- The ***LJ Optimization Procedure*** is one of the most reliable direct search methods[13]. The method is easy to program and handles the problem of multiple optima with high reliability. A important advantage of the method is its ability to handle multiple nonlinear constraints. The adaptation of the original LJ optimization procedure to parameter estimation problems for algebraic equation models is given next.

(i) Choose an initial guess for the p-dimensional unknown parameter vector, $\mathbf{k}^{(0)}$; the *region contraction coefficient*, δ (typically δ=0.95 is used); the number of random evaluations of the objective function, N_R (typically N_R=100 is used) within an iteration; the maximum number of iterations, j_{max} (typically j_{max}=200 is used) and an initial search region, $\mathbf{r}^{(0)}$ (a typical choice is $\mathbf{r}^{(0)} = \mathbf{k}_{max} - \mathbf{k}_{min}$).

(ii) Set the iteration index j=1 and $\mathbf{k}^{(j-1)} = \mathbf{k}^{(0)}$ and $\mathbf{r}^{(j-1)} = \mathbf{r}^{(0)}$.

(iii) Generate or read from a file, $N_R \times p$ random numbers (R_{ni}) uniformly distributed in [-0.5, 0.5]

(iv) For n=1,2,…,N_R, generate the corresponding random trial parameter vectors from

$$\mathbf{k}_n = \mathbf{k}^{(j-1)} + \boldsymbol{R}_n \mathbf{r}^{(j-1)} \qquad (5.24)$$

where $\boldsymbol{R}_n = diag(R_{n1}, R_{n2}, \ldots, R_{np})$.

(v) Find the parameter vector among the N_R trial ones that minimizes the LS Objective function

$$S_{LS}(\mathbf{k}) = \sum_{i=1}^{N} [\hat{\mathbf{y}}_i - \mathbf{f}(\mathbf{x}_i, \mathbf{k})]^T \mathbf{Q}_i [\hat{\mathbf{y}}_i - \mathbf{f}(\mathbf{x}_i, \mathbf{k})] \qquad (5.25)$$

(vi) Keep the best trial parameter vector, $\mathbf{k}^*$, up to now and the corresponding minimum value of the objective function, S*.

(vii) Set $\mathbf{k}^{(j)} = \mathbf{k}^*$ and compute the search region for the next iteration as

$$\mathbf{r}^{(j)} = \delta \times \mathbf{r}^{(j-1)} \qquad (5.26)$$

(viii) If $j < j_{max}$, increment j by 1 go to Step (iii); else STOP.

The algorithm can be more *efficient* if we choose a value for N_R which is a function of the number of unknown parameters e.g.

$$N_R = 50 + 10 \times p \qquad (5.27)$$

We may also use a slower contraction of the search region as p increases e.g.

$$\delta = (0.90)^{1/p} \qquad (5.28)$$

Since we have a minimization problem, significant computational savings can be realized by noting in the implementation of the LJ optimization procedure that for each trial parameter vector, we do not need to complete the summation in Equation 5.23 once the LS Objective function exceeds the smallest value found up to that point (S*), a new trial parameter vector can be selected.