00_setup_and_validation

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1 MetaboAnalystR Setup and Validation

This notebook verifies your MetaboAnalystR environment setup and validates the installation. It includes: 1. Environment verification 2. Package checks 3. Directory structure setup 4. Basic functionality test

Run each cell in sequence to validate your setup.

1.1 1. Initialize Project Structure

Set up the working directory and create a helper function for path management.

```
[2]: # Set working directory to project root
     project_root <- normalizePath("..")
     setwd(project_root)

     # Function to get subdirectory paths
     get_path <- function(subdir) {
         file.path(project_root, subdir)
     }

     print("Project root directory:")
     print(project_root)
```

```
[1] "Project root directory:"
[1] "/home/ubuntu/files/metaboanalystr-jupyter"
```

1.2 2. Environment Verification

Check R version, library paths, and locale settings.

```
[3]: # System information
     cat("\n1. System Information:\n")
     cat("R Version:", R.version.string, "\n")
     cat("Platform:", R.version$platform, "\n")
     cat("OS:", Sys.info()["sysname"], "\n")

     # Library paths
     cat("\n2. Library Paths:\n")
```

```r
print(.libPaths())

# Locale settings
cat("\n3. Locale Settings:\n")
print(Sys.getlocale())
```

```
1. System Information:
R Version: R version 4.3.3 (2024-02-29)
Platform: x86_64-conda-linux-gnu
OS: Linux

2. Library Paths:
[1] "/home/ubuntu/miniconda3/envs/metaboanalystr/lib/R/library"

3. Locale Settings:
[1] "LC_CTYPE=en_AU.UTF-8;LC_NUMERIC=C;LC_TIME=en_AU.UTF-8;LC_COLLATE=en_AU.UTF-
8;LC_MONETARY=en_AU.UTF-8;LC_MESSAGES=en_AU.UTF-8;LC_PAPER=en_AU.UTF-8;LC_NAME=C
;LC_ADDRESS=C;LC_TELEPHONE=C;LC_MEASUREMENT=en_AU.UTF-8;LC_IDENTIFICATION=C"
```

1.3 3. Package Verification

Check for required packages and their versions.

```r
[5]:  # Function to check package version
check_package <- function(pkg_name) {
    if (pkg_name %in% rownames(installed.packages())) {
        version <- packageVersion(pkg_name)
        cat(sprintf("%s: v%s []\n", pkg_name, version))
        return(TRUE)
    } else {
        cat(sprintf("%s: Not installed []\n", pkg_name))
        return(FALSE)
    }
}

# List of required packages
required_packages <- c(
    "MetaboAnalystR",
    "BiocManager",
    "Rserve",
    "IRkernel"
)

cat("Package Check:\n")
all_installed <- all(sapply(required_packages, check_package))

if (all_installed) {
```

```
    cat("\nAll required packages are installed! []\n")
} else {
    cat("\nWarning: Some packages are missing. Please install them before␣
  ↪proceeding. []\n")
}
```

Package Check:

MetaboAnalystR: v4.0.0 []
BiocManager: v1.30.25 []
Rserve: v1.8.13 []
IRkernel: v1.3.2 []

All required packages are installed! []

1.4   4. Directory Structure Setup

Create and verify the project directory structure.

```
[6]: # Define required directories
required_dirs <- c(
    "data",
    "data/processed",  # Subdirectory for processed data
    "plots",
    "results",
    "notebooks",
    "docs",
    "tests",
    "environment"
)

# Create and verify directories
cat("Directory Structure Check:\n")
for (dir in required_dirs) {
    dir_path <- get_path(dir)
    if (!dir.exists(dir_path)) {
        dir.create(dir_path, recursive = TRUE, showWarnings = FALSE)
        if (dir.exists(dir_path)) {
            cat(sprintf("%s: Created []\n", dir))
        } else {
            cat(sprintf("%s: Creation failed []\n", dir))
        }
    } else {
        cat(sprintf("%s: Already exists []\n", dir))
    }
}

# Verify write permissions
```

```r
cat("\nVerifying write permissions:\n")
for (dir in required_dirs) {
    dir_path <- get_path(dir)
    test_file <- file.path(dir_path, ".test_write")
    if (file.create(test_file)) {
        file.remove(test_file)
        cat(sprintf("%s: Writable []\n", dir))
    } else {
        cat(sprintf("%s: Not writable []\n", dir))
    }
}
```

```
Directory Structure Check:
data: Already exists []
data/processed: Already exists []
plots: Already exists []
results: Already exists []
notebooks: Already exists []
docs: Already exists []
tests: Already exists []
environment: Already exists []

Verifying write permissions:
data: Writable []
data/processed: Writable []
plots: Writable []
results: Writable []
notebooks: Writable []
docs: Writable []
tests: Writable []
environment: Writable []
```

1.5   5. MetaboAnalystR Functionality Test

Test basic MetaboAnalystR functionality.

```r
[7]: # Load MetaboAnalystR
     library(MetaboAnalystR)
     cat(sprintf("MetaboAnalystR v%s loaded successfully\n",
       packageVersion("MetaboAnalystR")))

     # Basic initialization test
     tryCatch({
         mSet <- InitDataObjects("pktable", "stat", FALSE)
         cat("InitDataObjects: Success []\n")

         # Test basic object properties
         if (!is.null(mSet$dataSet) && !is.null(mSet$analSet)) {
```

```
        cat("Object properties: Valid []\n")
    } else {
        cat("Object properties: Invalid []\n")
    }
}, error = function(e) {
    cat(sprintf("Initialization failed: %s []\n", e$message))
})
```

```
MetaboAnalystR 4.0.0 initialized Successfully !
https://github.com/xia-lab/MetaboAnalystR


MetaboAnalystR v4.0.0 loaded successfully
Starting Rserve:
 /home/ubuntu/miniconda3/envs/metaboanalystr/lib/R/bin/R CMD
/home/ubuntu/miniconda3/envs/metaboanalystr/lib/R/library/Rserve/libs//Rserve
--no-save

[1] "MetaboAnalyst R objects initialized …"
InitDataObjects: Success []
Object properties: Valid []
```

1.6   6. Save Environment Summary

Create a summary of the environment configuration.

```
[8]: # Create environment summary
summary <- c(
    "# MetaboAnalystR Environment Summary",
    paste("Date:", Sys.Date()),
    paste("R Version:", R.version.string),
    paste("MetaboAnalystR Version:", packageVersion("MetaboAnalystR")),
    paste("BiocManager Version:", packageVersion("BiocManager")),
    paste("Working Directory:", getwd()),
    "",
    "## Directory Structure:",
    paste("-", required_dirs),
    "",
    "## System Information:",
    paste("OS:", Sys.info()["sysname"]),
    paste("Platform:", R.version$platform),
    "",
    "## Session Information:"
)

# Add session info
session_info <- capture.output(sessionInfo())
summary <- c(summary, session_info)
```

```r
# Write summary to file
summary_file <- file.path(get_path("results"), "environment_summary.txt")
writeLines(summary, summary_file)
cat(sprintf("Environment summary saved to: %s\n", summary_file))
```

Environment summary saved to: /home/ubuntu/files/metaboanalystr-jupyter/results/environment_summary.txt

2 Setup Validation Complete

2.1 Setup Validation Complete

If you've reached this point without errors: 1. R is properly installed 2. Required packages are installed 3. Directory structure is set up 4. Basic MetaboAnalystR functionality is confirmed

2.1.1 Next Steps:

1. Proceed to `01_metabolomics_workflow.ipynb`
2. Start your metabolomics analysis

2.1.2 Troubleshooting:

If you encountered any errors: 1. Check the environment summary in `results/environment_summary.txt` 2. Consult the documentation in `docs/troubleshooting.md` 3. Verify R and package installations