SOP_V3 — Comprehensive Procedure for Proficiency Testing (PT) Data Analysis in R/Shiny

1. Purpose and Scope

This **Standard Operating Procedure (SOP)** defines the complete, unified workflow for the **PT Data Analysis Application**, built using R/Shiny, in compliance with **ISO/IEC 17043:2023** and **ISO 13528:2022**. It integrates the methodological rigor of **SOP_V2_Final**【74†source】 and the comparative sensitivity and analytical structure from **SOP_v_2.5_gem**【73†source】.

This SOP provides a single, comprehensive framework that ensures: - Accurate and reproducible estimation of **assigned values (x_{pt})** and **standard deviations for proficiency assessment (σ_{pt})** using **robust statistical methods**. - Full **homogeneity and stability validation** of PT items for each robust estimator. - **Comparative analysis** of results obtained by multiple robust methods to ensure reliability. - **Mandatory performance scoring** (z, z′, ζ, En) and transparent reporting.

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2. System Setup and Requirements

2.1 Software Environment

- **R version:** ≥ 4.2
- **Framework:** Shiny (web-based analytical interface)
- **Environment:** RStudio (recommended)

2.2 Required Packages

```
install.packages(c(
  "shiny", "tidyverse", "vroom", "DT", "rhandsontable", "shinythemes",
"outliers"
))
```

2.3 Directory Structure

```
/data           # Input files: homogeneity.csv, stability.csv,
participant_results.csv
/app            # Shiny app scripts (app.R, server.R)
/reports        # Outputs and generated results
```

2.4 Launch

Run the application using:

```
Rscript run_app.R
```

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3. Workflow Overview

The PT analysis follows a four-stage comparative and validation workflow:

1. **Compute four robust estimators** of x_{pt} and σ_{pt} (Median, MADe, nIQR, Algorithm A).
2. **Conduct homogeneity and stability tests** for each σ_{pt} version.
3. **Compare outcomes** to evaluate sensitivity and robustness across estimators.
4. **Select and apply the validated x_{pt} and σ_{pt}** to calculate participant performance scores.

This structured approach provides analytical transparency, ensuring robustness and reproducibility across PT schemes.

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4. Robust Estimation of x_{pt} and σ_{pt}

4.1 Methods Overview

Method	Description	Formula	Notes
Median	Robust location estimator	x_{pt1} = median(x)	Insensitive to outliers
MADe	Median Absolute Deviation (scaled)	σ_{pt2} = 1.4826·median(	x_i−median(x)
nIQR	Normalized Interquartile Range	$\sigma_{pt3} = 0.7413 \cdot (Q_3 - Q_1)$	ISO 13528 Annex C
Algorithm A	Iterative robust mean and SD	ISO 13528 §7.4	Preferred estimator for stability

4.2 Example R Implementations

```
mad_e_manual <- function(x){
  med <- median(x, na.rm = TRUE)
  1.4826 * median(abs(x - med), na.rm = TRUE)
}

nIQR_manual <- function(x){
  q <- quantile(x, probs = c(0.25, 0.75), na.rm = TRUE)
  0.7413 * (q[2] - q[1])
}

algorithm_A <- function(x, max_iter=100){
  x <- x[!is.na(x)]
```

```r
  x_star <- median(x); s_star <- mad(x, constant=1.4826)
  for(i in 1:max_iter){
    delta <- 1.5*s_star
    x_prime <- pmin(pmax(x, x_star-delta), x_star+delta)
    new_x <- mean(x_prime)
    new_s <- 1.134*sd(x_prime)
    if(abs(new_x - x_star) < 1e-6 && abs(new_s - s_star) < 1e-6) break
    x_star <- new_x; s_star <- new_s
  }
  list(robust_mean = x_star, robust_sd = s_star)
}
```

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5. Homogeneity and Stability Analysis (4×)

5.1 Purpose

To ensure that all PT samples are **statistically homogeneous and stable**, supporting valid participant performance comparisons.

5.2 Homogeneity Assessment (ISO 13528 Annex B)

Each σ_{pt} variant (1–4) is tested using ANOVA-based variance components:

1. Compute item means ($\bar{x}_i$) and overall mean ($\bar{\bar{x}}$).
2. Calculate sum of squares:
3. Between: $SSb = m \cdot \Sigma(\bar{x}_i - \bar{\bar{x}})^2$
4. Within: $SSw = \Sigma\Sigma(x_{i,k} - \bar{x}_i)^2$
5. Mean squares: $MSb = SSb/(g-1)$; $MSw = SSw/[g(m-1)]$
6. Between-item SD: $s_s = \sqrt{((MSb - MSw)/m)}$

Acceptance Criteria: - Primary: $s_s \leq 0.3 \cdot \sigma_{pti}$
- Expanded (if marginal): $MSb \leq F_1 \cdot (0.3\sigma_{pti})^2 + F_2 \cdot MSw$

5.3 Stability Assessment

Compare two time points (t_1, t_2): - Absolute mean difference: $|y_1 - y_2| \leq 0.3 \cdot \sigma_{pti}$
- Statistical test: t-test, $p > 0.05$ supports stability.

5.4 Comparative Reporting

For each method i = 1:4, produce: - Homogeneity table (MSb, MSw, s_s, criteria results) - Stability table ($|y_1 - y_2|$, t-test p-values, conclusion)

Summarize all results in a comparative matrix for decision-making.

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6. Selection of Operational x_{pt} and σ_{pt}

Decision Criteria: 1. Homogeneity and stability both confirmed.
2. σ_{pt} neither inflated nor unrealistically small.
3. Method aligns with previous PT rounds or standard practice (Algorithm A preferred).

The selected x_{pt} and σ_{pt} will be used for participant scoring.

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7. Performance Score Calculations (Mandatory)

After validation, participant results are evaluated using ISO 13528 formulas.

Score	Formula	Description	Criterion
z	$(x_i - x_{pt})/\sigma_{pt}$	Standard deviation-based	
z′	$(x_i - x_{pt})/\sqrt{(\sigma_{pt}^2 + u_{xpt}^2)}$	Accounts for x_{pt} uncertainty	2 <
ζ	$(x_i - x_{pt})/\sqrt{(u_{xpt}^2 + u(x_i)^2)}$	Includes both uncertainties	
En	$(x_i - x_{pt})/\sqrt{((k \cdot u_{xpt})^2 + (k \cdot u(x_i))^2)}$, k=2	Expanded uncertainty	

7.1 Outputs

- Individual score reports with color-coded thresholds.
- Graphical summaries: z/z′/ζ/En score charts and boxplots.
- Aggregated results for QA summaries.

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8. Reporting, Traceability, and QA

- Export numerical and graphical outputs (CSV, PDF, XLSX).
- Document the selected x_{pt}, σ_{pt}, and test results.
- Record software environment (R version, packages).
- Validate against reference datasets to ensure reproducibility.

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9. References

1. ISO/IEC 17043:2023 — *Conformity assessment – General requirements for proficiency testing.*
2. ISO 13528:2022 — *Statistical methods for proficiency testing by interlaboratory comparison.*
3. Eurachem Guide (2021) — *Selection, Use, and Interpretation of PT Schemes.*
4. Linsinger, M. G. (2018). *Use of robust statistical methods in proficiency testing. Accreditation and Quality Assurance*, 23, 399–403.
5. AMC Technical Brief No. 6 — *Robust Statistics*, Royal Society of Chemistry.

End of SOP_V3 — Comprehensive Edition (Gem+GPT Integration)