

Orthogonal Correction using PC1 of Batch and Order Effects

Tecla Duran Fort

2025-09-26

Contents

1. Load Data	1
2. Design Matrices	1
3. PCA of Batch and Order Reconstructions	2
Visualize PC1 Scores	2
4. Orthogonal Correction	2
5. Visualization of Correction	3
6. PCA Before and After Correction	4

1. Load Data

```
df <- read.csv("../data/peak_table_var.csv")

# Intensity matrix
X <- as.matrix(df %>% dplyr::select(starts_with("Cluster")))
```

2. Design Matrices

```
# One-hot encoding for batch
B <- model.matrix(~ 0 + factor(df$batch))
colnames(B) <- paste0("Batch_", sort(unique(df$batch)))

# Order index per batch
df <- df %>%
    arrange(batch, elapsed_time) %>%
    group_by(batch) %>%
    mutate(order_in_batch = row_number()) %>%
    ungroup()

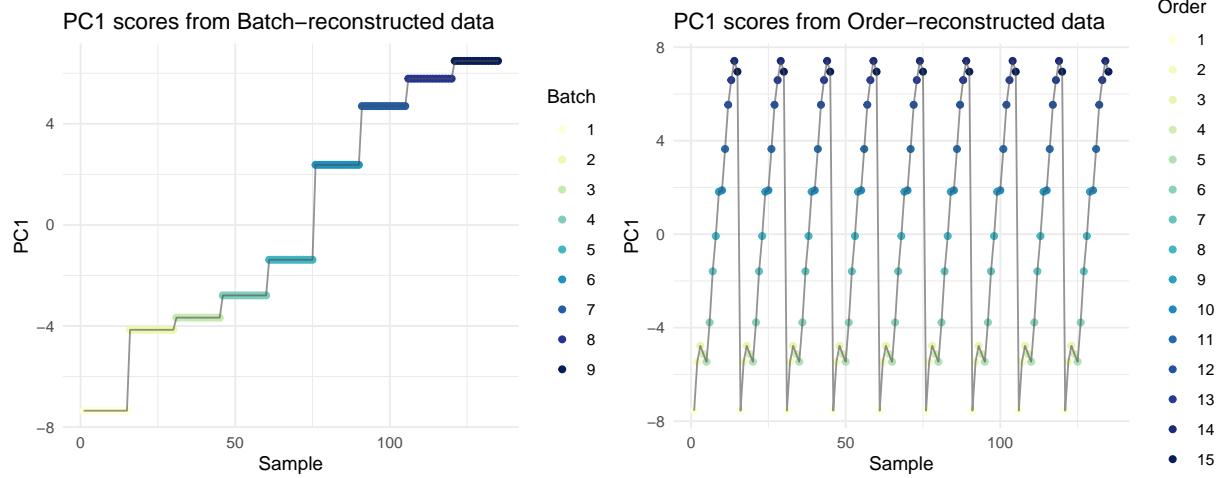
# One-hot encoding for order
O <- model.matrix(~ 0 + factor(df$order_in_batch))
colnames(O) <- paste0("Ord_", 1:max(df$order_in_batch))
```

3. PCA of Batch and Order Reconstructions

```
# Batch means and PCA
X_batch_means <- B %*% (solve(t(B)%*%B) %*% t(B) %*% X)
pca_batch <- prcomp(X_batch_means, scale. = TRUE)
pc1_batch <- pca_batch$x[,1, drop=FALSE]

# Order means and PCA
X_order_means <- O %*% (solve(t(O)%*%O) %*% t(O) %*% X)
pca_order <- prcomp(X_order_means, scale. = TRUE)
pc1_order <- pca_order$x[,1, drop=FALSE]
```

Visualize PC1 Scores

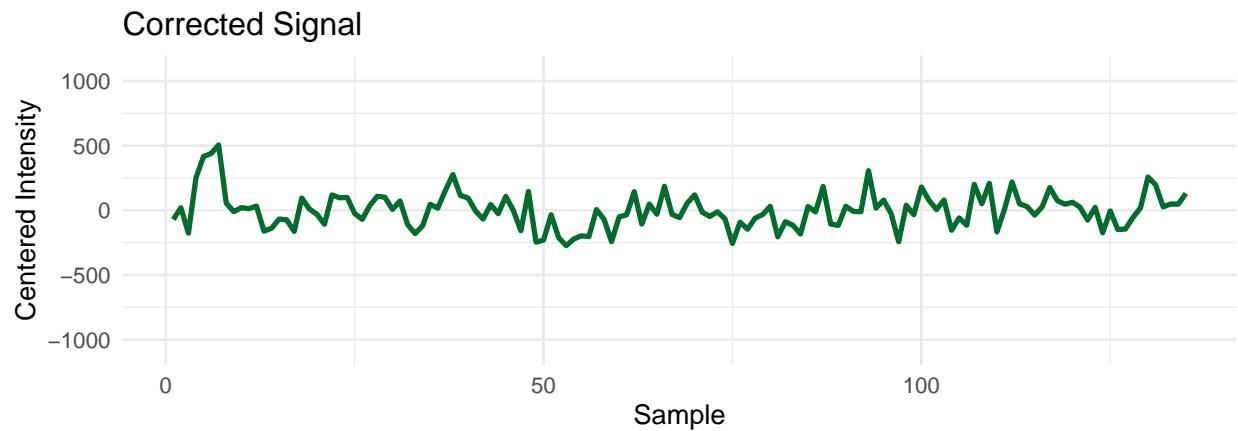
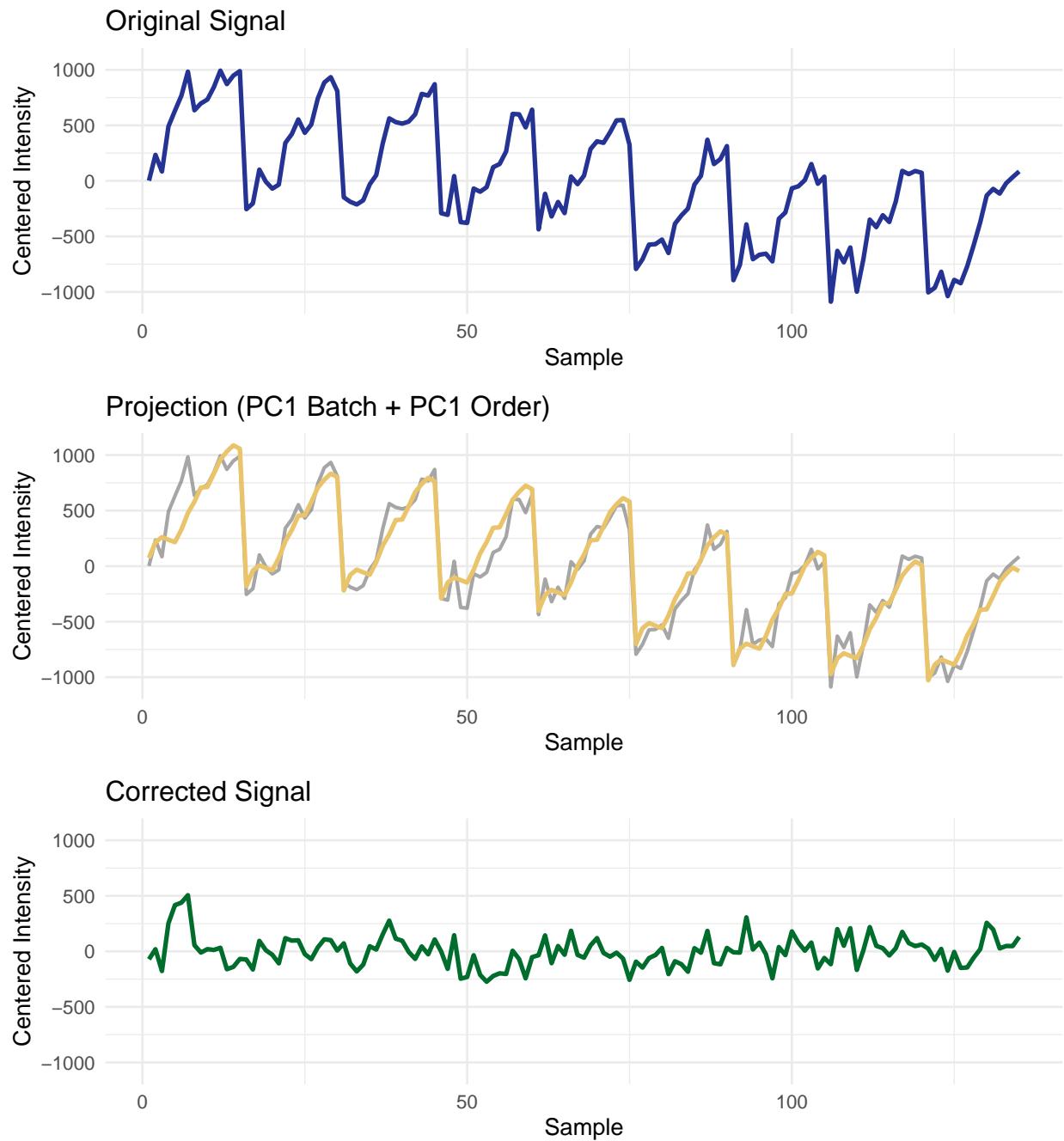


4. Orthogonal Correction

```
# Apply correction jointly with both directions as external variables
joint_corr <- orthogonal_correction(X, cbind(pc1_batch, pc1_order))

X_corr_joint <- joint_corr$corrected
proj_joint    <- joint_corr$projection
```

5. Visualization of Correction



6. PCA Before and After Correction

