_corr <- ggplot(var_df_corr, aes(x = PC, y = Variance)) +
  geom_col(fill = "#A8DADC") +
  theme_minimal(base_size = 13) +
  labs(title = "Corrected Data",
       x = "Principal Component", y = NULL) +
  theme(axis.text.x = element_text(size = 11),
        axis.title.y = element_blank(),
        plot.title = element_text(hjust = 0.5))

# Combine with generic title
final_plot <- (p_raw | p_corr) +
  plot_annotation(title = "PCA - Variance Explained") &
  theme(plot.title = element_text(size = 16, hjust = 0.5))

# Show in Rmd
final_plot
```



```
# Save to PNG with high resolution
ggsave("pca_variance_comparison.png", final_plot,
       width = 9, height = 5, dpi = 300)
```

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7. Conclusion

The applied correction successfully reduces the influence of time and batch effects. The PCA projection confirms that corrected data no longer follows the acquisition order. This confirms the effectiveness of the orthogonalization strategy when applied directly to the raw intensity matrix.