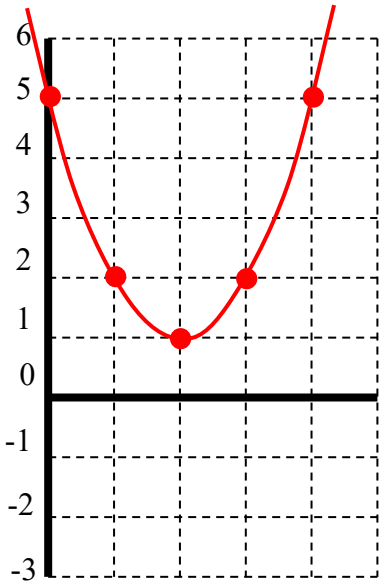
Numerical Optimization

Methods

- analytical
- exhaustive search
- gradient search
- non-gradient methods

$f(x) = x^2 - 4x + 5 \qquad \partial f / \partial x = 2x - 4 \qquad \min(f) \quad \text{for} \quad \partial f / \partial x = 0 \qquad x = 2$

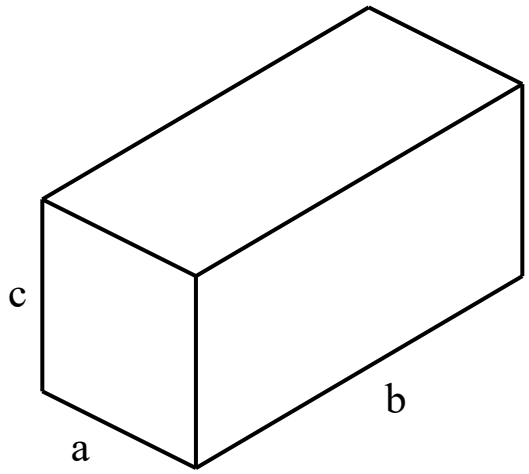
x	f(x)
0	5
1	2
2	1
3	2
4	5



Considerations

- multivariable
- multiple objective functions
- computational cost to evaluate objective function
- constraints
  - inequality
    - exact
    - penalty function
  - equality
- global versus local minima
- continuous versus discrete variables
- convergence

Lagrange Multiplier for Closed Box



Find minimum area of material A required to construct a closed box with given volume V

Minimize $A = 2ab + 2bc + 2ac$ Subject to $abc - V = 0$

$$L = (2ab + 2bc + 2ac) - \lambda(abc - V)$$

$$\frac{\partial L}{\partial a} = 2b + 2c - \lambda bc = 0 \qquad b = \frac{2c}{\lambda c - 2}$$

$$\frac{\partial L}{\partial b} = 2a + 2c - \lambda ac = 0 \qquad a = \frac{2c}{\lambda c - 2}$$

$$\frac{\partial L}{\partial c} = 2b + 2a - \lambda ab = 0$$

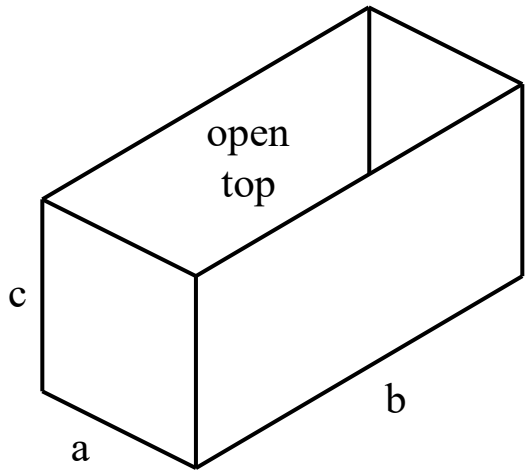
$$\frac{\partial L}{\partial \lambda} = abc - V = 0$$

$$\frac{4c}{\lambda c - 2} + \frac{4c}{\lambda c - 2} - \lambda \frac{4c^2}{(\lambda c - 2)^2} = 0$$

$$4c(\lambda c - 2) + 4c(\lambda c - 2) - \lambda(4c^2) = 0 \qquad 4c^2\lambda + 4c^2\lambda - 4c^2\lambda = 16c \qquad c = \frac{4}{\lambda}$$

$$a = \frac{4}{\lambda} \qquad b = \frac{4}{\lambda} \qquad V = abc = \frac{64}{\lambda^3} \qquad \lambda = \sqrt[3]{\frac{64}{V}}$$

Lagrange Multiplier for Open Box



Find minimum area of material A required to construct an open box with given volume V

Minimize $A = ab + 2bc + 2ac$ Subject to $abc - V = 0$

$$L = (ab + 2bc + 2ac) - \lambda(abc - V)$$

$$\frac{\partial L}{\partial a} = b + 2c - \lambda bc = 0 \qquad b = \frac{2c}{\lambda c - 1}$$

$$\frac{\partial L}{\partial b} = a + 2c - \lambda ac = 0 \qquad a = \frac{2c}{\lambda c - 1}$$

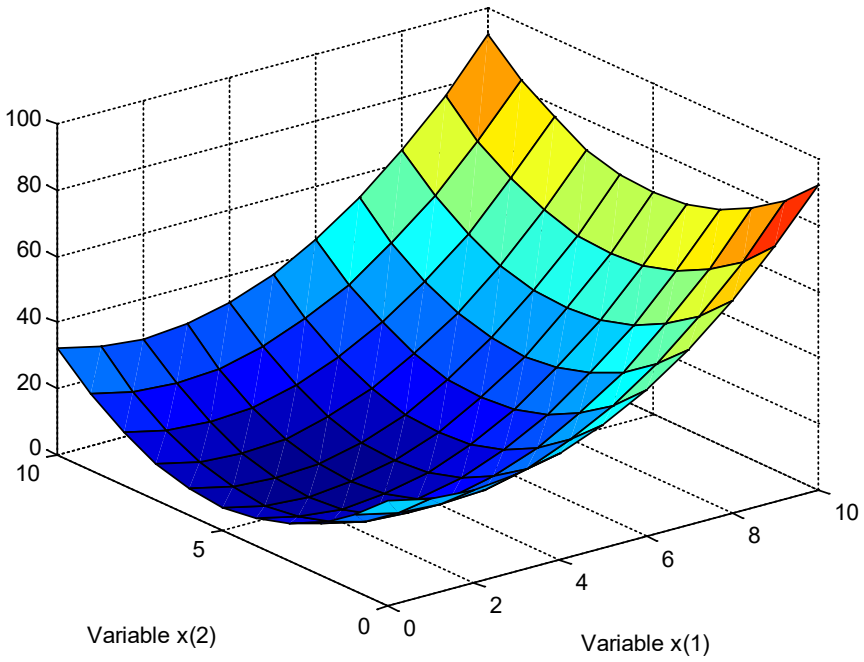
$$\frac{\partial L}{\partial c} = 2b + 2a - \lambda ab = 0$$

$$\frac{\partial L}{\partial \lambda} = abc - V = 0$$

$$\frac{4c}{\lambda c - 1} + \frac{4c}{\lambda c - 1} - \lambda \frac{4c^2}{(\lambda c - 1)^2} = 0$$

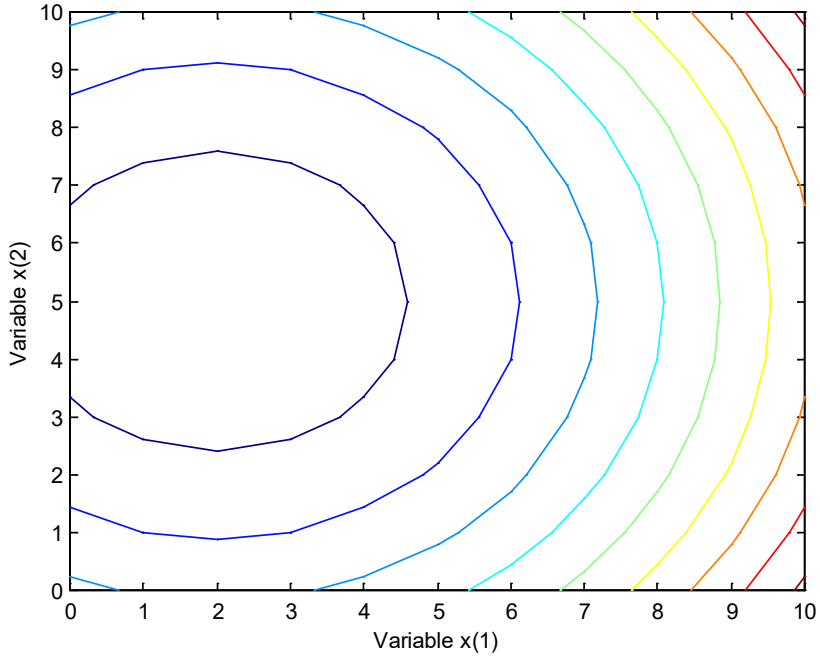
$$4c(\lambda c - 1) + 4c(\lambda c - 1) - \lambda(4c^2) = 0 \qquad c = \frac{2}{\lambda} \qquad a = \frac{4}{\lambda} \qquad b = \frac{4}{\lambda}$$

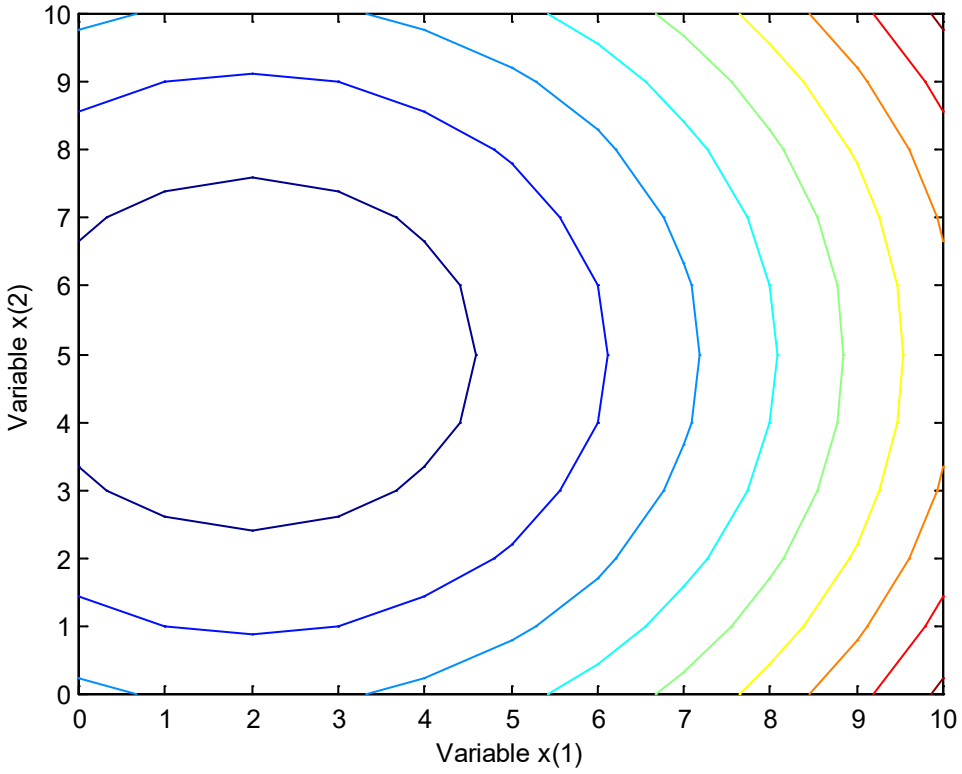
$$V = abc = \frac{32}{\lambda^3} \qquad \lambda = \sqrt[3]{\frac{32}{V}}$$

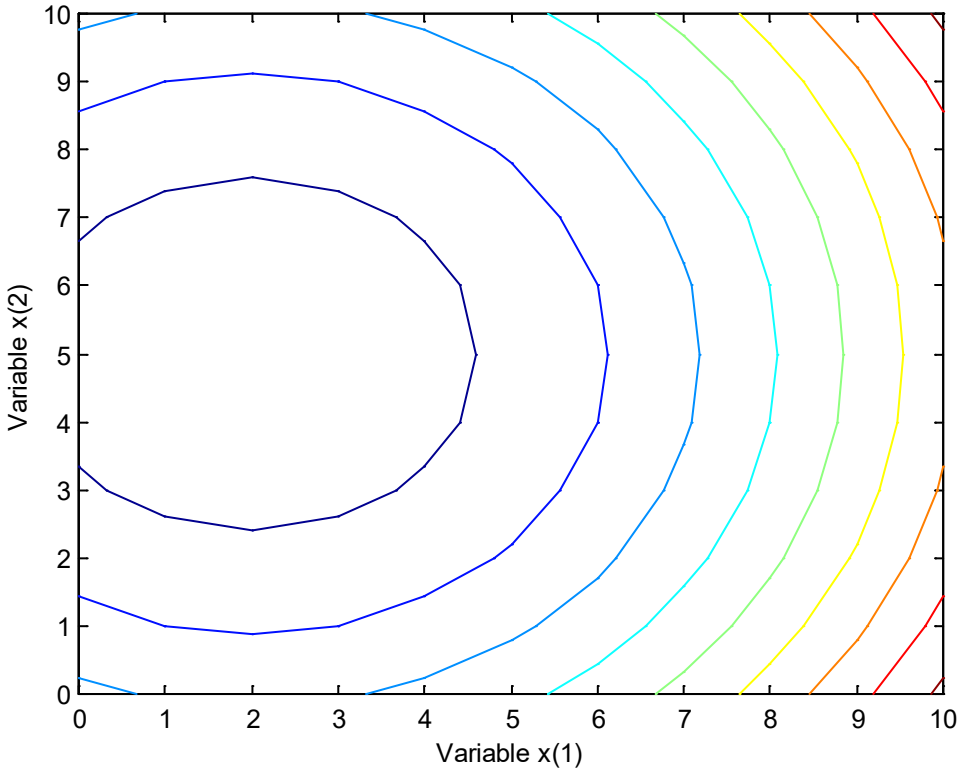


$$z = \left(x_1^2 - 4x_1 + 4\right) + \left(x_2^2 - 10x_2 + 25\right) + 3$$

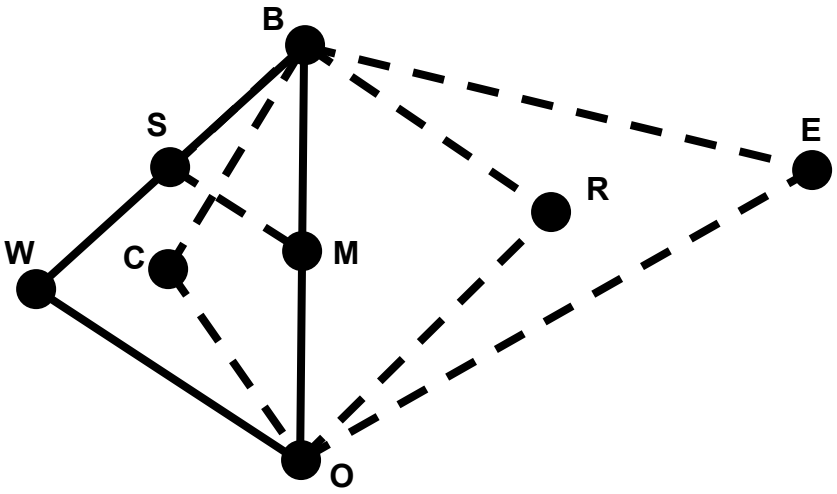
$$\partial z / \partial x_1 = 2x_1 - 4 \qquad \partial z / \partial x_2 = 2x_2 - 10$$




Variable x(2)
Variable x(1)
0
1
2
3
4
5
6
7
8
9
10


Variable x(2)
Variable x(1)
0
1
2
3
4
5
6
7
8
9
10

Simplex Minimization (Nelder-Mead)



current simplex
B = best
W = worst
O = others

new vertices
R = reflect
E = expand
C = contract
S = shrink

k = number of design parameters

$\{x\} = \{x_1 \quad x_2 \quad \cdots \quad x_i \quad \cdots \quad x_k\}^T$ = column vector of design parameters

n = k+1 = number of vertices for simplex

$\lfloor \{x\}_1 \quad \{x\}_2 \quad \cdots \quad \{x\}_j \quad \cdots \quad \{x\}_n \rfloor$ = list of vertices (for j=1 to n)

z_j = objective function evaluated at all $\{x\}_j$

$\{x\}_B$ = best vertex B based on objective function ($z_B < z_j < z_W$)

$\{x\}_W$ = worst vertex W based on objective function ($z_B < z_j < z_W$)

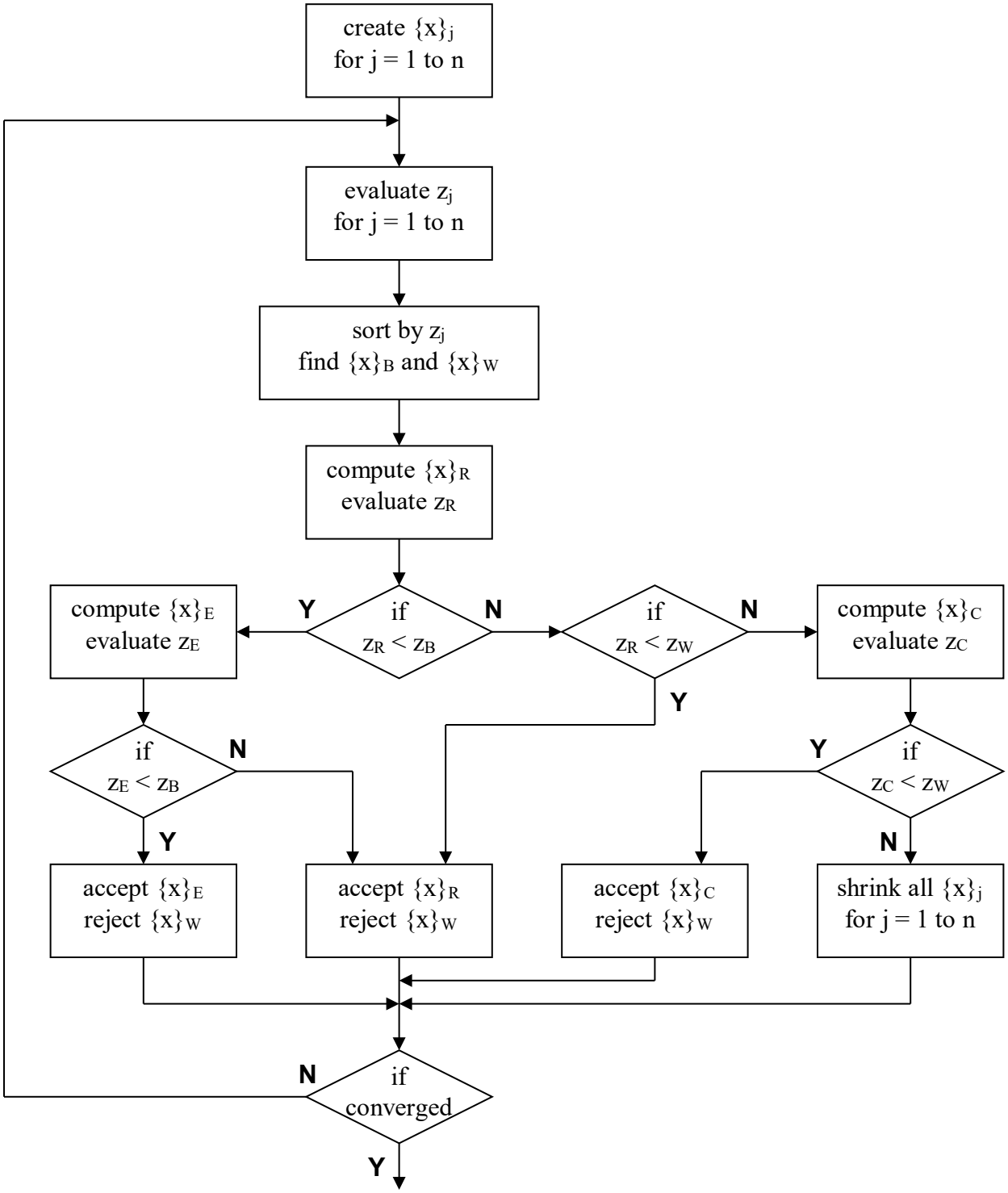
$$\{x\}_M = \left[\left(\sum_{j=1}^{n} \{x\}_j\right) - \{x\}_W\right] / (n-1)$$ = mean of vertices M excluding the worst

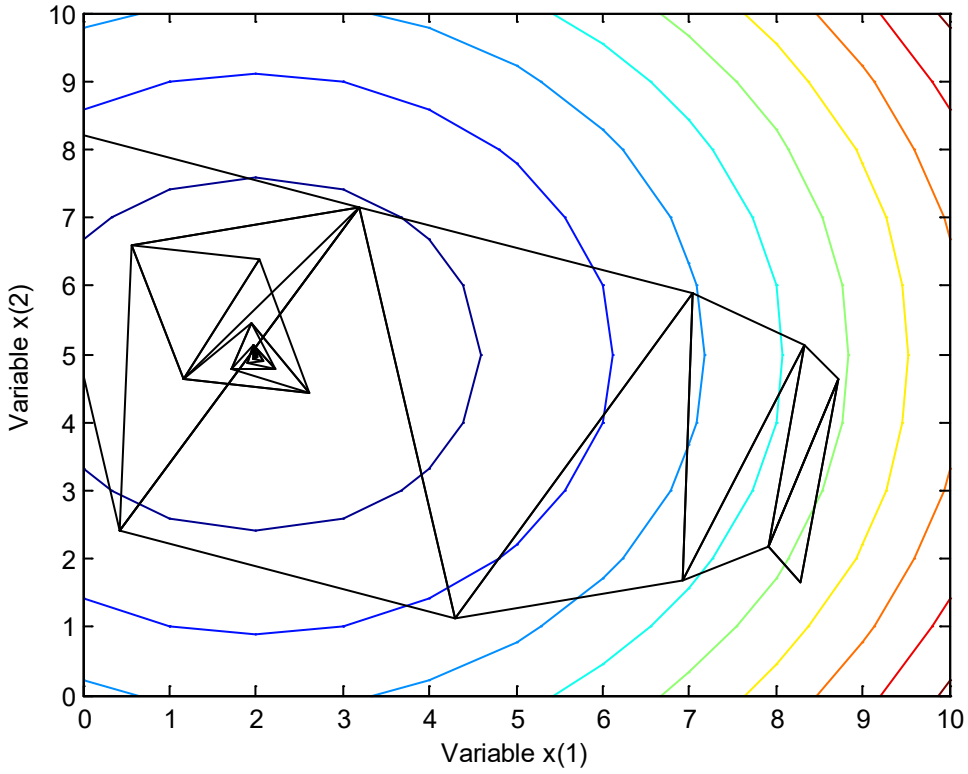
$$\{x\}_R = \{x\}_M + (\{x\}_M - \{x\}_W) = 2\{x\}_M - \{x\}_W$$ = new reflected vertex R

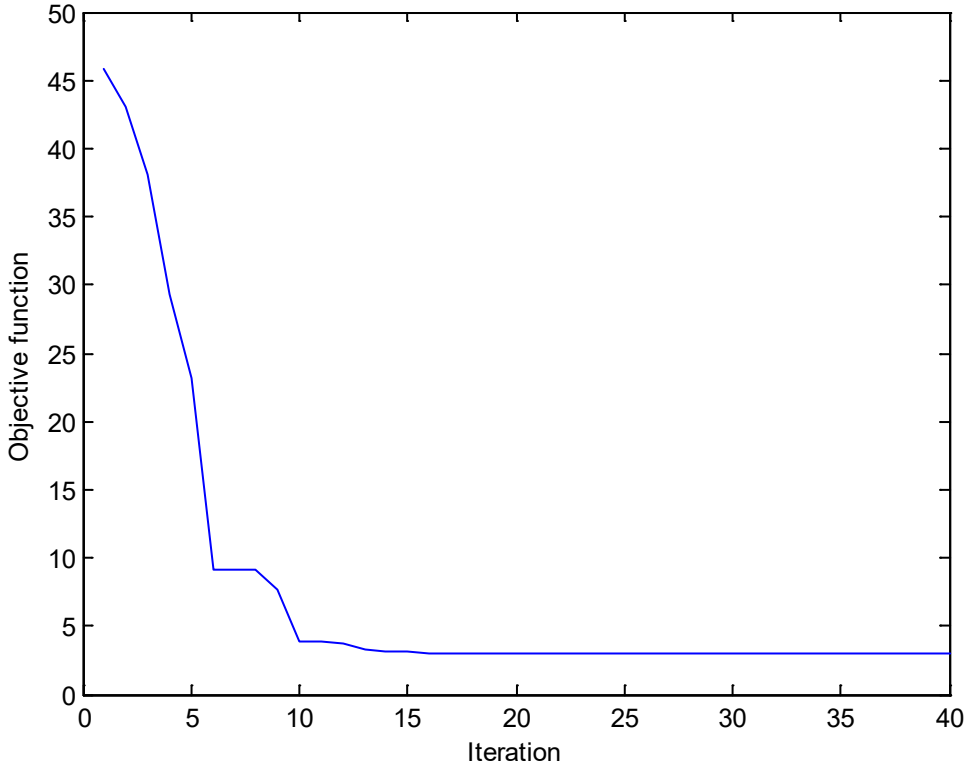
$$\{x\}_E = \{x\}_M + 2(\{x\}_M - \{x\}_W) = 3\{x\}_M - 2\{x\}_W$$ = new expanded vertex E

$$\{x\}_C = \{x\}_M - 0.5(\{x\}_M - \{x\}_W) = (\{x\}_M + \{x\}_W)/2$$ = new contracted vertex C

$$\{x\}_{j\_NEW} = (\{x\}_{j\_OLD} + \{x\}_B)/2$$ = new shrunken vertices S (for j = 1 to n)


create {x}j
for j = 1 to n
evaluate zj
for j = 1 to n
sort by zj
find {x}B and {x}W
compute {x}R
evaluate zR
if
zR < zB
Y
N
compute {x}E
evaluate zE
if
zR < zW
N
Y
compute {x}C
evaluate zC
if
zE < zB
N
Y
accept {x}E
reject {x}W
accept {x}R
reject {x}W
accept {x}C
reject {x}W
if
zC < zW
Y
N
shrink all {x}j
for j = 1 to n
if
converged
N
Y


Variable x(2)
Variable x(1)
0
1
2
3
4
5
6
7
8
9
10


Objective function
Iteration
0
5
10
15
20
25
30
35
40
45
50

```
% simplex.m - Simplex minimization per Kuester/Mize p. 298
% HJSIII, 12.10.15

clear

% 2D and 3D plots of biquadratic surface
% z = ( x(1)^2 - 4*x(1) + 4 ) + ( x(2)^2 - 10*x(2) + 25 ) + 3
biquad_surf

% maximum number of iterations
maxiter = 50;

% initial guess in column vector
guess = [  8  3  ]';     % 2D biquadratic example

% random radius around start
rad = 1;

% convergence distance
eps = 0.001;

% k = number of variables
% n = number of vertices in simplex
k = length( guess );
n = k + 1;

% random initial simplex
simp = guess*ones(1,n) + rad * randn(k,n);

% evaluate each vertex using external function
neval = 0;
for j = 1 : n,
  neval = neval + 1;
  z(1,j) = simplex_eval( simp(:,j) );   % external function
end

% plot initial simplex -  use countour plot from biquad_surf
hold on
h = patch( simp(1,:), simp(2,:), 'b');
set( h, 'FaceColor', 'none' )

% iteration loop
niter = 0;
while niter <= maxiter
  niter = niter + 1;

% check convergence
  del = max( max(simp') - min(simp') );
  if del < eps,
    break
  end

% plot each new iteration
  h = patch( simp(1,:), simp(2,:), 'b');
  set( h, 'FaceColor', 'none' )

% wait for keystroke
pause

% sort in ascending order to find min/max
  [ y, ind ] = sort( z );
  z_b = y(1);
  i_b = ind(1);
  x_b = simp(:,i_b);

  z_w = y(n);
  i_w = ind(n);
  x_w = simp(:,i_w);

% hold convergence history
  holdbest(niter) = z_b;
```

```
% reflect about centroid excluding the worst
  cen = ( sum(simp,2) - x_w ) / (n-1);
  d = cen - x_w;
  x_r = cen + d;

% evaluate reflection using external function
  neval = neval + 1;
  z_r = simplex_eval( x_r );   % external function

% try expansion if reflection is better than best
  if z_r < z_b,
    x_e = cen + 2 * d;

% evaluate expansion using external function
    neval = neval + 1;
    z_e = simplex_eval( x_e );   % external function

% keep the better of expansion or reflection
    if z_e < z_b,
      simp(:,i_w) = x_e;
      z(i_w) = z_e;
    else
      simp(:,i_w) = x_r;
      z(i_w) = z_r;
    end
  else

% keep reflection if better than worst
    if z_r < z_w,
      simp(:,i_w) = x_r;
      z(i_w) = z_r;
    else

% try contraction if reflection is worse than worst
      x_c = cen - 0.5 * d;

% evaluate contraction using external function
      neval = neval + 1;
      z_c = simplex_eval( x_c );   % external function

% keep contraction if better than worst
      if z_c < z_w,
        simp(:,i_w) = x_c;
        z(i_w) = z_c;
      else

% otherwise shrink toward best
        for j = 1:n,
          simp(:,j) = ( simp(:,j) + x_b ) / 2;

% evaluate each shrink using external function
          neval = neval + 1;
          z(1,j) = simplex_eval( simp(:,j) );   % external function
        end % shrink
      end % contraction
    end % expansion
  end % reflection

% next iteration
end

x_b

z_b

% plot convergence history
figure( 3 )
  clf
  plot( holdbest )
  xlabel( 'Iteration' )
```

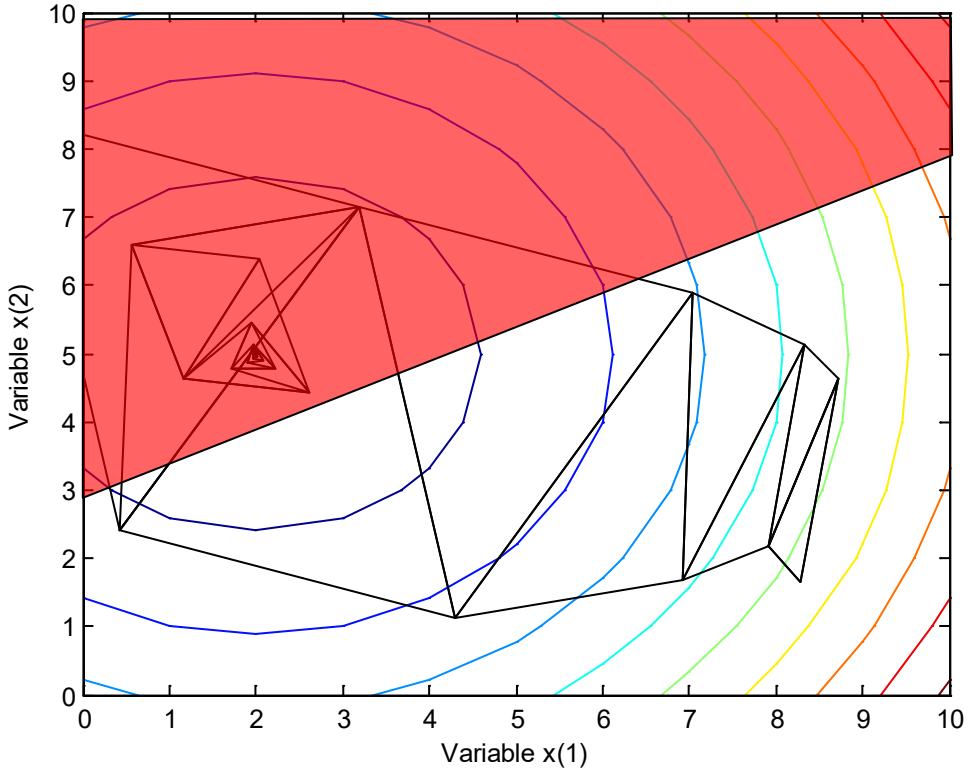
```
  ylabel( 'Objective function' )

% bottom - simplex
```

```
function z = simplex_eval( x )
% biquadratic test function for fminsearch
% HJSIII, 12.10.15

% unconstrained minimum = 3 at x(1)=2 and x(2)=5
z = ( x(1)^2 - 4*x(1) + 4 ) + ( x(2)^2 - 10*x(2) + 25 ) + 3;

% penalty function to provide inequality constraint
% constrained minimum = 3.8 at x(1)=2.4 and x(2)=4.2
%t = 0.5 * x(1) + 3;
%if x(2) > t,
%  z = z + 100;
%end

% bottom - simplex_eval
```

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

```
% biquad_surf.m - plot contours of biquadratic
% HJSIII, 12.10.15

clear

% design space
x1_val = ( 0 : 1 : 10 )';
x2_val = ( 0 : 1 : 10 )';
n1 = length( x1_val );
n2 = length( x2_val );

% exhaustive search
for i = 1 : n1,
  x(1) = x1_val(i);
  for j = 1 : n2;
    x(2) = x2_val(j);
    z_ij(i,j) = ( x(1)^2 - 4*x(1) + 4 ) + ( x(2)^2 - 10*x(2) + 25 ) + 3;
  end
end

% plot surface
z_ij = z_ij';
figure( 1 )
  clf
  h_surf = surf( x1_val, x2_val, z_ij );
  xlabel( 'Variable x(1)' )
  ylabel( 'Variable x(2)' )

% plot contours
figure( 2 )
  clf
  h_cont = contour( x1_val, x2_val, z_ij );
  xlabel( 'Variable x(1)' )
  ylabel( 'Variable x(2)' )

% bottom - biquad_surf
```

$x_2 < 0.5\, x_1 + 3$



add penalty function to objective if constraint is violated

```
>> help fminsearch
 FMINSEARCH Multidimensional unconstrained nonlinear minimization (Nelder-Mead).
    X = FMINSEARCH(FUN,X0) starts at X0 and attempts to find a local minimizer
    X of the function FUN.  FUN is a function handle.  FUN accepts input X and
    returns a scalar function value F evaluated at X. X0 can be a scalar, vector
    or matrix.

    X = FMINSEARCH(FUN,X0,OPTIONS)  minimizes with the default optimization
    parameters replaced by values in the structure OPTIONS, created
    with the OPTIMSET function.  See OPTIMSET for details.  FMINSEARCH uses
    these options: Display, TolX, TolFun, MaxFunEvals, MaxIter, FunValCheck,
    PlotFcns, and OutputFcn.

    X = FMINSEARCH(PROBLEM) finds the minimum for PROBLEM. PROBLEM is a
    structure with the function FUN in PROBLEM.objective, the start point
    in PROBLEM.x0, the options structure in PROBLEM.options, and solver
    name 'fminsearch' in PROBLEM.solver. The PROBLEM structure must have
    all the fields.

    [X,FVAL]= FMINSEARCH(...) returns the value of the objective function,
    described in FUN, at X.

    [X,FVAL,EXITFLAG] = FMINSEARCH(...) returns an EXITFLAG that describes
    the exit condition of FMINSEARCH. Possible values of EXITFLAG and the
    corresponding exit conditions are

     1  Maximum coordinate difference between current best point and other
        points in simplex is less than or equal to TolX, and corresponding
        difference in function values is less than or equal to TolFun.
     0  Maximum number of function evaluations or iterations reached.
    -1  Algorithm terminated by the output function.

    [X,FVAL,EXITFLAG,OUTPUT] = FMINSEARCH(...) returns a structure
    OUTPUT with the number of iterations taken in OUTPUT.iterations, the
    number of function evaluations in OUTPUT.funcCount, the algorithm name
    in OUTPUT.algorithm, and the exit message in OUTPUT.message.

    Examples
      FUN can be specified using @:
         X = fminsearch(@sin,3)
      finds a minimum of the SIN function near 3.
      In this case, SIN is a function that returns a scalar function value
      SIN evaluated at X.

      FUN can also be an anonymous function:
         X = fminsearch(@(x) norm(x),[1;2;3])
      returns a point near the minimizer [0;0;0].

    If FUN is parameterized, you can use anonymous functions to capture the
    problem-dependent parameters. Suppose you want to optimize the objective
    given in the function myfun, which is parameterized by its second argument c.
    Here myfun is an M-file function such as

      function f = myfun(x,c)
      f = x(1)^2 + c*x(2)^2;

    To optimize for a specific value of c, first assign the value to c. Then
    create a one-argument anonymous function that captures that value of c
    and calls myfun with two arguments. Finally, pass this anonymous function
    to FMINSEARCH:

      c = 1.5; % define parameter first
      x = fminsearch(@(x) myfun(x,c),[0.3;1])

    FMINSEARCH uses the Nelder-Mead simplex (direct search) method.

    See also optimset, fminbnd, function_handle.
```