

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 hybrid 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 hybrid 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 HYBRID DISTANCE

- Mahalanobis distance (continuous)
- Gower distance (discrete)
- Combine: $D_{\text{hybrid}} = \alpha D_{\text{mahal}} + (1-\alpha) D_{\text{gower}}$

↓

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 Hybrid 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  $D^2 = (x-x) S^{-1} (x-x)$ 
# - 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
#  $D_{\text{hybrid}} = \alpha \times D_{\text{mahalanobis}} + (1-\alpha) \times D_{\text{gower}}$ 
# where  $\alpha = 0.65$  (optimal from simulations)
```

4.1.3 The Code:

```
calc_hybrid_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_hybrid <- alpha * D_mahal_scaled + (1 - alpha) * D_gower

  return(list(
    distance = as.dist(D_hybrid),
    distance_matrix = D_hybrid,
    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: SYNONYMYZE (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 Hybrid Distance

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

# Calculate distances
hybrid_results <- calc_hybrid_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(hybrid_results$diagnostics)
```

6.1.4 STEP 4: Run Classification

```
# Classify specimens
classification <- classify_with_distance(
  distance_matrix = hybrid_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 = hybrid_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 <- hybrid_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 <- "SYNONYMYZE"
} 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: SYNONYIMIZE (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: SYNONYIMIZE (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)
hybrid_results <- calc_hybrid_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_hybrid_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: $n \geq 15$ per species for well-supported taxa
- ☐ Missing data: $<30\%$ per specimen, $<40\%$ per variable
- ☐ Outliers identified and investigated
- ☐ Measurement error estimated (should be $<0.5\text{mm SD}$)
- ☐ Taxonomic assignments verified against literature

9.2 Statistical Validation

- ☐ Cross-validation performed (k-fold, not just training accuracy)
- ☐ Multiple distance metrics compared (hybrid 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 hybrid distance metric combining Mahalanobis distance (accounting for covariance among continuous measurements) with Gowers coefficient (incorporating discrete morphological characters). The hybrid distance ($D_{\text{hybrid}} = \alpha \times D_{\text{Mahalanobis}} + (1 - \alpha) \times \text{Gowers coefficient}$) was calculated for 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
=====					
Au. afarensis-affricanus	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

Hybrid 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_hybrid_distance()  
# classify_with_distance()  
# cluster_with_distance()  
# analyze_temporal_variation()  
# analyze_geographic_variation()  
# make_taxonomic_decision()
```

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 ($n \geq 15$)
-

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