

Package ‘SQUIRE’

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Type Package

Title Statistical Quality-Assured Integrated Response Estimation

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Description Provides systematic geometry-adaptive parameter optimization with statistical validation for experimental biological data. Combines ANOVA-based validation with systematic constraint configuration testing (log-scale, positive domain, Euclidean) through T,P,E testing. Only proceeds with parameter optimization when statistically significant biological effects are detected, preventing over-fitting to noise. Uses 'GALAHAD' trust region methods with constraint projection from Conn et al. (2000) <[doi:10.1137/S1052623497325107](https://doi.org/10.1137/S1052623497325107)>, ANOVA-based validation following Fisher (1925) <[doi:10.1007/978-1-4612-4380-9_6](https://doi.org/10.1007/978-1-4612-4380-9_6)>, and effect size calculations per Cohen (1988, ISBN:0805802835). Designed for structured experimental data including kinetic curves, dose-response studies, and treatment comparisons where appropriate parameter constraints and statistical justification are important for meaningful biological interpretation. Developed at the Minnesota Center for Prion Research and Outreach at the University of Minnesota.

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Encoding UTF-8

Depends R (>= 4.2.0)

Imports stats, GALAHAD (>= 1.0.0), knitr

Suggests testthat (>= 3.0.0), rmarkdown

VignetteBuilder knitr

RoxygenNote 7.3.3

Config/testthat/edition 3

NeedsCompilation no

URL <https://github.com/RFeissIV/SQUIRE>
BugReports <https://github.com/RFeissIV/SQUIRE/issues>
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generate_example_data	<i>Generate Example Data for SQUIRE</i>
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Description

Creates a simple example dataset suitable for testing SQUIRE functionality. The data simulates a germination experiment with three treatments.

Usage

```
generate_example_data(n_time = 8, n_rep = 4, seed = NULL)
```

Arguments

n_time	Number of time points (default 8)
n_rep	Number of replicates per treatment (default 4)
seed	Random seed for reproducibility (default NULL)

Value

A data frame with columns: time, treatment, replicate, response

Examples

```
# Generate example data
example_data <- generate_example_data(seed = 123)
head(example_data)

# Check structure
str(example_data)
table(example_data$treatment, example_data$time)
```

optimize_simple

*Simple Parameter Optimization Without GALAHAD***Description**

A simplified version of parameter optimization that doesn't require GALAHAD. Used for examples and testing when GALAHAD is not available.

Usage

```
optimize_simple(data, constraints = "positive")
```

Arguments

data	Data frame with time and response columns
constraints	Character vector specifying constraints ("positive", "none")

Value

Named vector of parameters: rate, offset, scale

Examples

```
# Create simple growth data
simple_data <- data.frame(
  time = rep(0:7, 4),
  response = rnorm(32, mean = rep(seq(0, 50, length.out = 8), 4), sd = 2)
)

# Optimize parameters
params <- optimize_simple(simple_data, constraints = "positive")
print(params)
```

print.SQUIRE

*Print SQUIRE Results***Description**

Print SQUIRE Results

Usage

```
## S3 method for class 'SQUIRE'
print(x, ...)
```

Arguments

x	SQUIRE results object
...	Additional arguments

SQUIRE

*SQUIRE: Statistical Quality-Assured Integrated Response Estimation***Description**

Systematic adaptive GALAHAD framework: 1. Statistical validation 2. Systematic T->P->E geometry discovery (3 focused runs) 3. Final optimization with discovered optimal settings 4. Done!

Usage

```
SQUIRE(
  data,
  treatments,
  control_treatment = treatments[1],
  validation_level = 0.05,
  min_timepoints = 5,
  min_replicates = 3,
  verbose = TRUE
)
```

Arguments

data	Data frame with columns: time, response, treatment, replicate
treatments	Character vector of treatment names
control_treatment	Name of control treatment for comparisons
validation_level	Statistical significance level (default: 0.05)
min_timepoints	Minimum timepoints required for fitting (default: 5)
min_replicates	Minimum replicates per treatment (default: 3)
verbose	Logical, print progress messages

Value

List with validation results, systematic GALAHAD discovery, and final parameters

Examples

```
# Synthetic germination data for demonstration
test_data <- data.frame(
  time = rep(c(0, 1, 2, 3, 4, 5, 6, 7), times = 12),
  treatment = rep(c("Control", "Contaminant_A", "Contaminant_B"), each = 32),
  replicate = rep(rep(1:4, each = 8), times = 3),
  response = c(
    0, 5, 15, 28, 45, 62, 75, 82,      # Control
    0, 4, 12, 26, 43, 60, 73, 80,
    0, 6, 17, 30, 47, 64, 77, 84,
    0, 5, 14, 27, 44, 61, 74, 81,
    0, 2, 8, 18, 32, 48, 60, 68,      # Contaminant_A
    0, 3, 7, 16, 30, 46, 58, 66,
    0, 2, 9, 19, 34, 50, 62, 70,
    0, 3, 8, 17, 31, 47, 59, 67,
    0, 8, 22, 38, 55, 72, 85, 92,      # Contaminant_B
    0, 7, 20, 36, 53, 70, 83, 90,
    0, 9, 24, 40, 57, 74, 87, 94,
    0, 8, 21, 37, 54, 71, 84, 91
  )
)

result <- SQUIRE(test_data, c("Control", "Contaminant_A", "Contaminant_B"))
if (result$optimization_performed) {
  print(result$parameters$parameter_matrix)
}
```

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