Package 'GALAHAD'

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Type Package

Title Geometry-Adaptive Lyapunov-Assured Hybrid Optimizer with Softplus Reparameterization and Trust-Region Control

Version 2.0.0

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Description Implements the GALAHAD algorithm (Geometry-Adaptive Lyapunov-Assured Hybrid Optimizer), updated in version 2 to replace the hard-clamp positivity constraint of v1 with a numerically smooth softplus reparameterization, add rho-based trust-region adaptation (actual vs. predicted objective reduction), extend convergence detection to include both absolute and relative function-stall criteria, and enrich the per-iteration history with Armijo backtrack counts and trust-region quality ratios. Parameters constrained to be positive (rates, concentrations, scale parameters) are handled in a transformed z-space via the softplus map so that gradients remain well-defined at the constraint boundary. A two-partition API (positive / euclidean) replaces the three-way T/P/E partition of v1; the legacy form is still accepted for backwards compatibility. Designed for biological modeling problems (germination, dose-response, prion RT-QuIC, survival) where rates, concentrations, and unconstrained coefficients coexist. Developed at the Minnesota Center for Prion Research and Outreach (MNPRO), University of Minnesota. Based on Conn et al. (2000) <doi:10.1137/1.9780898719857>, Barzilai and Borwein (1988) <doi:10.1093/imanum/8.1.141>, Xu and An (2024) <doi:10.48550/arXiv.2409.14383>, Polyak (1969) <doi:10.1016/0041-5553(69)90035-4>, Nocedal and Wright (2006, ISBN:978-0-387-30303-1), and Dugas et al. (2009) <https://www.jmlr.org/papers/v10/dugas09a.html>.

URL https://github.com/RFeissIV/GALAHAD

BugReports https://github.com/RFeissIV/GALAHAD/issues

Note Development followed an iterative human-machine collaboration where all algorithmic design, statistical methodologies, and biological validation logic were conceptualized, tested, and iteratively refined by Richard A. Feiss through repeated cycles of running experimental data, evaluating analytical outputs, and selecting among candidate algorithms and approaches. AI systems ('Anthropic Claude' and 'OpenAI GPT') served as coding assistants and analytical sounding boards under continuous human direction. The selection of statistical methods, evaluation of biological plausibility, and all final methodology decisions were made by the human author. AI systems did not independently originate algorithms, statistical approaches, or scientific methodologies.

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GALAHAD *GALAHAD: Geometry-Adaptive Optimizer with Softplus Reparameterization*

Description

Minimises a smooth objective $V(\theta)$ over a mixed-geometry parameter space. Parameters declared as **positive** are handled via a softplus reparameterization so that positivity is guaranteed analytically and gradients remain smooth at the constraint boundary. Parameters declared as **euclidean** are unconstrained.

The algorithm combines:

- Diagonal Hessian preconditioning via a secant-based exponential moving average.
- Adaptive step-size selection: Polyak (when `V_star` is supplied) -> Barzilai-Borwein -> constant default.
- Armijo backtracking line-search with a configurable monotone or rho-accept mode.
- Trust-region projection with rho-based radius adaptation (actual vs. predicted reduction).
- Dual convergence criterion: gradient + step tolerance (primary) and absolute or relative function-stall over five iterations (secondary).

Usage

```
GALAHAD(V, gradV, theta0, parts, control = list(), callback = NULL)
```

Arguments

`V`	Objective function: `function(theta) -> scalar`. Must return a finite numeric scalar for any `theta` encountered during optimization.
`gradV`	Gradient function: `function(theta) -> numeric vector` of length p. Must return finite values. A finite-difference approximation (e.g., `galahad_numgrad`) may be substituted when an analytical gradient is unavailable.
`theta0`	Initial parameter vector, numeric of length p. Elements indexed by `parts$positive` must be strictly positive.
`parts`	Named list specifying the parameter partition. See section *Parameter partitions* above.
`control`	Optional named list of control parameters. See section *Control parameters* above.
`callback`	Optional function called at the end of each iteration. Receives a list with elements `iter` (integer), `theta` (numeric vector), `value` (scalar), and `grad_norm` (scalar). Errors inside the callback are silently suppressed.

Value

A named list with the following elements:

`theta` Numeric vector; final parameter estimate in the original θ space (`theta[positive] > 0` is guaranteed).

`value` Scalar; $V(\theta)$ at the final iterate.

`grad_inf` Sup-norm of the gradient at the final iterate.

`converged` Logical; `TRUE` if any convergence criterion was satisfied before `max_iter`.

`status` Character; `"converged"` or `"max_iter"`.

`reason` Character; one of `"GRAD_TOL"`, `"FUNC_STALL_ABS"`, `"FUNC_STALL_REL"`, `"MAX_ITER"`.

`iterations` Integer; number of iterations performed.

`history` A `data.frame` with one row per iteration and columns `iter`, `f`, `g_inf`, `step_norm`, `df` (change in V), `eta`, `method` (step-size method: `"POLYAK"`, `"BB"`, or `"DEFAULT"`), `armijo_iters`, `pred_red` (predicted reduction), and `rho` (actual / predicted reduction).

`diagnostics` List with `mean_L_hat` (mean diagonal Hessian estimate at termination), `final_delta` (final trust radius), `enforce_monotone`, `use_rho_accept`, and `parameterization` (`"softplus"`).

`certificate` List with `converged` and `reason`; a compact convergence certificate.

Parameter partitions

The `parts` argument partitions the indices `1:p` (where $p =$ length(theta0)) into two groups.

Preferred form:

`positive` Integer indices of parameters constrained to $(0, \infty)$. Typical examples: rate constants, concentrations, standard deviations, Hill coefficients. Internally reparameterized via $\theta_i = \text{softplus}(z_i)$.

`euclidean` Integer indices of unconstrained parameters. Typical examples: location parameters, regression coefficients, log-EC50.

Legacy form (v1 compatibility): `list(T = ..., P = ..., E = ...)` is also accepted. Indices in `T` and `P` are mapped to `positive`; indices in `E` are mapped to `euclidean`.

All indices must appear exactly once and cover `1:p`.

Control parameters

Pass as named elements of the `control` list. Any omitted element takes the default shown below.

`max_iter` Maximum iterations (default: `2000`).

`tol_g` Convergence: sup-norm of gradient $\leq$ `tol_g` (default: `1e-6`).

`tol_x` Convergence: step norm $\leq$ `tol_x` (default: `1e-9`).

`tol_f` Stall: absolute change in V over last five iterations $\leq$ `tol_f` (default: `1e-12`).

`tol_f_rel` Stall: relative change in V over last five iterations $\leq$ `tol_f_rel` (default: `1e-9`).

`delta` Initial trust-region radius (default: `1.0`).

`delta_min` Minimum trust-region radius (default: `1e-6`).

`delta_max` Maximum trust-region radius (default: `1e3`).

`eta0` Initial / fallback step size (default: `1.0`).

`eta_min` Minimum step size (default: `1e-8`).

`eta_max` Maximum step size (default: `10.0`).

`c1` Armijo sufficient-decrease constant (default: `1e-4`).

`armijo_max` Maximum Armijo backtrack steps (default: `20`).

`L_est` Initial diagonal Hessian estimate (default: `1.0`).

`l_min`, `l_max` Bounds for Hessian diagonal entries (defaults: `1e-8`, `1e8`).

`V_star` Known or estimated minimum value of V, used to compute Polyak step sizes. `NULL` disables Polyak steps (default: `NULL`).

`lambda` L2 regularization coefficient; adds $\lambda\|\theta\|^2$ to the objective (default: `0`).

`enforce_monotone` Logical; if `TRUE` (default), the Armijo condition must be satisfied. Set to `FALSE` together with `use_rho_accept = TRUE` to use rho-accept mode instead.

`use_rho_accept` Logical; if `TRUE`, accept a step when $\rho \geq$ `rho_accept` rather than requiring Armijo decrease (default: `FALSE`).

`rho_accept` Minimum acceptable rho for step acceptance in rho-accept mode (default: `0.1`).

`rho_shrink` Trust-radius shrinks when $\rho <$ `rho_shrink` (default: `0.25`).

`rho_grow` Trust-radius grows when $\rho >$ `rho_grow` and step fills the region (default: `0.75`).

`shrink_factor` Multiplicative shrink factor for trust radius (default: `0.5`).

`grow_factor` Multiplicative growth factor for trust radius (default: `1.5`).

`softplus_cap` Upper threshold in the softplus overflow guard (default: `700`). Rarely needs changing.

References

Barzilai, J., & Borwein, J. M. (1988). Two-point step size gradient methods. *IMA Journal of Numerical Analysis*, 8(1), 141–148. doi:10.1093/imanum/8.1.141

Conn, A. R., Gould, N. I. M., & Toint, P. L. (2000). *Trust-Region Methods*. SIAM. doi:10.1137/1.9780898719857

Dugas, C., Bengio, Y., Belisle, F., Nadeau, C., & Garcia, R. (2009). Incorporating functional knowledge in neural networks. *Journal of Machine Learning Research*, 10(42), 1239–1262. https://www.jmlr.org/papers/v10/dugas09a.html

Nocedal, J., & Wright, S. J. (2006). *Numerical Optimization* (2nd ed.). Springer. ISBN 978-0-387-30303-1.

Polyak, B. T. (1969). The conjugate gradient method in extremal problems. *USSR Computational Mathematics and Mathematical Physics*, 9(4), 94–112. doi:10.1016/00415553(69)900354

Xu, X., & An, C. (2024). A trust region method with regularized Barzilai-Borwein step-size for large-scale unconstrained optimization. *arXiv preprint*. doi:10.48550/arXiv.2409.14383

See Also

`galahad_numgrad` for finite-difference gradient approximation; `galahad_parts` for a helper that builds the `parts` list.

Examples

```
## -- Example 1: purely positive parameters (exponential decay) ----------
set.seed(1)
t  <- seq(0, 5, by = 0.5)
y  <- 3 * exp(-0.8 * t) + rnorm(length(t), sd = 0.05)

obj <- function(theta) sum((y - theta[1] * exp(-theta[2] * t))^2)
grd <- function(theta) {
  r  <- y - theta[1] * exp(-theta[2] * t)
  dA <- -2 * sum(r * exp(-theta[2] * t))
  dk <- -2 * sum(r * (-t) * theta[1] * exp(-theta[2] * t))
  c(dA, dk)
}

fit <- GALAHAD(V      = obj,
               gradV  = grd,
               theta0 = c(A = 2, k = 0.5),
               parts  = list(positive  = c(1L, 2L),
                             euclidean = integer(0)))
fit$theta      # close to c(3, 0.8)
```

```
fit$converged
fit$reason

## -- Example 2: mixed geometry (4PL dose-response) -----------------------

set.seed(42)
dose  <- c(0.01, 0.1, 1, 5, 10, 50, 100)
y4pl  <- 10 + (90 - 10) / (1 + exp(-1.5 * (log(dose) - log(5)))) +
         rnorm(length(dose), sd = 2)

## theta = c(bottom, hill, logEC50, top)
## hill > 0 is positive; bottom, logEC50, top are unconstrained
obj4 <- function(th) {
  pred <- th[1] + (th[4] - th[1]) / (1 + exp(-th[2] * (log(dose) - th[3])))
  sum((y4pl - pred)^2)
}
grd4 <- function(th) galahad_numgrad(obj4, th)

fit4 <- GALAHAD(V      = obj4,
                gradV  = grd4,
                theta0 = c(bottom = 15, hill = 1, logEC50 = log(5), top = 80),
                parts  = list(positive  = 2L,        # hill must be > 0
                              euclidean = c(1L, 3L, 4L)))
fit4$theta
fit4$converged


## -- Example 3: legacy v1 partition syntax (backwards compatible) --------

set.seed(7)
p <- 10
theta_true <- abs(rnorm(p)) + 0.5
V_q  <- function(th) sum((th - theta_true)^2)
gV_q <- function(th) 2 * (th - theta_true)

## Old-style T / P / E partition -- still accepted in v2
fit_legacy <- GALAHAD(V      = V_q,
                      gradV  = gV_q,
                      theta0 = rep(1, p),
                      parts  = list(T = 1:3, P = 4:7, E = 8:10))
fit_legacy$converged
```

`galahad_numgrad` *Finite-difference gradient approximation*

Description

Computes a central-difference numerical gradient of `f` at `theta`. Useful when an analytical gradient is not available.

Usage

```
galahad_numgrad(f, theta, eps = 1e-07)
```

Arguments

f	Scalar-valued function of a numeric vector.
theta	Numeric vector at which to evaluate the gradient.
eps	Step size scaling factor (default 1e-7). The actual step for parameter i is eps * (|theta[i]| + 1).

Value

Numeric gradient vector of the same length as theta.

Examples

```
f <- function(th) sum((th - c(2, 3))^2)
galahad_numgrad(f, c(0, 0))   # should be close to c(-4, -6)
```

---

galahad_parts *Build a GALAHAD parts list*

Description

Convenience constructor that validates and assembles the parts argument for GALAHAD.

Usage

```
galahad_parts(positive = integer(0), euclidean = integer(0), p = NULL)
```

Arguments

positive	Integer vector of indices (1-based) for parameters that must be positive. May be integer(0) if there are no positive constraints.
euclidean	Integer vector of indices for unconstrained parameters. May be integer(0).
p	Total number of parameters. If supplied, indices are validated against 1:p.

Value

A named list list(positive = ..., euclidean = ...).

Examples

```
galahad_parts(positive = c(1L, 2L), euclidean = 3L, p = 3)
```

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