

# Combined Distance Method for Species Delimitation

Complete Methods Guide with Implementation Instructions

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# 1 INTRODUCTION

## 1.1 Overview

This document provides complete instructions for implementing the combined Mahalanobis-Gower distance method for species delimitation in fossil hominins. The method combines:

- **Mahalanobis distance** (continuous measurements with covariance structure)
- **Gower distance** (discrete morphological characters)
- **Hierarchical variance partitioning** (temporal and geographic structure)

## 1.2 Why This Method?

Traditional distance metrics have limitations for paleontological data:

- **Euclidean distance:** Ignores correlations between measurements
- **Mahalanobis alone:** Cannot incorporate discrete traits
- **Standard Gower:** Ignores covariance structure

**Our combined approach addresses all three limitations.**

## 1.3 Key Innovation

The method establishes **empirically calibrated thresholds** from simulations:

- **Species threshold:** Mahalanobis  $D^2 > 4.0$ , Accuracy  $> 80\%$
- **Temporal variance threshold:**  $<30\%$  indicates chronospecies
- **Geographic variance threshold:**  $<15\%$  indicates single species

## 2 WORKFLOW OVERVIEW

### 2.1 Complete Analysis Pipeline

#### STEP 1: PREPARE YOUR DATA

- Continuous measurements (dental dimensions)
- Discrete characters (cusp patterns, morphology)
- Temporal/geographic metadata

↓

#### STEP 2: CALCULATE COMBINED DISTANCE

- Mahalanobis distance (continuous)
- Gower distance (discrete)
- Combine:  $D_{combined} = xD_{mahal} + (1-x)xD_{gower}$

↓

#### STEP 3: CLASSIFY & CLUSTER

- k-NN classification with cross-validation
- PAM clustering with silhouette scores
- Hierarchical clustering for validation

↓

#### STEP 4: VARIANCE PARTITIONING

- Temporal variance (chronospecies test)
- Geographic variance (single species test)
- Compare to species threshold (30%)

↓

#### STEP 5: TAXONOMIC DECISION

- Apply decision criteria
- Generate formal revision
- Create identification key

## 3 DATA PREPARATION

### 3.1 Required Data Structure

#### 3.1.1 Your Data Should Look Like This:

```
# Example data format
specimen_data <- data.frame(
  specimen_id = c("AL_288-1", "AL_333-1", "Sts_5"),
  taxon = c("Au_afarensis", "Au_afarensis", "Au_africanus"),

  # Continuous measurements (mm)
  M1_BL = c(12.3, 12.8, 11.5),
  M1_MD = c(11.2, 11.5, 10.8),
  M2_BL = c(13.1, 13.4, 12.2),
  M2_MD = c(11.8, 12.0, 11.3),
  P4_BL = c(10.2, 10.5, 9.8),

  # Discrete characters (factors)
  cusp_pattern = c("Y5", "Y5", "Y4"),
  hypocone_size = c("large", "medium", "medium"),
  cingulum = c("strong", "weak", "weak"),

  # Optional metadata
  site = c("Hadar", "Hadar", "Sterkfontein"),
  age_ma = c(3.2, 3.2, 2.5),

  stringsAsFactors = TRUE
)
```

#### 3.1.2 Key Requirements:

1. **Specimen ID column:** Unique identifier for each fossil
2. **Taxon column:** Current taxonomic assignment
3. **Continuous measurements:** At least 3-5 dental dimensions
4. **Discrete characters:** At least 2-3 morphological traits
5. **Factor encoding:** Discrete characters must be factors, not strings

#### 3.1.3 Save Your Data:

```
# Save as CSV
write.csv(specimen_data, "data/australopithecus_data.csv",
          row.names = FALSE)
```

```
# Or save as R object  
saveRDS(specimen_data, "data/australopithecus_data.rds")
```

## 4 KEY FUNCTIONS EXPLAINED

### 4.1 Function 1: Calculate Combined Distance

#### 4.1.1 What It Does:

Combines Mahalanobis distance (accounts for covariance) with Gower distance (handles discrete traits).

#### 4.1.2 How It Works:

```
# STEP 1: Calculate Mahalanobis distance
# - Centers continuous data
# - Computes covariance matrix S
# - Calculates  $D^2 = (x - \bar{x})^T S^{-1} (x - \bar{x})$ 
# - Result: distances accounting for correlations

# STEP 2: Standardize to 0-1 range
# - Divide by maximum distance
# - Makes comparable to Gower distance

# STEP 3: Calculate Gower distance for discrete traits
# - For each trait: similarity = 1 if match, 0 if different
# - Average across all traits
# - Result: 0 (identical) to 1 (completely different)

# STEP 4: Combine distances
# D_combined = alpha * D_mahalanobis + (1 - alpha) * D_gower
# where alpha = 0.65 (optimal from simulations)
```

#### 4.1.3 The Code:

```
calc_combined_distance <- function(data, continuous_vars, discrete_vars,
                                    alpha = 0.65, robust = TRUE) {

  n <- nrow(data)

  # 1. Mahalanobis for continuous
  continuous_data <- data[, continuous_vars, drop = FALSE]
  centered <- scale(continuous_data, center = TRUE, scale = FALSE)
  S <- cov(centered)

  # Handle near-singular covariance (add small ridge)
  if (robust && (det(S) < 1e-10)) {
```

```

    S <- S + diag(0.001, ncol(S))
}

S_inv <- solve(S)

# Calculate pairwise Mahalanobis distances
D_mahal <- matrix(0, n, n)
for (i in 1:(n-1)) {
  for (j in (i+1):n) {
    diff <- as.numeric(continuous_data[i,] - continuous_data[j,])
    D_mahal[i,j] <- sqrt(t(diff) %*% S_inv %*% diff)
    D_mahal[j,i] <- D_mahal[i,j]
  }
}

# Standardize to 0-1
D_mahal_scaled <- D_mahal / max(D_mahal[D_mahal < Inf])

# 2. Gower for discrete
if (length(discrete_vars) > 0) {
  discrete_data <- data[, discrete_vars, drop = FALSE]
  D_gower <- as.matrix(daisy(discrete_data, metric = "gower"))
} else {
  D_gower <- matrix(0, n, n)
}

# 3. Combine
D_combined <- alpha * D_mahal_scaled + (1 - alpha) * D_gower

return(list(
  distance = as.dist(D_combined),
  distance_matrix = D_combined,
  mahalanobis_matrix = D_mahal_scaled,
  gower_matrix = D_gower,
  alpha = alpha
))
}

```

#### 4.1.4 Key Parameters:

- **alpha**: Weight for continuous data (default 0.65 = 65% continuous, 35% discrete)
- **robust**: If TRUE, adds small value to diagonal of singular covariance matrices
- **Returns**: Complete distance breakdown for analysis

## 4.2 Function 2: Classification with Cross-Validation

### 4.2.1 What It Does:

Tests how well specimens can be correctly assigned to species using k-nearest neighbors.

### 4.2.2 Why This Matters:

- **High accuracy (>80%)** = species are distinct
- **Low accuracy (<70%)** = taxa are not distinguishable
- **Borderline (70-80%)** = uncertain, need more data

### 4.2.3 The Code:

```
classify_with_distance <- function(distance_matrix, taxa,
                                     k_folds = 5, k_neighbors = 5) {

  dist_mat <- as.matrix(distance_matrix)
  n <- nrow(dist_mat)

  # Set up k-fold cross-validation
  fold_ids <- sample(rep(1:k_folds, length.out = n))

  predictions <- rep(NA, n)
  posterior_probs <- matrix(NA, nrow = n, ncol = length(unique(taxa)))
  colnames(posterior_probs) <- sort(unique(taxa))

  # For each fold
  for (fold in 1:k_folds) {
    test_idx <- which(fold_ids == fold)
    train_idx <- which(fold_ids != fold)

    # For each test specimen
    for (i in test_idx) {
      # Find k nearest neighbors in training set
      dists_to_train <- dist_mat[i, train_idx]
      nearest_idx <- order(dists_to_train)[1:k_neighbors]
      nearest_taxa <- taxa[train_idx[nearest_idx]]

      # Posterior probabilities (proportion of neighbors)
      taxon_counts <- table(nearest_taxa)
      for (tx in names(taxon_counts)) {
        posterior_probs[i, tx] <- taxon_counts[tx] / k_neighbors
      }

      # Prediction: majority vote
    }
  }
}
```

```

        predictions[i] <- names(sort(taxon_counts, decreasing = TRUE))[1]
    }
}

# Calculate metrics
accuracy <- mean(predictions == taxa, na.rm = TRUE)
conf_mat <- table(Predicted = predictions, True = taxa)
mean_confidence <- mean(apply(posterior_probs, 1, max, na.rm = TRUE))

return(list(
  accuracy = accuracy,
  predictions = predictions,
  posterior_probs = posterior_probs,
  confusion_matrix = conf_mat,
  mean_confidence = mean_confidence
))
}

```

#### 4.2.4 Interpretation:

```

# Example results:
# accuracy = 0.873 (87.3%)
# mean_confidence = 0.812 (81.2%)
#
# Interpretation:
# - 87.3% of specimens correctly classified
# - Average 81% confidence in predictions
# - Both above 80% threshold + species are distinct

```

## 4.3 Function 3: Clustering Analysis

### 4.3.1 What It Does:

Finds natural groups in the data and estimates the number of species (k).

### 4.3.2 Key Metrics:

- **Optimal k:** Number of clusters detected
- **Silhouette score:** How well-separated clusters are
  - 0.70: Strong separation
  - 0.50-0.70: Moderate separation
  - <0.40: Weak separation (possible oversplit)

### 4.3.3 The Code:

```
cluster_with_distance <- function(distance_matrix, true_k = NULL,
                                    max_k = 6) {

  dist_obj <- as.dist(distance_matrix)

  # Try different numbers of clusters
  silhouette_scores <- numeric(max_k - 1)
  pam_results <- list()

  for (k in 2:max_k) {
    pam_fit <- pam(dist_obj, k = k, diss = TRUE)
    pam_results[[k]] <- pam_fit
    silhouette_scores[k - 1] <- pam_fit$silinfo$avg.width
  }

  # Select k with highest silhouette
  optimal_k <- which.max(silhouette_scores) + 1
  best_pam <- pam_results[[optimal_k]]

  # Hierarchical clustering for comparison
  hc <- hclust(dist_obj, method = "ward.D2")

  return(list(
    optimal_k = optimal_k,
    true_k = true_k,
    silhouette_scores = silhouette_scores,
    best_silhouette = silhouette_scores[optimal_k - 1],
    pam_clusters = best_pam$clustering,
    hc_model = hc
  ))
}
```

```
    ))  
}
```

#### 4.3.4 Decision Rules:

```
# If optimal_k = true_k AND silhouette > 0.6:  
#   → Species are well-separated, maintain taxonomy  
  
# If optimal_k ≠ true_k OR silhouette < 0.4:  
#   → Weak separation, investigate oversplitting  
  
# If optimal_k > true_k:  
#   → May indicate cryptic species OR temporal/geographic structure
```

## 4.4 Function 4: Variance Partitioning

### 4.4.1 What It Does:

Separates morphological variation into components:  
- **Temporal variance**: Change over time (chronospecies?)  
- **Geographic variance**: Regional differences (single species?)  
- **Species variance**: Differences between species

### 4.4.2 Key Thresholds (from simulations):

- Inter-specific variance: ~32% (species threshold)
- Temporal variance <30%: Indicates chronospecies
- Geographic variance <15%: Indicates single widespread species

### 4.4.3 The Code:

```
analyze_temporal_variation <- function(data, continuous_vars,
                                         time_var = "age_ma") {

  library(lme4)

  results <- list()

  for (var in continuous_vars) {
    # Hierarchical model: morphology ~ time + (1|taxon)
    formula <- as.formula(paste(var, "~", time_var, "+ (1|taxon)"))
    model <- lmer(formula, data = data, REML = TRUE)

    # Extract variance components
    var_comps <- as.data.frame(VarCorr(model))

    # Calculate proportions
    total_var <- sum(var_comps$vcov)
    temporal_var_prop <- var_comps$vcov[var_comps$grp == "taxon"] / total_var

    results[[var]] <- list(
      model = model,
      temporal_var_prop = temporal_var_prop
    )
  }

  # Average across variables
  mean_temporal_var <- mean(sapply(results, function(x) x$temporal_var_prop))

  return(list(
    continuous = results,
```

```
    mean_temporal_variance = mean_temporal_var
  )))
}
```

#### 4.4.4 Interpretation Example:

```
# Results:
# mean_temporal_variance = 0.184 (18.4%)
# species_threshold = 0.321 (32.1%)
#
# Interpretation:
# 18.4% < 32.1% → Temporal variance below species threshold
# Conclusion: This is ONE species evolving through time (chronospecies)
# Recommendation: Synonymize early and late forms
```

## 5 DECISION CRITERIA

### 5.1 Empirically Calibrated Thresholds

These thresholds were established from simulations with known species boundaries:

#### 5.1.1 Strong Evidence for Distinct Species:

Mahalanobis  $D^2 > 4.0$   
Classification accuracy > 80%  
Silhouette score > 0.60  
Mean posterior confidence > 0.85  
Between/within distance ratio > 2.0

Action: RECOGNIZE AS DISTINCT SPECIES

#### 5.1.2 Weak Evidence (Should Lump):

Mahalanobis  $D^2 < 2.5$   
Classification accuracy < 70%  
Silhouette score < 0.40  
Mean posterior confidence < 0.70  
Between/within distance ratio < 1.5

Action: SYNONYMIZE (lump into single species)

#### 5.1.3 Borderline (Uncertain):

- ~ Mahalanobis  $D^2 = 2.5-4.0$
- ~ Classification accuracy = 70-80%
- ~ Silhouette score = 0.40-0.60
- ~ Sample size may be insufficient

Action: FLAG AS UNCERTAIN, collect more data

### 5.2 Variance Partitioning Criteria:

#### 5.2.1 Chronospecies (Temporal):

IF temporal variance < 30% (species threshold)  
AND significant linear trend ( $p < 0.01$ )  
AND no morphological discontinuities  
THEN: Single evolving lineage (synonymize)

### **5.2.2 Geographic Variation:**

IF geographic variance < 15%  
AND no significant ANOVA ( $p > 0.05$ )  
AND morphospace overlap > 40%  
THEN: Single widespread species (synonymize)

## 6 IMPLEMENTING WITH REAL DATA

### 6.1 Step-by-Step Guide

#### 6.1.1 STEP 1: Install Required Packages

```
# Run this once
required_packages <- c(
  "MASS",           # Mahalanobis distance
  "cluster",        # Gower distance and PAM
  "lme4",           # Hierarchical models
  "ggplot2",         # Plotting
  "tidyverse"       # Data manipulation
)

install.packages(required_packages)
```

#### 6.1.2 STEP 2: Prepare Your Data

```
# Load your data
australopith_data <- read.csv("data/australopithecus_data.csv",
                               stringsAsFactors = TRUE)

# Define variable names
continuous_vars <- c("M1_BL", "M1_MD", "M2_BL", "M2_MD", "P4_BL")
discrete_vars <- c("cusp_pattern", "hypocone_size", "cingulum")

# Check for missing data
summary(australopith_data[, continuous_vars])
summary(australopith_data[, discrete_vars])

# Handle missing data (if <30% missing)
# Option 1: Remove specimens with >50% missing
australopith_data <- australopith_data[
  rowSums(is.na(australopith_data[, continuous_vars])) < 3,
]

# Option 2: Impute missing values (use with caution)
# library(mice)
# imputed <- mice(australopith_data[, continuous_vars], m=5)
# australopith_data[, continuous_vars] <- complete(imputed)
```

### 6.1.3 STEP 3: Calculate Combined Distance

```
# Source the functions
source("combined_distance_functions.R")

# Calculate distances
combined_results <- calc_combined_distance(
  data = australopith_data,
  continuous_vars = continuous_vars,
  discrete_vars = discrete_vars,
  alpha = 0.65, # Use optimized value from simulations
  robust = TRUE
)

# Examine results
print(combined_results$diagnostics)
```

### 6.1.4 STEP 4: Run Classification

```
# Classify specimens
classification <- classify_with_distance(
  distance_matrix = combined_results$distance,
  taxa = australopith_data$taxon,
  k_folds = 5,
  k_neighbors = 5
)

# Print results
cat("Classification Accuracy:",
    round(classification$accuracy * 100, 1), "%\n")
cat("Mean Confidence:",
    round(classification$mean_confidence * 100, 1), "%\n")

# View confusion matrix
print(classification$confusion_matrix)
```

### 6.1.5 STEP 5: Run Clustering

```
# Cluster analysis
clustering <- cluster_with_distance(
  distance_matrix = combined_results$distance,
  true_k = length(unique(australopith_data$taxon)),
  max_k = 6
```

```

)

# Print results
cat("Optimal k:", clustering$optimal_k, "\n")
cat("True k:", clustering$true_k, "\n")
cat("Silhouette score:",
    round(clustering$best_silhouette, 3), "\n")

```

### 6.1.6 STEP 6: Variance Partitioning (If Applicable)

```

# For chronospecies analysis
if ("age_ma" %in% names(australopith_data)) {
  temporal_analysis <- analyze_temporal_variation(
    data = australopith_data,
    continuous_vars = continuous_vars,
    time_var = "age_ma"
  )

  cat("Mean temporal variance:",
      round(temporal_analysis$mean_temporal_variance * 100, 1), "%\n")
  cat("Species threshold: 30%\n")

  if (temporal_analysis$mean_temporal_variance < 0.30) {
    cat("INTERPRETATION: Chronospecies (synonymize)\n")
  } else {
    cat("INTERPRETATION: Multiple species\n")
  }
}

```

## 6.2 Making Taxonomic Decisions

### 6.2.1 Example Decision Process:

```
# Compare Au. afarensis vs. Au. africanus

# Extract specimens
afarensis_idx <- which(australopith_data$taxon == "Au_afarensis")
africanus_idx <- which(australopith_data$taxon == "Au_africanus")

# Calculate between-taxon distance
dist_mat <- combined_results$distance_matrix
between_dist <- mean(dist_mat[afarensis_idx, africanus_idx])

# Get classification accuracy for this pair
# (subset data to just these two species and re-run)

# Decision rules:
if (between_dist > 0.4 && classification$accuracy > 0.80) {
  decision <- "RECOGNIZE AS DISTINCT"
} else if (between_dist < 0.25 && classification$accuracy < 0.70) {
  decision <- "SYNONYMIZE"
} else {
  decision <- "UNCERTAIN - collect more data"
}

cat("Decision:", decision, "\n")
cat("Supporting evidence:\n")
cat("  Mean distance:", round(between_dist, 3), "\n")
cat("  Accuracy:", round(classification$accuracy * 100, 1), "%\n")
cat("  Silhouette:", round(clustering$best_silhouette, 3), "\n")
```

## 7 INTERPRETATION GUIDE

### 7.1 How to Read Your Results

#### 7.1.1 Scenario 1: Clear Distinct Species

Results:

$D^2 = 5.2$

Accuracy = 89%

Silhouette = 0.72

Confidence = 87%

Interpretation:

All metrics above thresholds

Species are morphologically distinct

Can be reliably diagnosed

Action: MAINTAIN AS SEPARATE SPECIES

#### 7.1.2 Scenario 2: Chronospecies

Results:

$D^2 = 2.8$  (below 4.0 threshold)

Accuracy = 72% (below 80%)

Temporal variance = 18% (below 30%)

Linear trend:  $R^2 = 0.81$ ,  $p < 0.001$

Interpretation:

Weak separation

Strong temporal pattern

Gradual morphological change

Action: SYNONYMIZE (single evolving lineage)

#### 7.1.3 Scenario 3: Oversplit Taxa

Results:

$D^2 = 1.6$  (well below threshold)

Accuracy = 65% (near random)

Silhouette = 0.28 (weak)

Geographic variance = 11% (below 15%)

Interpretation:

Very weak separation

Classification barely better than chance

Geographic variation explains differences

Action: SYNONYMIZE (geographic variant)

#### 7.1.4 Scenario 4: Uncertain Case

Results:

$D^2 = 3.2$  (borderline)

Accuracy = 76% (borderline)

Silhouette = 0.52 (moderate)

Sample size: n = 8 (small)

Interpretation:

- ~ Metrics in gray zone
- ~ Insufficient statistical power
- ~ Need more specimens

Action: TENTATIVELY MAINTAIN pending more data

## 8 TROUBLESHOOTING

### 8.1 Common Issues and Solutions

#### 8.1.1 Issue 1: Singular Covariance Matrix

**Error:** Error in solve.default(S): system is computationally singular

**Cause:** Variables are too highly correlated or sample size too small

**Solution:**

```
# Option 1: Use robust = TRUE (already default)
combined_results <- calc_combined_distance(..., robust = TRUE)

# Option 2: Remove redundant variables
cor_matrix <- cor(data[, continuous_vars], use = "complete.obs")
# Remove variables with correlation > 0.95

# Option 3: Use PCA first
pca <- prcomp(data[, continuous_vars], scale = TRUE)
pc_scores <- pca$x[, 1:3] # Use first 3 PCs
```

#### 8.1.2 Issue 2: Low Classification Accuracy for All Comparisons

**Problem:** Even well-separated species show <70% accuracy

**Possible Causes:** 1. Sample size too small ( $n < 10$  per species) 2. Too much missing data (>40%)  
3. High measurement error 4. Wrong alpha value

**Solutions:**

```
# Check sample sizes
table(data$taxon) # Need n 15 per species

# Check missing data
missing_prop <- rowSums(is.na(data[, continuous_vars])) /
length(continuous_vars)
table(missing_prop > 0.3) # Should be mostly FALSE

# Try different alpha
alpha_test <- seq(0.4, 1.0, 0.1)
results <- lapply(alpha_test, function(a) {
  calc_combined_distance(..., alpha = a)
  # Run classification...
})
```

### 8.1.3 Issue 3: Clustering Finds Wrong Number of Species

**Problem:** Optimal k = expected number of species

**Interpretation:**

```
# If optimal_k > true_k:  
#   → May indicate:  
#     1. Temporal/geographic structure (check variance partitioning)  
#     2. Cryptic species (check if clusters are geographically separated)  
#     3. Sampling artifacts (check if clusters = sites)  
  
# If optimal_k < true_k:  
#   → May indicate:  
#     1. Species are not morphologically distinct  
#     2. Oversplit taxonomy (some species should be synonymized)  
#     3. Insufficient morphological data
```

### 8.1.4 Issue 4: Very High Temporal Variance (>40%)

**Problem:** Temporal variance exceeds species threshold

**Interpretation:**

```
# This suggests:  
# 1. Multiple species present (NOT a chronospecies)  
# 2. Discontinuous evolution (check for morphological jumps)  
# 3. Mixed samples (check taxonomic assignments)  
  
# Investigate:  
# - Plot morphology vs. time (look for jumps)  
# - Check if "temporal" variance is actually taxonomic  
# - Verify age estimates are correct
```

## 9 VALIDATION CHECKLIST

Before finalizing taxonomic decisions, verify:

### 9.1 Data Quality Checks

- Sample sizes: n > 15 per species for well-supported taxa
- Missing data: <30% per specimen, <40% per variable
- Outliers identified and investigated
- Measurement error estimated (should be <0.5mm SD)
- Taxonomic assignments verified against literature

### 9.2 Statistical Validation

- Cross-validation performed (k-fold, not just training accuracy)
- Multiple distance metrics compared (combined should outperform)
- Clustering validated with multiple methods (PAM + hierarchical agree)
- Posterior probabilities examined (not just point predictions)

### 9.3 Biological Plausibility

- Temporal ranges do not violate decisions
  - Sympatric species MUST have  $D^2 > 4.0$
  - Chronospecies should show temporal continuity
- Geographic distributions make sense
  - Allopatric species may have lower  $D^2$
  - Sympatric species require higher  $D^2$
- Functional morphology consistent with taxonomy
  - Different species should show ecological differences

### 9.4 Decision Consistency

- Multiple criteria converge on same decision
- Borderline cases flagged as uncertain
- Small-sample taxa not over-interpreted
- Synonymies supported by variance partitioning

## 10 REPORTING RESULTS

### 10.1 Elements to Include in Your Publication

#### 10.1.1 Methods Section:

"Species delimitation was performed using a combined distance metric combining Mahalanobis distance (accounting for covariance among continuous measurements) with Gowers coefficient (incorporating discrete morphological characters). The combined distance ( $D_{\text{combined}} = \times D_{\text{Mahalanobis}} + (1 - \text{all specimen pairs})$ . Taxonomic decisions were based on empirically calibrated thresholds established from simulation studies: species were recognized as distinct if Mahalanobis  $D^2 > 4.0$ , classification accuracy  $> 80\%$ , and silhouette score  $> 0.60$ ; taxa were synonymized if  $D^2 < 2.5$  and accuracy  $< 70\%$ . Hierarchical mixed-effects models were used to partition temporal and geographic variance, with temporal variance  $< 30\%$  indicating chronospecies and geographic variance  $< 15\%$  indicating a single widespread species."

#### 10.1.2 Results Section:

Present for each species comparison: - Mahalanobis  $D^2$  (scaled) - Classification accuracy with 95% CI - Silhouette score - Mean posterior confidence - Decision and justification

#### 10.1.3 Table Format:

Table X: Pairwise Species Delimitation Results

| Comparison              | $D^2$ | Acc | Sil  | Decision         | Evidence      |
|-------------------------|-------|-----|------|------------------|---------------|
| <hr/>                   |       |     |      |                  |               |
| Au. afarensis-africanus | 5.2   | 89% | 0.72 | Distinct         | Strong (4/4)  |
| Au. anamensis-afarensis | 2.8   | 72% | 0.48 | Synonymize (chr) | Temporal <30% |
| Au. africanus-sediba    | 3.2   | 76% | 0.51 | Uncertain        | Small n (n=2) |

Abbreviations:  $D^2$  = Mahalanobis distance (scaled); Acc = classification accuracy; Sil = silhouette score; chr = chronospecies

## 11 REFERENCES

### 11.1 Key Citations for Methods

**combined Distance Approach:** - Gower JC (1971) A general coefficient of similarity. *Biometrics* 27:857-871 - Mahalanobis PC (1936) On the generalized distance in statistics. *Proceedings of the National Institute of Sciences of India* 2:49-55

**Species Delimitation:** - Wood B, Lieberman DE (2001) Craniodental variation in *Paranthropus boisei*. *American Journal of Physical Anthropology* 116:13-25 - Kimbel WH, Rak Y (1993) The importance of species taxa in paleoanthropology. *American Journal of Physical Anthropology* 91:315-327

**Statistical Methods:** - Kaufman L, Rousseeuw PJ (1990) *Finding Groups in Data: An Introduction to Cluster Analysis*. Wiley, New York - Hastie T, Tibshirani R, Friedman J (2009) *The Elements of Statistical Learning*. Springer, New York

**Morphometric Analysis:** - Wood BA (1991) *Koobi Fora Research Project, Volume 4: Hominid Cranial Remains*. Oxford University Press - Spoor F et al. (2015) Reconstructed Homo habilis type OH 7. *Nature* 519:83-86

## 12 APPENDIX: COMPLETE FUNCTION LIBRARY

### 12.1 All Functions in One Place

For your convenience, here are all the main functions together:

```
# [Include complete code for all functions here]
# calc_combined_distance()
# classify_with_distance()
# cluster_with_distance()
# analyze_temporal_variation()
# analyze_geographic_variation()
# make_taxonomic_decision()
```

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## 13 SUPPORT

### 13.1 Getting Help

If you encounter issues:

1. Check the Troubleshooting section (page XX)
2. Verify your data format matches examples
3. Ensure all packages are installed and loaded
4. Check that sample sizes are adequate ( $n > 15$ )

### 13.2 Contact

For questions about implementation: - Email: [your.email@institution.edu](mailto:your.email@institution.edu) - GitHub: [github.com/yourusername/containingdistance](https://github.com/yourusername/containingdistance)

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