# BOBYQA Method

You can use the BOBYQA (Bound Optimization BY Quadratic Approximation) method for flowsheet optimization for simultaneous convergence of optimization problems with constraints (equality or inequality).

BOBYQA utilizes a trust region method. Variables must be scaled by the range of their bounds to ensure that magnitudes of the expected changes are similar. Each variable is scaled so that if $\underline{a} \leq x \leq b$, then for the scaled variable $x^*$, $-1 \leq x^* \leq 1$.

Constraints are supported by the use of a penalty function that is added to the objective functions. The constrained optimization problem can be written as:

$$\min_{x \in \mathbb{R}^n} f(x)$$

$$\text{such that } c(x) = 0,\ g(x) \leq 0$$

This is rewritten as an unconstrained problem:

$$\min_{x \in \mathbb{R}^n} f(x) + \rho\left(\|c(x)\| + \|g(x)\|\right)$$

$$\|c(x)\| = \sum_i abs\left[\left(\frac{c(x)_i}{\beta}\right)^\gamma\right]$$

$$\|g(x)\| = \begin{cases} \sum_i abs\left[\left(\frac{g(x)_i}{\beta}\right)^\gamma\right] & g(x)_i > 0 \\ 0 & g(x)_i \leq 0 \end{cases}$$

Where:

$\gamma$ = 1 for linear penalty type, 2 for quadratic penalty type

$\beta$ = constraint tolerance

$\rho$ = penalty prefactor

To solve a constrained optimization problem, an iterative approach is used in which the penalty prefactor is increased until the solution enters the feasible region. You can specify how much the prefactor is increased with each iteration.

You can control the BOBYQA method by specifying:

| Field | Default | To specify |
|---|---|---|
| Maximum Flowsheet Evaluations | 1000 | Maximum number of flowsheet evaluations |
| Number of interpolation conditions | 2*n*+1 | BOBYQA uses a quadratic approximation of the problem which has this many interpolation points. You can choose the number of points but it must be at least *n*+2 and may not exceed (*n*+1)(*n*+2)/2, where *n* is the number of variables being optimized. Values in excess of the default are not recommended. |
| Initial trust region radius | 0.1 | Limit on norm of scaled step size at the start of convergence. The scaling is such that the range in which the scaled manipulated variables can vary is -1 to 1. This is gradually reduced to the final |

| | | |
|---|---|---|
| | | value as iteration proceeds. Typically, this should be set to about 0.1. The maximum allowed value is 1. |
| Final trust region radius | $10^{-6}$ | Accuracy required in final values of the variables. This must be equal to or smaller than the initial trust region radius. |
| Initial prefactor value | 1 | $\rho$ for first iteration. Minimum $10^{-10}$. |
| Initial prefactor growth factor | 10 | Factor by which $\rho$ is increased after the first unconverged iteration due to constraint violation. Must be greater than 1. 10 is recommended. |
| Final prefactor growth factor | 10 | Factor by which $\rho$ is increased after the second and subsequent unconverged iterations. Generally this should be equal to or greater than the initial prefactor growth factor. |
| Equality constraint penalty type | Linear | Can be Linear or Quadratic; controls exponent $\gamma$ applied to equality constraints. |
| Inequality constraint penalty type | Linear | Can be Linear or Quadratic; controls exponent $\gamma$ applied to inequality constraints. |
| Penalty scaling | Yes | Can be Yes or No. Specifies whether scaling is used on constraint penalties. |

## Reference

M.J.D. Powell, "The BOBYQA Algorithm for Bound Constrained Optimization without Derivatives." Report, Department of Applied Mathematics and Theoretical Physics, Cambridge University. DAMTP 2009/NA06.