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# **Fides Documentation**

***Release 0.4.1***

**The Fides developers**

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Version: 0.4.1

Source code: <https://github.com/Fides-dev/fides>



## **ABOUT FIDES**

Fides implements an Interior Trust Region Reflective for boundary constrained optimization problems based on the papers [ColemanLi1994] and [ColemanLi1996]. Accordingly, Fides is named after the Roman goddess of trust and reliability. In contrast to other optimizers, Fides solves the full trust -region subproblem exactly, which can yield higher quality proposal steps, but is computationally more expensive. This makes Fides particularly attractive for optimization problems with objective functions that are computationally expensive to evaluate and the computational cost of solving the trust -region subproblem is negligible.

### **1.1 Features**

- Boundary constrained interior trust-region optimization
- Recursive Reflective and Truncated constraint management
- Full and 2D subproblem solution solvers
- BFGS, DFP and SR1 Hessian Approximations





## FIDES PYTHON API

### Modules

<i>fides</i>	Fides
<i>fides.minimize</i>	Minimization
<i>fides.trust_region</i>	Trust Region Step Evaluation
<i>fides.subproblem</i>	Subproblem Solvers
<i>fides.hessian_approximation</i>	Hessian Update Strategies
<i>fides.logging</i>	Logging
<i>fides.constants</i>	Constants

## 2.1 Fides

Fides is an interior trust-region reflective optimizer

## 2.2 Minimization

This module performs the optimization given a step proposal.

### Classes Summary

<i>Optimizer</i> (fun, ub, lb[, verbose, options, ...])	Performs optimization
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### Classes

**class** `fides.minimize.Optimizer` (*fun, ub, lb, verbose=10, options=None, funargs=None, hessian\_update=None*)

Performs optimization

#### Variables

- **fun** – Objective function
- **funargs** – Keyword arguments that are passed to the function
- **lb** – Lower optimization boundaries

- **ub** – Upper optimization boundaries
- **options** – Options that configure convergence checks
- **delta\_iter** – Trust region radius that was used for the current step
- **delta** – Updated trust region radius
- **x** – Current optimization variables
- **fval** – Objective function value at x
- **grad** – Objective function gradient at x
- **x\_min** – Optimal optimization variables
- **fval\_min** – Objective function value at x\_min
- **grad\_min** – Objective function gradient at x\_min
- **hess** – Objective function Hessian (approximation) at x
- **hessian\_update** – Object that performs hessian updates
- **starttime** – Time at which optimization was started
- **iteration** – Current iteration
- **converged** – Flag indicating whether optimization has converged
- **exitflag** – ExitFlag to indicate reason for termination
- **verbose** – Verbosity level for logging
- **logger** – logger instance

`__init__` (*fun, ub, lb, verbose=10, options=None, funargs=None, hessian\_update=None*)  
Create an optimizer object

#### Parameters

- **fun** (`typing.Callable`) – This is the objective function, if no *hessian\_update* is provided, this function must return a tuple (fval, grad), otherwise this function must return a tuple (fval, grad, Hessian)
- **ub** (`numpy.ndarray`) – Upper optimization boundaries. Individual entries can be set to `np.inf` for respective variable to have no upper bound
- **lb** (`numpy.ndarray`) – Lower optimization boundaries. Individual entries can be set to `-np.inf` for respective variable to have no lower bound
- **verbose** (`typing.Optional[int]`) – Verbosity level, pick from logging.[DEBUG,INFO,WARNING,ERROR]
- **options** (`typing.Optional[typing.Dict]`) – Options that control termination of optimization. See *minimize* for details.
- **funargs** (`typing.Optional[typing.Dict]`) – Additional keyword arguments that are to be passed to fun for evaluation
- **hessian\_update** (`typing.Optional[fides.hessian_approximation.HessianApproximation]`) – Subclass of *fides.hessian\_update.HessianApproximation* that performs the hessian updates in every iteration.

#### `check_continue()`

Checks whether minimization should continue based on convergence, iteration count and remaining computational budget

**Return type** `bool`

**Returns** flag indicating whether minimization should continue

**check\_convergence** (*step*, *fval*, *grad*)

Check whether optimization has converged.

**Parameters**

- **step** (`fides.steps.Step`) – update to optimization variables
- **fval** (`float`) – updated objective function value
- **grad** (`numpy.ndarray`) – updated objective function gradient

**Return type** `None`

**check\_finite** (*grad*=`None`, *hess*=`None`)

Checks whether objective function value, gradient and Hessian (approximation) have finite values and optimization can continue.

**Parameters**

- **grad** (`typing.Optional[numpy.ndarray]`) – gradient to be checked for finiteness, if not provided, current one will be checked
- **hess** (`typing.Optional[numpy.ndarray]`) – Hessian (approximation) to be checked for finiteness, if not provided, current one will be checked

**Raises** `RuntimeError` if any of the variables have non-finite entries

**check\_in\_bounds** (*x*=`None`)

Checks whether the current optimization variables are all within the specified boundaries

**Raises** `RuntimeError` if any of the variables are not within boundaries

**get\_affine\_scaling** ()

Computes the vector *v* and *dv*, the diagonal of its Jacobian. For the definition of *v*, see Definition 2 in [Coleman-Li1994]

**Return type** `typing.Tuple[numpy.ndarray, numpy.ndarray]`

**Returns** *v* scaling vector *dv* diagonal of the Jacobian of *v* wrt *x*

**log\_header** ()

Prints the header for diagnostic information, should complement `Optimizer.log_step()`.

**log\_step** (*accepted*, *step*, *fval*)

Prints diagnostic information about the current step to the log

**Parameters**

- **accepted** (`bool`) – flag indicating whether the current step was accepted
- **step** (`fides.steps.Step`) – proposal step
- **fval** (`float`) – new fval if step is accepted

**log\_step\_initial** ()

Prints diagnostic information about the initial step to the log

**make\_non\_degenerate** (*eps*=`2.220446049250313e-14`)

Ensures that *x* is non-degenerate, this should only be necessary for initial points.

**Parameters** **eps** – degeneracy threshold

**Return type** `None`

**minimize** (*x0*)

Minimize the objective function using the interior trust-region reflective algorithm described by [ColemanLi1994] and [ColemanLi1996]. Convergence with respect to function value is achieved when  $|f_{k+1} - f_k| < \text{options}[\text{f\_atol}] - f_k \text{ options}[\text{f\_rtol}]$ . Similarly, convergence with respect to optimization variables is achieved when  $\|x_{k+1} - x_k\| < \text{options}[\text{x\_tol}] x_k$  (note that this is checked in transformed coordinates that account for distance to boundaries). Convergence with respect to the gradient is achieved when  $\|g_k\| < \text{options}[\text{g\_atol}]$  or  $\|g_k\| < \text{options}[\text{g\_rtol}] * f_k$ . Other than that, optimization can be terminated when iterations exceed  $\text{options}[\text{maxiter}]$  or the elapsed time is expected to exceed  $\text{options}[\text{maxtime}]$  on the next iteration.

**Parameters** **x0** (`numpy.ndarray`) – initial guess

**Returns** **fval**: final function value, **x**: final optimization variable values, **grad**: final gradient, **hess**: final Hessian (approximation)

**track\_minimum** (*x\_new*, *fval\_new*, *grad\_new*)

Function that tracks the optimization variables that have minimal function value independent of whether the step is accepted or not.

**Parameters**

- **x\_new** (`numpy.ndarray`) –
- **fval\_new** (`float`) –
- **grad\_new** (`numpy.ndarray`) –

**Return type** `None`

**Returns****update** (*step*, *x\_new*, *fval\_new*, *grad\_new*, *hess\_new=None*)

Update self according to employed step

**Parameters**

- **step** (`fides.steps.Step`) – Employed step
- **x\_new** (`numpy.ndarray`) – New optimization variable values
- **fval\_new** (`float`) – Objective function value at **x\_new**
- **grad\_new** (`numpy.ndarray`) – Objective function gradient at **x\_new**
- **hess\_new** (`typing.Optional[numpy.ndarray]`) – (Approximate) objective function Hessian at **x\_new**

**Return type** `None`

**update\_tr\_radius** (*fval*, *grad*, *step*, *dv*)

Update the trust region radius

**Parameters**

- **fval** (`float`) – new function value if step defined by **step\_sx** is taken
- **grad** (`numpy.ndarray`) – new gradient value if step defined by **step\_sx** is taken
- **step** (`fides.steps.Step`) – step
- **dv** (`numpy.ndarray`) – derivative of scaling vector **v** wrt **x**

**Return type** `bool`

**Returns** flag indicating whether the proposed step should be accepted

## 2.3 Trust Region Step Evaluation

This module provides the machinery to evaluate different trust-region( -reflective) step proposals and select among them based on to their performance according to the quadratic approximation of the objective function

### Functions Summary

<code>trust_region(x, g, hess, scaling, delta, dv, ...)</code>	Compute a step according to the solution of the trust-region subproblem.
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### Functions

`fides.trust_region.trust_region(x, g, hess, scaling, delta, dv, theta, lb, ub, subspace_dim, step-back_strategy, refine_stepback, logger)`

Compute a step according to the solution of the trust-region subproblem. If step-back is necessary, gradient and reflected trust region step are also evaluated in terms of their performance according to the local quadratic approximation

#### Parameters

- **x** (`numpy.ndarray`) – Current values of the optimization variables
- **g** (`numpy.ndarray`) – Objective function gradient at x
- **hess** (`numpy.ndarray`) – (Approximate) objective function Hessian at x
- **scaling** (`scipy.sparse.csc.csc_matrix`) – Scaling transformation according to distance to boundary
- **delta** (`float`) – Trust region radius, note that this applies after scaling transformation
- **dv** (`numpy.ndarray`) – derivative of scaling transformation
- **theta** (`float`) – parameter regulating stepback
- **lb** (`numpy.ndarray`) – lower optimization variable boundaries
- **ub** (`numpy.ndarray`) – upper optimization variable boundaries
- **subspace\_dim** (`fides.constants.SubSpaceDim`) – Subspace dimension in which the subproblem will be solved. Larger subspaces require more compute time but can yield higher quality step proposals.
- **stepback\_strategy** (`fides.constants.StepBackStrategy`) – Strategy that is applied when the proposed step exceeds the optimization boundary.
- **refine\_stepback** (`bool`) – If set to True, proposed steps that are computed via the specified stepback\_strategy will be refined via optimization.
- **logger** (`logging.Logger`) – logging.Logger instance to be used for logging

**Return type** `fides.steps.Step`

**Returns** s: proposed step, ss: rescaled proposed step, qpval: expected function value according to local quadratic approximation, subspace: computed subspace for reuse if proposed step is not accepted, steptype: type of step that was selected for proposal

## 2.4 Subproblem Solvers

This module provides the machinery to solve 1- and N-dimensional trust-region subproblems.

### Functions Summary

<code>dsecular(lam, w, eigvals, eigvecs, delta)</code>	Derivative of the secular equation
<code>dslam(lam, w, eigvals, eigvecs)</code>	Computes the derivative of the solution $s(\lambda)$ with respect to lambda, where $s$ is the subproblem solution according to
<code>get_1d_trust_region_boundary_solution(B, g, ...)</code>	
<code>quadratic_form(Q, p, x)</code>	Computes the quadratic form $x^T Q x + x^T p$
<code>secular(lam, w, eigvals, eigvecs, delta)</code>	Secular equation
<code>slam(lam, w, eigvals, eigvecs)</code>	Computes the solution $s(\lambda)$ as subproblem solution according to
<code>solve_1d_trust_region_subproblem(B, g, s, ...)</code>	Solves the special case of a one-dimensional subproblem
<code>solve_nd_trust_region_subproblem(B, g, delta)</code>	This function exactly solves the n-dimensional subproblem.

### Functions

`fides.subproblem.dsecular(lam, w, eigvals, eigvecs, delta)`

Derivative of the secular equation

$$\phi(\lambda) = \frac{1}{\|s\|} - \frac{1}{\Delta}$$

with respect to  $\lambda$

#### Parameters

- **lam** (`float`) –  $\lambda$
- **w** (`numpy.ndarray`) – precomputed eigenvector coefficients for -g
- **eigvals** (`numpy.ndarray`) – precomputed eigenvalues of B
- **eigvecs** (`numpy.ndarray`) – precomputed eigenvectors of B
- **delta** (`float`) – trust region radius  $\Delta$

**Returns**  $\frac{\partial \phi(\lambda)}{\partial \lambda}$

`fides.subproblem.dslam(lam, w, eigvals, eigvecs)`

Computes the derivative of the solution  $s(\lambda)$  with respect to lambda, where  $s$  is the subproblem solution according to

$$-(B + \lambda I)s = g$$

#### Parameters

- **lam** (`float`) –  $\lambda$
- **w** (`numpy.ndarray`) – precomputed eigenvector coefficients for -g
- **eigvals** (`numpy.ndarray`) – precomputed eigenvalues of B

- **eigvecs** (`numpy.ndarray`) – precomputed eigenvectors of B

**Returns**  $\frac{\partial s(\lambda)}{\partial \lambda}$

`fides.subproblem.get_1d_trust_region_boundary_solution` (*B*, *g*, *s*, *s0*, *delta*)

`fides.subproblem.quadratic_form` (*Q*, *p*, *x*)

Computes the quadratic form  $x^T Q x + x^T p$

**Parameters**

- **Q** (`numpy.ndarray`) – Matrix
- **p** (`numpy.ndarray`) – Vector
- **x** (`numpy.ndarray`) – Input

**Return type** `float`

**Returns** Value of form

`fides.subproblem.secular` (*lam*, *w*, *eigvals*, *eigvecs*, *delta*)

Secular equation

$$\phi(\lambda) = \frac{1}{\|s\|} - \frac{1}{\Delta}$$

Subproblem solutions are given by the roots of this equation

**Parameters**

- **lam** (`float`) –  $\lambda$
- **w** (`numpy.ndarray`) – precomputed eigenvector coefficients for -g
- **eigvals** (`numpy.ndarray`) – precomputed eigenvalues of B
- **eigvecs** (`numpy.ndarray`) – precomputed eigenvectors of B
- **delta** (`float`) – trust region radius  $\Delta$

**Returns**  $\phi(\lambda)$

`fides.subproblem.slam` (*lam*, *w*, *eigvals*, *eigvecs*)

Computes the solution  $s(\lambda)$  as subproblem solution according to

$$-(B + \lambda I)s = g$$

**Parameters**

- **lam** (`float`) –  $\lambda$
- **w** (`numpy.ndarray`) – precomputed eigenvector coefficients for -g
- **eigvals** (`numpy.ndarray`) – precomputed eigenvalues of B
- **eigvecs** (`numpy.ndarray`) – precomputed eigenvectors of B

**Return type** `numpy.ndarray`

**Returns**  $s(\lambda)$

`fides.subproblem.solve_1d_trust_region_subproblem` (*B*, *g*, *s*, *delta*, *s0*)

Solves the special case of a one-dimensional subproblem

**Parameters**

- **B** (`numpy.ndarray`) – Hessian of the quadratic subproblem
- **g** (`numpy.ndarray`) – Gradient of the quadratic subproblem

- **s** (`numpy.ndarray`) – Vector defining the one-dimensional search direction
- **delta** (`float`) – Norm boundary for the solution of the quadratic subproblem
- **s0** (`numpy.ndarray`) – reference point from where search is started, also counts towards norm of step

**Return type** `numpy.ndarray`

**Returns** Proposed step-length

`fides.subproblem.solve_nd_trust_region_subproblem(B, g, delta, logger=None)`

This function exactly solves the n-dimensional subproblem.

$$\operatorname{argmin}_s \{s^T B s + s^T g = 0 : \|s\| \leq \Delta, s \in \mathbb{R}^n\}$$

The solution is characterized by the equation  $-(B + \lambda I)s = g$ . If B is positive definite, the solution can be obtained by  $\lambda = 0$  if  $Bs = -g$  satisfies  $\|s\| \leq \Delta$ . If B is indefinite or  $Bs = -g$  satisfies  $\|s\| > \Delta$  and an appropriate  $\lambda$  has to be identified via 1D rootfinding of the secular equation

$$\phi(\lambda) = \frac{1}{\|s(\lambda)\|} - \frac{1}{\Delta} = 0$$

with  $s(\lambda)$  computed according to an eigenvalue decomposition of B. The eigenvalue decomposition, although being more expensive than a cholesky decomposition, has the advantage that eigenvectors are invariant to changes in  $\lambda$  and eigenvalues are linear in  $\lambda$ , so factorization only has to be performed once. We perform the linesearch via Newton's algorithm and Brent-Q as fallback. The hard case is treated separately and serves as general fallback.

#### Parameters

- **B** (`numpy.ndarray`) – Hessian of the quadratic subproblem
- **g** (`numpy.ndarray`) – Gradient of the quadratic subproblem
- **delta** (`float`) – Norm boundary for the solution of the quadratic subproblem
- **logger** (`typing.Optional[logging.Logger]`) – Logger instance to be used for logging

**Return type** `typing.Tuple[numpy.ndarray, str]`

**Returns** `s`: Selected step, `step_type`: Type of solution that was obtained

## 2.5 Hessian Update Strategies

This module provides various generic Hessian approximation strategies that can be employed when the calculating the exact Hessian or an approximation is computationally too demanding.

### Classes Summary

<code>BFGS([hess_init])</code>	Broyden-Fletcher-Goldfarb-Shanno update strategy.
<code>DFP([hess_init])</code>	Davidon-Fletcher-Powell update strategy.
<code>HessianApproximation([hess_init])</code>	Abstract class from which Hessian update strategies should subclass
<code>HybridUpdate([happ, hess_init, ...])</code>	
<code>SR1([hess_init])</code>	Symmetric Rank 1 update strategy.



## Classes

```

class fides.hessian_approximation.BFGS (hess_init=None)
    Broyden-Fletcher-Goldfarb-Shanno update strategy. This is a rank 2 update strategy that always yields positive-semidefinite hessian approximations.

class fides.hessian_approximation.DFP (hess_init=None)
    Davidon-Fletcher-Powell update strategy. This is a rank 2 update strategy that always yields positive-semidefinite hessian approximations. It usually does not perform as well as the BFGS strategy, but included for the sake of completeness.

class fides.hessian_approximation.HessianApproximation (hess_init=None)
    Abstract class from which Hessian update strategies should subclass

    __init__ (hess_init=None)
        Create a Hessian update strategy instance

        Parameters hess_init (typing.Optional[numpy.ndarray]) – Initial guess for the Hessian, if empty Identity matrix will be used

    get_mat ()
        Getter for the Hessian approximation :rtype: numpy.ndarray :return:

    init_mat (dim)
        Initializes this approximation instance and checks the dimensionality

        Parameters dim (int) – dimension of optimization variables

    set_init (hess_init)
        Create a Hessian update strategy instance

        Parameters hess_init (numpy.ndarray) – Initial guess for the Hessian, if empty Identity matrix will be used

class fides.hessian_approximation.HybridUpdate (happ=None, hess_init=None,
                                                init_with_hess=False,
                                                switch_iteration=None)

    __init__ (happ=None, hess_init=None, init_with_hess=False, switch_iteration=None)
        Create a Hybrid Hessian update strategy which is generated from the start but only applied after a certain iteration, while Hessian computed by the objective function is used until then.

        Parameters

        • happ (typing.Optional[fides.hessian_approximation.HessianApproximation]) – Hessian Update Strategy (default: BFGS)

        • switch_iteration (typing.Optional[int]) – Iteration after which this approximation is used (default: 2*dim)

        • (default (init_with_hess) – False) Whether the hybrid update strategy should be initialized according to the user-provided objective function

        • hess_init (typing.Optional[numpy.ndarray]) – Initial guess for the Hessian. (default: eye)

    get_mat ()
        Getter for the Hessian approximation :rtype: numpy.ndarray :return:

    init_mat (dim)
        Initializes this approximation instance and checks the dimensionality

        Parameters dim (int) – dimension of optimization variables

```

**set\_init** (*hess\_init*)

Create a Hessian update strategy instance

**Parameters** **hess\_init** (`numpy.ndarray`) – Initial guess for the Hessian, if empty Identity matrix will be used

**class** `fides.hessian_approximation.SR1` (*hess\_init=None*)

Symmetric Rank 1 update strategy. This updating strategy may yield indefinite hessian approximations.

## 2.6 Logging

This module provides the machinery that is used to display progress of the optimizer as well as debugging information

**var logger** `logging.Logger` instance that can be used throughout fides

### Functions Summary

---

<code>create_logger(level)</code>	Creates a logger instance.
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---

### Functions

`fides.logging.create_logger` (*level*)

Creates a logger instance. To avoid unnecessary locks during multithreading, different logger instance should be created for every

**Parameters** **level** (`int`) – logging level

**Return type** `logging.Logger`

**Returns** logger instance

## 2.7 Constants

This module provides a central place to define native python enums and constants that are used in multiple other modules

### Classes Summary

---

<code>ExitFlag(value)</code>	Defines possible exitflag values for the optimizer to indicate why optimization exited.
<code>Options(value)</code>	Defines all the fields that can be specified in Options to Optimizer
<code>StepBackStrategy(value)</code>	Defines the possible choices of search refinement if proposed step reaches optimization boundary
<code>SubSpaceDim(value)</code>	Defines the possible choices of subspace dimension in which the subproblem will be solved.

---

## Classes

**class** fides.constants.**ExitFlag**(*value*)

Defines possible exitflag values for the optimizer to indicate why optimization exited. Negative value indicate errors while positive values indicate convergence.

**DELTA\_TOO\_SMALL** = -5

Trust Region Radius too small to proceed

**DID\_NOT\_RUN** = 0

Optimizer did not run

**EXCEEDED\_BOUNDARY** = -4

Exceeded specified boundaries

**FTOL** = 1

Converged according to fval difference

**GTOL** = 3

Converged according to gradient norm

**MAXITER** = -1

Reached maximum number of allowed iterations

**MAXTIME** = -2

Expected to reach maximum allowed time in next iteration

**NOT\_FINITE** = -3

Encountered non-finite fval/grad/hess

**XTOL** = 2

Converged according to x difference

**class** fides.constants.**Options**(*value*)

Defines all the fields that can be specified in Options to Optimizer

**DELTA\_INIT** = 'delta\_init'

initial trust region radius

**FATOL** = 'fatol'

absolute tolerance for convergence based on fval

**FRTOL** = 'frtol'

relative tolerance for convergence based on fval

**GATOL** = 'gatol'

absolute tolerance for convergence based on grad

**GRTOL** = 'grtol'

relative tolerance for convergence based on grad

**MAXITER** = 'maxiter'

maximum number of allowed iterations

**MAXTIME** = 'maxtime'

maximum amount of walltime in seconds

**STEPBACK\_STRAT** = 'stepback\_strategy'

method to use for stepback

**SUBSPACE\_DIM** = 'subspace\_solver'

trust region subproblem subspace

**THETA\_MAX** = 'theta\_max'  
maximal fraction of step that would hit bounds

**XTOL** = 'xtol'  
tolerance for convergence based on x

**class** fides.constants.**StepBackStrategy**(*value*)  
Defines the possible choices of search refinement if proposed step reaches optimization boundary

**MIXED** = 'mixed'  
mix reflections and truncations

**REFLECT** = 'reflect'  
recursive reflections at boundary

**SINGLE\_REFLECT** = 'reflect\_single'  
single reflection at boundary

**TRUNCATE** = 'truncate'  
truncate step at boundary and resolve subproblem

**class** fides.constants.**SubSpaceDim**(*value*)  
Defines the possible choices of subspace dimension in which the subproblem will be solved.

**FULL** = 'full'  
Full  $\mathbb{R}^n$

**STEIHAUG** = 'scg'  
CG subspace via Steihaug's method

**TWO** = '2D'  
Two dimensional Newton/Gradient subspace

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