

## `::opt::`

1.0

Opt is a tcl package used for multiparameter minimization of a Tcl function. The minimization kernel is based on Nelder and Meads simplex algorithm. Routines are supplied to minimize, scan, fix and release parameters, and for confidence interval calculations.

Opt acts by creating a number of commands, e.g., `opt::minimize`. The user creates a number of parameters to optimize and specifies the procedure to optimize.

Table 1. Commands available in the Opt package.

<code>opt::newpar</code>	Create a new parameter
<code>opt::function</code>	Specifies the function to minimize
<code>opt::fix</code>	Fix a parameter in the minimization
<code>opt::release</code>	Release a fixed parameter
<code>opt::setpar</code>	Set parameter value
<code>opt::scan</code>	Scan a parameter
<code>opt::minimize</code>	Run a simplex minimization
<code>opt::confidence</code>	Perform a confidence interval calculation
<code>opt::c_data</code>	Get data from confidence interval calculation
<code>opt::c_calculate</code>	Calculate confidence based on input

`opt::newpar` <parname> <value> <stepsize> ?<min> <max>?

This command creates a new parameter with name `parname` and the specified initial value. The step size is used for setting up the initial simplex and when scanning the parameter. The ranges are optional. The command has no return value.

`opt::function` <funcname>

This command specifies which function to minimize. The Tcl procedure named `funcname` must return the value to minimize. The command has no return value.

`opt::fix` <parname>

Fixes the specified parameter in subsequent minimizations. The command has no return value.

`opt::release` <parname>

Releases a fixed parameter. The command has no return value.

`opt::setpar` <parname> <value>

Assigns a new value to the parameter `parname`. The command has no return value.

*min\_func\_val* **opt::scan** <parname>

Scan the parameter *parname* in a linear fashion. If limits are specified for the parameter, the command performs 21 function evaluations with the parameter taking values between min and max. If no limits are specified, the parameter is incremented by its step size. Once finished, *parname* takes the value yielding the smallest value of the minimization function. The command returns the minimum function value (*min\_func\_val*).

*min\_func\_val* **opt::minimize** ?<tolerance>?

Perform a simplex minimization. Optionally, a convergence tolerance may be specified. This defaults to  $10^{-3}$ . The command returns the minimum function value.

*confidence\_interval* **opt::confidence** <parname>

Calculate the 95% confidence interval for the specified parameter. This is done by scanning the parameter in 11 steps around its current value, and for each value perform an optimization of the remaining parameters. The plot of the optimized function value (*y*) versus the parameter value (*x*) should give a parabolic curve ( $y = ax^2 + bx + c$ ), and the confidence interval is given by  $C_{95} = 2/\sqrt{a}$ . If  $a > 0$ , the command returns the confidence interval, otherwise it returns 0.

*data* **opt::c\_data**

Returns the data from the previous confidence interval calculation. The data is in the form of a list of *x,y* values.

{*C95* {*a b c*}} **opt::c\_calculate** <data>

This command takes data in the form of a list of *x,y* values as input and fits the data to a parabolic function. The parameter returns the 95% confidence interval and the three parameters *a*, *b*, and *c* defining the parabolic function.

### *Acknowledgements*

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Linear algebra algorithms for solving sets of linear equations are taken from the `::math::linearalgebra` package of TCLLIB.