Constrained Nonlinear Optimization Examples

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Example: Nonlinear Inequality Constraints

If inequality constraints are added to Equation 6–16, the resulting problem can be solved by the $\underline{\text{fmincon}}$ function. For example, find x that solves

$$\min_{x} f(x) = e^{x_1} \left(4x_1^2 + 2x_2^2 + 4x_1x_2 + 2x_2 + 1 \right). \tag{6-57}$$

subject to the constraints

$$\begin{array}{l} x_{_{1}}x_{_{2}}-x_{_{1}}-x_{_{2}}\leq -1.5,\\ x_{_{1}}x_{_{2}}\geq -10. \end{array}$$

Because neither of the constraints is linear, you cannot pass the constraints to $\underline{\mathtt{fmincon}}$ at the command line. Instead you can create a second file, $\mathtt{confun.m}$, that returns the value at both constraints at the current x in a vector c. The constrained optimizer, $\mathtt{fmincon}$, is then invoked. Because $\mathtt{fmincon}$ expects the constraints to be written in the form $c(x) \leq 0$, you must rewrite your constraints in the form

$$x_1 x_2 - x_1 - x_2 + 1.5 \le 0,$$
 (6-58)
 $-x_1 x_2 - 10 \le 0.$

Step 1: Write a file objfun.m for the objective function.

```
function f = objfun(x)

f = exp(x(1))*(4*x(1)^2 + 2*x(2)^2 + 4*x(1)*x(2) + 2*x(2) + 1);
```

Step 2: Write a file confun.m for the constraints.

```
function [c, ceq] = confun(x)
% Nonlinear inequality constraints
c = [1.5 + x(1)*x(2) - x(1) - x(2);
     -x(1)*x(2) - 10];
% Nonlinear equality constraints
ceq = [];
```

Step 3: Invoke constrained optimization routine.

```
x0 = [-1,1]; % Make a starting guess at the solution
```

```
options = optimset('Algorithm', 'active-set');
[x,fval] = ...
fmincon(@objfun,x0,[],[],[],[],[],[],@confun,options);
```

fmincon produces the solution x with function value fval:

```
x,fval
x =
    -9.5474  1.0474
fval =
    0.0236
```

You can evaluate the constraints at the solution by entering

```
[c,ceq] = confun(x)
```

This returns numbers close to zero, such as

```
c =
  1.0e-007 *
  -0.9032
   0.9032
ceq =
[]
```

Note that both constraint values are, to within a small tolerance, less than or equal to 0; that is, x satisfies $c(x) \le 0$.

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Example: Bound Constraints

The variables in x can be restricted to certain limits by specifying simple bound constraints to the constrained optimizer function. For fmincon, the command

```
x = fmincon(@objfun, x0,[],[],[],[],lb,ub,@confun,options);
```

limits x to be within the range $lb \le x \le ub$.

To restrict x in Equation 6-57 to be greater than 0 (i.e., $x_1 \ge 0$, $x_1 \ge 0$), use the commands

Note that to pass in the lower bounds as the seventh argument to $\underline{\texttt{fmincon}}$, you must specify values for the third through sixth arguments. In this example, we specified [] for these arguments since there are no linear inequalities or linear equalities.

fmincon produces the following results:

When 1b or ub contains fewer elements than x, only the first corresponding elements in x are bounded. Alternatively, if only some of the variables are bounded, then use -inf in 1b for unbounded below variables and inf in ub for unbounded above variables. For example,

```
lb = [-inf 0];
ub = [10 inf];
```

bounds $x_1 \le 10$, $x_2 \ge 0$. x_1 has no lower bound, and x_2 has no upper bound. Using inf and -inf give better numerical results than using a very large positive number or a very large negative number to imply lack of bounds.

Note that the number of function evaluations to find the solution is reduced because we further restricted the search space. Fewer function evaluations are usually taken when a problem has more constraints and bound limitations because the optimization makes better decisions regarding step size and regions of feasibility than in the unconstrained case. It is, therefore, good practice to bound and constrain problems, where possible, to promote fast convergence to a solution.

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Example: Constraints With Gradients

Ordinarily the medium-scale minimization routines use numerical gradients calculated by finite-difference approximation. This procedure systematically perturbs each of the variables in order to calculate function and constraint partial derivatives. Alternatively, you can provide a function to compute partial derivatives analytically. Typically, the problem is solved more accurately and efficiently if such a function is provided.

To solve Equation 6–57 using analytically determined gradients, do the following.

Step 1: Write a file for the objective function and gradient.

```
function [f,G] = objfungrad(x)
f = \exp(x(1))*(4*x(1)^2+2*x(2)^2+4*x(1)*x(2)+2*x(2)+1);
% Gradient of the objective function
if nargout > 1
   G = [ f + \exp(x(1)) * (8*x(1) + 4*x(2)),
       exp(x(1))*(4*x(1)+4*x(2)+2)];
end
```

Step 2: Write a file for the nonlinear constraints and the gradients of the nonlinear constraints.

```
function [c,ceq,DC,DCeq] = confungrad(x) c(1) = 1.5 + x(1) * x(2) - x(1) - x(2); %Inequality constraints <math>c(2) = -x(1) * x(2)-10; % No nonlinear equality constraints ceq=[]; % Gradient of the constraints if nargout > 2 DC=[x(2)-1, -x(2); x(1)-1, -x(1)]; DCeq=[]; end
```

G contains the partial derivatives of the objective function, f, returned by objfungrad(x), with respect to each of the elements in x:

$$\nabla f = \begin{bmatrix} e^{x_1} \left(4x_1^2 + 2x_2^2 + 4x_1x_2 + 2x_2 + 1 \right) + e^{x_1} \left(8x_1 + 4x_2 \right) \\ e^{x_1} \left(4x_1 + 4x_2 + 2 \right) \end{bmatrix}. \tag{6-59}$$

The columns of DC contain the partial derivatives for each respective constraint (i.e., the ith column of DC is the partial derivative of the ith constraint with respect to x). So in the above example, DC is

$$\begin{bmatrix} \frac{\partial c_1}{\partial x_1} & \frac{\partial c_2}{\partial x_1} \\ \frac{\partial c_1}{\partial x_2} & \frac{\partial c_2}{\partial x_2} \end{bmatrix} = \begin{bmatrix} x_2 - 1 & -x_2 \\ x_1 - 1 & -x_1 \end{bmatrix}. \tag{6-60}$$

Since you are providing the gradient of the objective in objfungrad.m and the gradient of the constraints in confungrad.m, you must tell <u>fmincon</u> that these files contain this additional information. Use <u>optimset</u> to turn the options GradObj and GradConstr to 'on' in the example's existing options structure:

```
options = optimset(options, 'GradObj', 'on', 'GradConstr', 'on');
```

If you do not set these options to 'on' in the options structure, $\frac{fmincon}{}$ does not use the analytic gradients.

The arguments 1b and ub place lower and upper bounds on the independent variables in x. In this example, there are no bound constraints and so they are both set to [].

Step 3: Invoke the constrained optimization routine.

The results:

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Example: Constrained Minimization Using fmincon's Interior-Point Algorithm with Analytic Hessian

The fmincon interior-point algorithm can accept a Hessian function as an input. When you supply a Hessian, you may obtain a faster, more accurate solution to a constrained minimization problem.

The constraint set for this example is the intersection of the interior of two cones—one pointing up, and one pointing down. The constraint function c is a two-component vector, one component for each cone. Since this is a three-dimensional example, the gradient of the constraint c is a 3-by-2 matrix.

```
function [c ceq gradc gradceq] = twocone(x)
% This constraint is two cones, z > -10 + r
% and z < 3 - r

ceq = [];
r = sqrt(x(1)^2 + x(2)^2);
c = [-10+r-x(3);
    x(3)-3+r];

if nargout > 2

    gradceq = [];
    gradc = [x(1)/r,x(1)/r;
        x(2)/r,x(2)/r;
        -1,1];
end
```

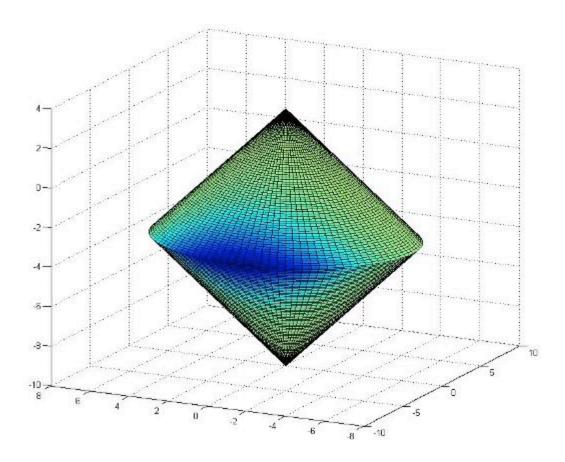
The objective function grows rapidly negative as the x(1) coordinate becomes negative. Its gradient is a three-element vector.

```
function [f gradf] = bigtoleft(x)
% This is a simple function that grows rapidly negative
% as x(1) gets negative
%
f=10*x(1)^3+x(1)*x(2)^2+x(3)*(x(1)^2+x(2)^2);

if nargout > 1

   gradf=[30*x(1)^2+x(2)^2+2*x(3)*x(1);
        2*x(1)*x(2)+2*x(3)*x(2);
        (x(1)^2+x(2)^2)];
end
```

Here is a plot of the problem. The shading represents the value of the objective function. You can see that the objective function is minimized near x = [-6.5, 0, -3.5]:



Code for generating the figure

The Hessian of the Lagrangian is given by the equation:

$$\nabla^2_{xx}L(x,\lambda) = \nabla^2 f(x) + \sum \lambda_i \nabla^2 c_i(x) + \sum \lambda_i \nabla^2 ceq_i(x).$$

The following function computes the Hessian at a point ${\bf x}$ with Lagrange multiplier structure lambda:

```
function h = hessinterior(x,lambda)

h = [60*x(1)+2*x(3),2*x(2),2*x(1);
    2*x(2),2*(x(1)+x(3)),2*x(2);
    2*x(1),2*x(2),0];% Hessian of f

r = sqrt(x(1)^2+x(2)^2);% radius

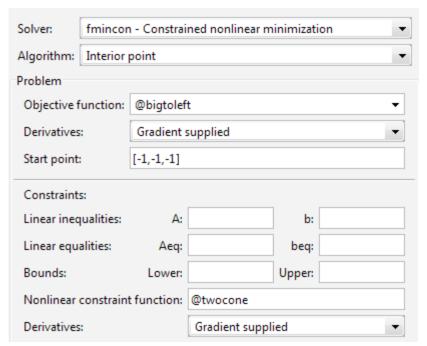
rinv3 = 1/r^3;

hessc = [(x(2))^2*rinv3,-x(1)*x(2)*rinv3,0;
    -x(1)*x(2)*rinv3,x(1)^2*rinv3,0;
    0,0,0];% Hessian of both c(1) and c(2)

h = h + lambda.ineqnonlin(1)*hessc + lambda.ineqnonlin(2)*hessc;
```

Run this problem using the interior-point algorithm in fmincon. To do this using the Optimization Tool:

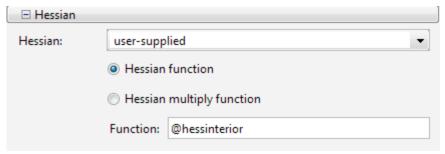
1. Set the problem as in the following figure.



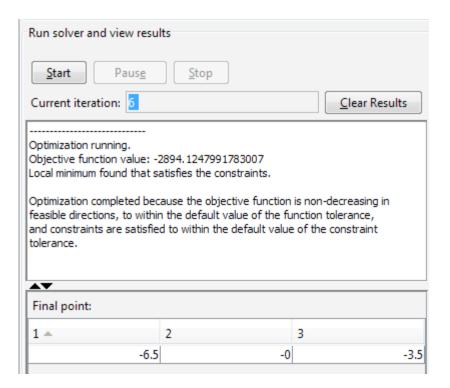
2. For iterative output, scroll to the bottom of the **Options** pane and select **Level of display**, iterative.



3. In the **Options** pane, give the analytic Hessian function handle.



4. Under Run solver and view results, click Start.



To perform the minimization at the command line:

1. Set options as follows:

2. Run fmincon with starting point [-1,-1,-1], using the options structure:

```
[x fval mflag output]=fmincon(@bigtoleft,[-1,-1,-1],...
[],[],[],[],[],@twocone,options)
```

The output is:

				First-order	Norm of
Iter	F-cour	f(x)	Feasibility	optimality	step
0	1	-1.300000e+001	0.000e+000	3.067e+001	
1	2	-2.011543e+002	0.000e+000	1.739e+002	1.677e+000
2	3	-1.270471e+003	9.844e-002	3.378e+002	2.410e+000
3	4	-2.881667e+003	1.937e-002	1.079e+002	2.206e+000
4	5	-2.931003e+003	2.798e-002	5.813e+000	6.006e-001
5	6	-2.894085e+003	0.000e+000	2.352e-002	2.800e-002
6	7	-2.894125e+003	0.000e+000	5.981e-005	3.048e-005
_					

Local minimum found that satisfies the constraints.

Optimization completed because the objective function is non-decreasing in feasible directions, to within the default value of the function tolerance, and constraints are satisfied to within the default value of the constraint tolera

```
x =
-6.5000 -0.0000 -3.5000

fval =
```

```
-2.8941e+003
   mflaq =
        1
   output =
            iterations: 6
             funcCount: 7
       constrviolation: 0
              stepsize: 3.0479e-005
             algorithm: 'interior-point'
         firstorderopt: 5.9812e-005
          cgiterations: 3
               message: [1x782 char]
If you do not use a Hessian function, fmincon takes 9 iterations to converge, instead of 6:
   options = optimset('Algorithm', 'interior-point',...
           'Display', 'iter', 'GradObj', 'on', 'GradConstr', 'on');
   [x fval mflag output]=fmincon(@bigtoleft,[-1,-1,-1],...
              [],[],[],[],[],@twocone,options)
                                          First-order
                                                         Norm of
   Iter F-count
                        f(x) Feasibility optimality
                                                             step
     0 1 -1.300000e+001 0.000e+000 3.067e+001
     1
           2 -7.259551e+003 2.495e+000 2.414e+003 8.344e+000
           3 -7.361301e+003 2.529e+000 2.767e+001 5.253e-002
     2
          4 -2.978165e+003 9.392e-002 1.069e+003 2.462e+000
     3
     4
          8 -3.033486e+003 1.050e-001 8.282e+002 6.749e-001
          9 -2.893740e+003 0.000e+000 4.186e+001 1.053e-001
     5
         10 -2.894074e+003 0.000e+000 2.637e-001 3.565e-004
     6
     7
         11 -2.894124e+003 0.000e+000 2.340e-001 1.680e-004
         12 -2.894125e+003 2.830e-008 1.180e-001 6.374e-004
         13 -2.894125e+003 2.939e-008 1.423e-004 6.484e-004
   Local minimum found that satisfies the constraints.
   Optimization completed because the objective function is non-decreasing in
   feasible directions, to within the default value of the function tolerance,
   and constraints are satisfied to within the default value of the constraint tolera
   x =
      -6.5000 -0.0000 -3.5000
   fval =
    -2.8941e+003
   mflag =
        1
   output =
            iterations: 9
             funcCount: 13
       constrviolation: 2.9391e-008
              stepsize: 6.4842e-004
```

algorithm: 'interior-point'

firstorderopt: 1.4235e-004

```
cgiterations: 0
    message: [1x782 char]
```

Both runs lead to similar solutions, but the F-count and number of iterations are lower when using an analytic Hessian.

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Example: Equality and Inequality Constraints

For routines that permit equality constraints, nonlinear equality constraints must be computed with the nonlinear inequality constraints. For linear equalities, the coefficients of the equalities are passed in through the matrix Aeq and the right-hand-side vector beq.

For example, if you have the nonlinear equality constraint $x_1^2 + x_2 = 1$ and the nonlinear inequality constraint $x_1 x_2 \ge -10$, rewrite them as

$$x_1^2 + x_2 - 1 = 0,$$

 $-x_1x_2 - 10 \le 0,$

and then solve the problem using the following steps.

Step 1: Write a file objfun.m.

```
function f = objfun(x)

f = exp(x(1))*(4*x(1)^2+2*x(2)^2+4*x(1)*x(2)+2*x(2)+1);
```

Step 2: Write a file confuneq.m for the nonlinear constraints.

```
function [c, ceq] = confuneq(x)
% Nonlinear inequality constraints
c = -x(1)*x(2) - 10;
% Nonlinear equality constraints
ceq = x(1)^2 + x(2) - 1;
```

Step 3: Invoke constrained optimization routine.

```
x0 = [-1,1]; % Make a starting guess at the solution
options = optimset('Algorithm', 'active-set');
[x,fval] = fmincon(@objfun,x0,[],[],[],[],[],[],...
@confuneq.options);
```

After 21 function evaluations, the solution produced is

```
x,fval
x =
     -0.7529     0.4332
fval =
     1.5093

[c,ceq] = confuneq(x) % Check the constraint values at x
c =
     -9.6739
ceq =
     6.3038e-009
```

Note that ceq is equal to 0 within the default tolerance on the constraints of 1.0e-006 and that c is less than or equal to 0 as desired.

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Example: Nonlinear Minimization with Bound Constraints and Banded Preconditioner

The goal in this problem is to minimize the nonlinear function

$$f(x) = 1 + \sum_{i=1}^{n} \left| \left(3 - 2x_{i}\right) x_{i} - x_{i-1} - x_{i+1} + 1 \right|^{p} + \sum_{i=1}^{n/2} \left| x_{i} + x_{i+n/2} \right|^{p},$$

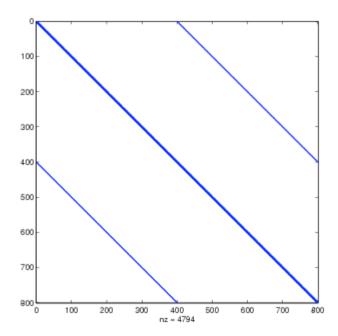
such that $-10.0 \le x_i \le 10.0$, where n is 800 (n should be a multiple of 4), p = 7/3, and $x_0 = x_{n+1} = 0$.

Step 1: Write a file tbroyfg.m that computes the objective function and the gradient of the objective

The tbroyfg.m file computes the function value and gradient. This file is long and is not included here. You can see the code for this function using the command

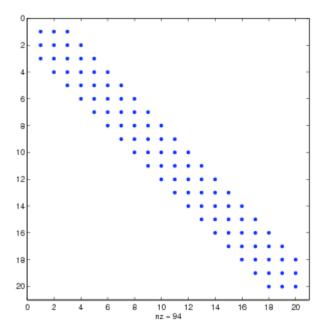
The sparsity pattern of the Hessian matrix has been predetermined and stored in the file tbroyhstr.mat. The sparsity structure for the Hessian of this problem is banded, as you can see in the following spy plot.

load tbroyhstr
spy(Hstr)



In this plot, the center stripe is itself a five-banded matrix. The following plot shows the matrix more clearly:

```
spy(Hstr(1:20,1:20))
```



Use <u>optimset</u> to set the HessPattern parameter to Hstr. When a problem as large as this has obvious sparsity structure, not setting the HessPattern parameter requires a huge amount of unnecessary memory and computation. This is because <u>fmincon</u> attempts to use finite differencing on a full Hessian matrix of 640,000 nonzero entries.

You must also set the GradObj parameter to 'on' using <u>optimset</u>, since the gradient is computed in tbroyfg.m. Then execute fmincon as shown in <u>Step 2</u>.

Step 2: Call a nonlinear minimization routine with a starting point xstart.

After seven iterations, the exitflag, fval, and output values are

```
exitflag =
    3

fval =
    270.4790

output =
    iterations: 7
    funcCount: 8
    cgiterations: 18
    firstorderopt: 0.0163
        algorithm: 'trust-region-reflective'
```

```
message: [1x471 char]
constrviolation: 0
```

For bound constrained problems, the first-order optimality is the infinity norm of v.*g, where v is defined as in Box Constraints, and g is the gradient.

Because of the five-banded center stripe, you can improve the solution by using a five-banded preconditioner instead of the default diagonal preconditioner. Using the optimset function, reset the PrecondBandWidth parameter to 2 and solve the problem again. (The bandwidth is the number of upper (or lower) diagonals, not counting the main diagonal.)

The number of iterations actually goes up by two; however the total number of CG iterations drops from 18 to 15. The first-order optimality measure is reduced by a factor of 1e-3:

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Example: Nonlinear Minimization with Equality Constraints

The trust-region reflective method for $\underline{\mathtt{fmincon}}$ can handle equality constraints if no other constraints exist. Suppose you want to minimize the same objective as in $\underline{\mathtt{Equation 6-17}}$, which is coded in the function $\mathtt{brownfgh.m}$, where $\mathtt{n} = 1000$, such that $Aeq \cdot x = beq$ for Aeq that has 100 equations (so Aeq is a 100-by-1000 matrix).

Step 1: Write a file brownfgh.m that computes the objective function, the gradient of the objective, and the sparse tridiagonal Hessian matrix.

The file is lengthy so is not included here. View the code with the command

```
type brownfgh
```

Because brownfgh computes the gradient and Hessian values as well as the objective function, you need to use optimset to indicate that this information is available in brownfgh, using the GradObj and

Hessian options.

The sparse matrix Aeq and vector beq are available in the file browneq.mat:

```
load browneq
```

The linear constraint system is 100-by-1000, has unstructured sparsity (use $\underline{spy}(Aeq)$ to view the sparsity structure), and is not too badly ill-conditioned:

```
condest(Aeq*Aeq')
ans =
  2.9310e+006
```

Step 2: Call a nonlinear minimization routine with a starting point xstart.

fmincon prints the following exit message:

```
Local minimum possible.
```

fmincon stopped because the final change in function value relative to its initial value is less than the default value of the function tolerance.

The exitflag value of 3 also indicates that the algorithm terminated because the change in the objective function value was less than the tolerance TolFun. The final function value is given by fval.

```
exitflag, fval, output

exitflag =
    3

fval =
    205.9313

output =
    iterations: 22
    funcCount: 23
    cgiterations: 30
    firstorderopt: 0.0027
        algorithm: 'trust-region-reflective'
        message: [1x471 char]
    constrviolation: 2.2249e-013
```

The linear equalities are satisfied at x.

```
norm(Aeq*x-beq)
ans =
  1.1957e-012
```

Example: Nonlinear Minimization with a Dense but Structured Hessian and Equality Constraints

The <u>fmincon</u> interior-point and trust-region reflective algorithms, and the <u>fminunc</u> large-scale algorithm can solve problems where the Hessian is dense but structured. For these problems, fmincon and fminunc do not compute H^*Y with the Hessian H directly, because forming H would be memory-intensive. Instead, you must provide fmincon or fminunc with a function that, given a matrix Y and information about H, computes $W = H^*Y$.

In this example, the objective function is nonlinear and linear equalities exist so fmincon is used. The description applies to the trust-region reflective algorithm; the fminunc large-scale algorithm is similar. For the interior-point algorithm, see the 'HessMult' option in Hessian. The objective function has the structure

$$f(x) = \hat{f}(x) - \frac{1}{2}x^T V V^T x,$$

where V is a 1000-by-2 matrix. The Hessian of f is dense, but the Hessian of \hat{f} is sparse. If the Hessian of \hat{f} is \hat{H} , then H, the Hessian of f, is

$$H = \hat{H} - VV^T$$
.

To avoid excessive memory usage that could happen by working with H directly, the example provides a Hessian multiply function, hmfleq1. This function, when passed a matrix Y, uses sparse matrices Hinfo, which corresponds to \hat{H} , and V to compute the Hessian matrix product

$$W = H*Y = (Hinfo - V*V')*Y$$

In this example, the Hessian multiply function needs \hat{H} and v to compute the Hessian matrix product. v is a constant, so you can capture v in a function handle to an anonymous function.

However, \hat{H} is not a constant and must be computed at the current x. You can do this by computing \hat{H} in the objective function and returning \hat{H} as Hinfo in the third output argument. By using optimset to set the 'Hessian' options to 'on', fmincon knows to get the Hinfo value from the objective function and pass it to the Hessian multiply function hmfleg1.

Step 1: Write a file brownvv.m that computes the objective function, the gradient, and the sparse part of the Hessian.

The example passes brownvv to fmincon as the objective function. The <u>brownvv.m</u> file is long and is not included here. You can view the code with the command

type brownvv

Because brownvv computes the gradient and part of the Hessian as well as the objective function, the example (Step 3) uses optimset to set the GradObj and Hessian options to 'on'.

Step 2: Write a function to compute Hessian-matrix products for H given a matrix Y.

Now, define a function hmfleq1 that uses Hinfo, which is computed in brownvv, and V, which you can capture in a function handle to an anonymous function, to compute the Hessian matrix product W where W = H*Y = (Hinfo - V*V')*Y. This function must have the form

```
W = hmfleq1(Hinfo,Y)
```

The first argument must be the same as the third argument returned by the objective function brownvv. The second argument to the Hessian multiply function is the matrix Y (of W = H*Y).

Because fmincon expects the second argument Y to be used to form the Hessian matrix product, Y is always a matrix with n rows where n is the number of dimensions in the problem. The number of columns in Y can vary. Finally, you can use a function handle to an anonymous function to capture V, so V can be the third argument to 'hmfleqq'.

```
function W = hmfleq1(Hinfo,Y,V);
%HMFLEQ1 Hessian-matrix product function for BROWNVV objective.
% W = hmfleq1(Hinfo,Y,V) computes W = (Hinfo-V*V')*Y
% where Hinfo is a sparse matrix computed by BROWNVV
% and V is a 2 column matrix.
W = Hinfo*Y - V*(V'*Y);
```

Note The function hmfleq1 is available in the optimdemos folder as hmfleq1.m.

Step 3: Call a nonlinear minimization routine with a starting point and linear equality constraints.

Load the problem parameter, V, and the sparse equality constraint matrices, Aeq and beq, from fleq1.mat, which is available in the optimdemos folder. Use optimset to set the GradObj and Hessian options to 'on' and to set the HessMult option to a function handle that points to hmfleq1. Call fmincon with objective function brownvv and with V as an additional parameter:

```
function [fval, exitflag, output, x] = runfleq1
% RUNFLEQ1 demonstrates 'HessMult' option for
% FMINCON with linear equalities.
용
    Copyright 1984-2006 The MathWorks, Inc.
    $Revision: 1.1.6.29.2.1 $ $Date: 2011/12/02 18:22:02 $
problem = load('fleq1'); % Get V, Aeq, beq
V = problem.V; Aeq = problem.Aeq; beq = problem.beq;
n = 1000;
                      % problem dimension
xstart = -ones(n,1); xstart(2:2:n,1) = ones(length(2:2:n),1);
% starting point
options = optimset('GradObj','on','Hessian','on','HessMult',...
@(Hinfo,Y)hmfleq1(Hinfo,Y,V) ,'Display','iter','TolFun',1e-9);
[x, fval, exitflag, output] = fmincon(@(x)brownvv(x, V), ...
xstart,[],[],Aeq,beq,[],[], [],options);
```

To run the preceding code, enter

```
[fval,exitflag,output,x] = runfleq1;
```

Because the iterative display was set using optimset, this command generates the following iterative display:

	Norm of	First-order	
f(x)	step	optimality	CG-iterations
1997.07		916	
1072.57	6.31716	465	1
480.247	8.19711	201	2
136.982	10.3039	78.1	2
	1997.07 1072.57 480.247	f(x) step 1997.07 1072.57 6.31716 480.247 8.19711	f(x) step optimality 1997.07 916 1072.57 6.31716 465 480.247 8.19711 201

4	44.416	9.04685	16.7	2
5	44.416	100	16.7	2
6	44.416	25	16.7	0
7	-9.05631	6.25	52.9	0
8	-317.437	12.5	91.7	1
9	-405.381	12.5	1.11e+003	1
10	-451.161	3.125	327	4
11	-482.688	0.78125	303	5
12	-547.427	1.5625	187	5
13	-610.42	1.5625	251	7
14	-711.522	1.5625	143	3
15	-802.98	3.125	165	3
16	-820.431	1.13329	32.9	3
17	-822.996	0.492813	7.61	2
18	-823.236	0.223154	1.68	3
19	-823.245	0.056205	0.529	3
20	-823.246	0.0150139	0.0342	5
21	-823.246	0.00479085	0.0152	7
22	-823.246	0.00353697	0.00828	9
23	-823.246	0.000884242	0.005	9
24	-823.246	0.0012715	0.00125	9
25	-823.246	0.000317876	0.0025	9

Local minimum possible.

fmincon stopped because the final change in function value relative to its initial value is less than the selected value of the function tolerance.

Convergence is rapid for a problem of this size with the PCG iteration cost increasing modestly as the optimization progresses. Feasibility of the equality constraints is maintained at the solution.

```
problem = load('fleq1'); % Get V, Aeq, beq
V = problem.V; Aeq = problem.Aeq; beq = problem.beq;
norm(Aeq*x-beq,inf)
ans =
  2.4869e-014
```

Preconditioning

In this example, fmincon cannot use H to compute a preconditioner because H only exists implicitly. Instead of H, fmincon uses Hinfo, the third argument returned by brownvv, to compute a preconditioner. Hinfo is a good choice because it is the same size as H and approximates H to some degree. If Hinfo were not the same size as H, fmincon would compute a preconditioner based on some diagonal scaling matrices determined from the algorithm. Typically, this would not perform as well.

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Example: Using Symbolic Math Toolbox Functions to Calculate Gradients and Hessians

If you have a license for Symbolic Math Toolbox functions, you can use these functions to calculate analytic gradients and Hessians for objective and constraint functions. There are two relevant Symbolic Math Toolbox functions:

• <u>jacobian</u> generates the gradient of a scalar function, and generates a matrix of the partial derivatives of a vector function. So, for example, you can obtain the Hessian matrix, the second

derivatives of the objective function, by applying jacobian to the gradient. Part of this example shows how to use jacobian to generate symbolic gradients and Hessians of objective and constraint functions.

• <u>matlabFunction</u> generates either an anonymous function or a file that calculates the values of a symbolic expression. This example shows how to use <u>matlabFunction</u> to generate files that evaluate the objective and constraint function and their derivatives at arbitrary points.

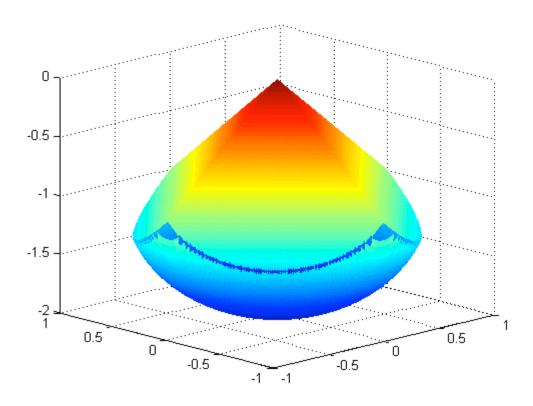
Consider the electrostatics problem of placing 10 electrons in a conducting body. The electrons will arrange themselves so as to minimize their total potential energy, subject to the constraint of lying inside the body. It is well known that all the electrons will be on the boundary of the body at a minimum. The electrons are indistinguishable, so there is no unique minimum for this problem (permuting the electrons in one solution gives another valid solution). This example was inspired by Dolan, Moré, and Munson [58].

This example is a conducting body defined by the following inequalities:

$$z \le -|x| - |y| \tag{6-61}$$

$$x^2 + y^2 + (z+1)^2 \le 1. ag{6-62}$$

This body looks like a pyramid on a sphere.



Code for Generating the Figure

There is a slight gap between the upper and lower surfaces of the figure. This is an artifact of the general plotting routine used to create the figure. This routine erases any rectangular patch on one surface that touches the other surface.

The syntax and structures of the two sets of toolbox functions differ. In particular, symbolic variables are real or complex scalars, but Optimization Toolbox functions pass vector arguments. So there are several steps to take to generate symbolically the objective function, constraints, and all their requisite derivatives, in a form suitable for the interior-point algorithm of fmincon:

- 1. Create the Variables
- 2. Include the Linear Constraints
- 3. Create the Nonlinear Constraints, Their Gradients and Hessians
- 4. Create the Objective Function, Its Gradient and Hessian
- 5. Create the Objective Function File
- 6. Create the Constraint Function File
- 7. Generate the Hessian Files
- 8. Run the Optimization
- 9. Clear the Symbolic Variable Assumptions

To see the efficiency in using gradients and Hessians, see <u>Compare to Optimization Without Gradients and Hessians</u>.

Create the Variables

Generate a symbolic vector \mathbf{x} as a 30-by-1 vector composed of real symbolic variables \mathbf{xij} , \mathbf{i} between 1 and 10, and \mathbf{j} between 1 and 3. These variables represent the three coordinates of electron \mathbf{i} : $\mathbf{xi1}$ corresponds to the x coordinate, $\mathbf{xi2}$ corresponds to the y coordinate, and $\mathbf{xi3}$ corresponds to the z coordinate.

```
x = cell(3, 10);
for i = 1:10
    for j = 1:3
        x{j,i} = sprintf('x%d%d',i,j);
    end
end
x = x(:); % now x is a 30-by-1 vector
x = sym(x, 'real');
```

The vector x is:

х x = x11 x12 x13 x21 x22 x23 x31 x32 x33 x41 x42 x43 x51 x52 x53 x61 x62 x63 x71 x72 x73

> x81 x82

```
x83
x91
x92
x93
x101
x102
x103
```

Include the Linear Constraints

Write the linear constraints in Equation 6-61,

```
z \leq -|x| - |y|,
```

as a set of four linear inequalities for each electron:

```
xi3 - xi1 - xi2 \le 0

xi3 - xi1 + xi2 \le 0

xi3 + xi1 - xi2 \le 0

xi3 + xi1 + xi2 \le 0
```

Therefore there are a total of 40 linear inequalities for this problem.

Write the inequalities in a structured way:

```
B = [1,1,1;-1,1,1;1,-1,1;-1,-1,1];
A = zeros(40,30);
for i=1:10
A(4*i-3:4*i,3*i-2:3*i) = B;
end
b = zeros(40,1);
```

You can see that $A*x \le b$ represents the inequalities:

```
A*x
ans =
    x11 + x12 + x13
    x12 - x11 + x13
    x11 - x12 + x13
    x13 - x12 - x11
    x21 + x22 + x23
    x22 - x21 + x23
    x21 - x22 + x23
    x23 - x22 - x21
    x31 + x32 + x33
    x32 - x31 + x33
    x31 - x32 + x33
    x33 - x32 - x31
    x41 + x42 + x43
    x42 - x41 + x43
    x41 - x42 + x43
    x43 - x42 - x41
    x51 + x52 + x53
    x52 - x51 + x53
    x51 - x52 + x53
    x53 - x52 - x51
```

```
x61 + x62 + x63
   x62 - x61 + x63
   x61 - x62 + x63
   x63 - x62 - x61
   x71 + x72 + x73
   x72 - x71 + x73
   x71 - x72 + x73
   x73 - x72 - x71
   x81 + x82 + x83
   x82 - x81 + x83
   x81 - x82 + x83
   x83 - x82 - x81
   x91 + x92 + x93
   x92 - x91 + x93
   x91 - x92 + x93
   x93 - x92 - x91
x101 + x102 + x103
x102 - x101 + x103
x101 - x102 + x103
x103 - x102 - x101
```

Create the Nonlinear Constraints, Their Gradients and Hessians

The nonlinear constraints in Equation 6-62,

$$x^2 + y^2 + (z+1)^2 \le 1$$
,

are also structured. Generate the constraints, their gradients, and Hessians as follows:

```
c = sym(zeros(1,10));
i = 1:10;
c = (x(3*i-2).^2 + x(3*i-1).^2 + (x(3*i)+1).^2 - 1).';
gradc = jacobian(c,x).'; % .' performs transpose
hessc = cell(1, 10);
for i = 1:10
    hessc{i} = jacobian(gradc(:,i),x);
end
```

The constraint vector c is a row vector, and the gradient of c(i) is represented in the ith column of the matrix grade. This is the correct form, as described in Nonlinear Constraints.

The Hessian matrices, $hessc{1}...hessc{10}$, are square and symmetric. It is better to store them in a cell array, as is done here, than in separate variables such as $hessc{1}$, ..., $hessc{10}$.

Use the .' syntax to transpose. The ' syntax means conjugate transpose, which has different symbolic derivatives.

Create the Objective Function, Its Gradient and Hessian

The objective function, potential energy, is the sum of the inverses of the distances between each electron pair:

energy =
$$\sum_{i < j} \frac{1}{|x_i - x_j|}.$$

The distance is the square root of the sum of the squares of the differences in the components of the

vectors.

Calculate the energy, its gradient, and its Hessian as follows:

```
energy = sym(0);
for i = 1:3:25
    for j = i+3:3:28
        dist = x(i:i+2) - x(j:j+2);
        energy = energy + 1/sqrt(dist.'*dist);
    end
end

gradenergy = jacobian(energy,x).';
hessenergy = jacobian(gradenergy,x);
```

Create the Objective Function File

The objective function should have two outputs, energy and gradenergy. Put both functions in one vector when calling matlabfunction to reduce the number of subexpressions that matlabfunction generates, and to return the gradient only when the calling function (fmincon in this case) requests both outputs. This example shows placing the resulting files in your current folder. Of course, you can place them anywhere you like, as long as the folder is on the MATLAB path.

```
currdir = [pwd filesep]; % You may need to use currdir = pwd
filename = [currdir,'demoenergy.m'];
matlabFunction(energy,gradenergy,'file',filename,'vars',{x});
```

This syntax causes matlabFunction to return energy as the first output, and gradenergy as the second. It also takes a single input vector $\{x\}$ instead of a list of inputs x11, ..., x103.

The resulting file demoenergy.m contains, in part, the following lines or similar ones:

```
function [energy,gradenergy] = demoenergy(in1)
%DEMOENERGY
%    [ENERGY,GRADENERGY] = DEMOENERGY(IN1)
...
x101 = in1(28,:);
...
energy = 1./t140.^(1./2) + ...;
if nargout > 1
    ...
    gradenergy = [(t174.*(t185 - 2.*x11))./2 - ...];
end
```

This function has the correct form for an objective function with a gradient; see <u>Writing Scalar Objective Functions</u>.

Create the Constraint Function File

Generate the nonlinear constraint function, and put it in the correct format.

```
filename = [currdir,'democonstr.m'];
matlabFunction(c,[],gradc,[],'file',filename,'vars',{x},...
'outputs',{'c','ceq','gradc','gradceq'});
```

The resulting file democonstr.m contains, in part, the following lines or similar ones:

```
function [c,ceq,gradc,gradceq] = democonstr(in1)
```

```
%DEMOCONSTR
%     [C,CEQ,GRADC,GRADCEQ] = DEMOCONSTR(IN1)
...
x101 = in1(28,:);
...
c = [t417.^2 + ...];
if nargout > 1
     ceq = [];
end
if nargout > 2
     gradc = [2.*x11,...];
end
if nargout > 3
     gradceq = [];
end
```

This function has the correct form for a constraint function with a gradient; see Nonlinear Constraints.

Generate the Hessian Files

To generate the Hessian of the Lagrangian for the problem, first generate files for the energy Hessian and for the constraint Hessians.

The Hessian of the objective function, hessenergy, is a very large symbolic expression, containing over 150,000 symbols, as evaluating size(char(hessenergy)) shows. So it takes a substantial amount of time to run matlabFunction(hessenergy).

To generate a file hessenergy.m, run the following two lines:

```
filename = [currdir,'hessenergy.m'];
matlabFunction(hessenergy,'file',filename,'vars',{x});
```

In contrast, the Hessians of the constraint functions are small, and fast to compute:

```
for i = 1:10
    ii = num2str(i);
    thename = ['hessc',ii];
    filename = [currdir,thename,'.m'];
    matlabFunction(hessc{i},'file',filename,'vars',{x});
end
```

After generating all the files for the objective and constraints, put them together with the appropriate Lagrange multipliers in a file hessfinal.m as follows:

```
function H = hessfinal(X,lambda)
%
% Call the function hessenergy to start
H = hessenergy(X);
% Add the Lagrange multipliers * the constraint Hessians
H = H + hessc1(X) * lambda.ineqnonlin(1);
H = H + hessc2(X) * lambda.ineqnonlin(2);
H = H + hessc3(X) * lambda.ineqnonlin(3);
H = H + hessc4(X) * lambda.ineqnonlin(4);
H = H + hessc5(X) * lambda.ineqnonlin(5);
H = H + hessc6(X) * lambda.ineqnonlin(6);
H = H + hessc7(X) * lambda.ineqnonlin(7);
H = H + hessc8(X) * lambda.ineqnonlin(8);
```

```
H = H + hessc9(X) * lambda.ineqnonlin(9);
H = H + hessc10(X) * lambda.ineqnonlin(10);
```

Run the Optimization

Start the optimization with the electrons distributed randomly on a sphere of radius 1/2 centered at [0,0,-1]:

```
rng('default'); % for reproducibility
Xinitial = randn(3,10); % columns are normal 3-D vectors
for j=1:10
    Xinitial(:,j) = Xinitial(:,j)/norm(Xinitial(:,j))/2;
    % this normalizes to a 1/2-sphere
end
Xinitial(3,:) = Xinitial(3,:) - 1; % center at [0,0,-1]
Xinitial = Xinitial(:); % Convert to a column vector
```

Set the options to use the interior-point algorithm, and to use gradients and the Hessian:

```
options = optimset('Algorithm','interior-point','GradObj','on',...
'GradConstr','on','Hessian','user-supplied',...
'HessFcn',@hessfinal,'Display','final');
```

Call fmincon:

```
[xfinal fval exitflag output] = fmincon(@demoenergy,Xinitial,...
A,b,[],[],[],[democonstr,options)
```

The output is as follows:

Local minimum found that satisfies the constraints.

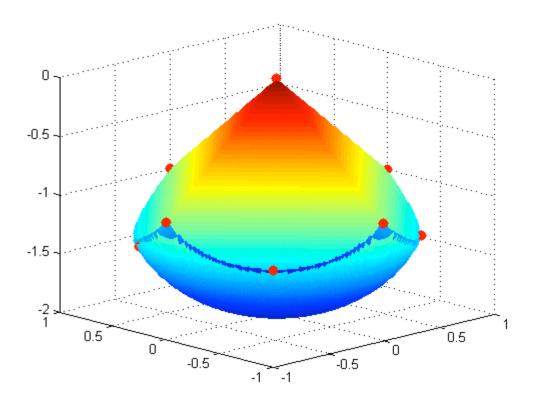
Optimization completed because the objective function is non-decreasing in feasible directions, to within the default value of the function tolerance, and constraints are satisfied to within the default value of the constraint tolera

```
xfinal =
   -0.0317
    0.0317
   -1.9990
    0.6356
   -0.6356
   -1.4381
    0.0000
   -0.0000
   -0.0000
    0.0000
   -1.0000
   -1.0000
    1.0000
   -0.0000
   -1.0000
   -1.0000
   -0.0000
   -1.0000
    0.6689
    0.6644
```

-1.3333

```
-0.6667
    0.6667
   -1.3333
    0.0000
    1.0000
   -1.0000
   -0.6644
   -0.6689
   -1.3333
fval =
   34.1365
exitflag =
     1
output =
         iterations: 19
          funcCount: 28
    constrviolation: 0
           stepsize: 4.0372e-005
          algorithm: 'interior-point'
      firstorderopt: 4.0015e-007
       cgiterations: 55
            message: [1x777 char]
```

Even though the initial positions of the electrons were random, the final positions are nearly symmetric:



▶ Code for Generating the Figure

Compare to Optimization Without Gradients and Hessians

The use of gradients and Hessians makes the optimization run faster and more accurately. To compare with the same optimization using no gradient or Hessian information, set the options not to use gradients and Hessians:

```
options = optimset('Algorithm','interior-point',...
    'Display','final');
[xfinal2 fval2 exitflag2 output2] = fmincon(@demoenergy,Xinitial,...
    A,b,[],[],[],@democonstr,options)
```

The output shows that fmincon found an equivalent minimum, but took more iterations and many more function evaluations to do so:

Local minimum found that satisfies the constraints.

Optimization completed because the objective function is non-decreasing in feasible directions, to within the default value of the function tolerance, and constraints are satisfied to within the default value of the constraint tolera

```
0.0000
    1.0000
   -1.0000
    0.6690
   -0.6644
   -1.3333
   -0.6644
   0.6690
   -1.3333
    0.0000
   -1.0000
   -1.0000
   0.6356
   0.6356
   -1.4381
   -0.0317
   -0.0317
   -1.9990
   1.0000
   0.0000
   -1.0000
   -1.0000
   0.0000
   -1.0000
    0.0000
   0.0000
   -0.0000
   -0.6667
   -0.6667
   -1.3333
fval2 =
   34.1365
exitflag2 =
     1
```

xfinal2 =

```
output2 =
    iterations: 87
    funcCount: 2745
constrviolation: 0
    stepsize: 1.4494e-06
    algorithm: 'interior-point'
firstorderopt: 2.9480e-06
    cgiterations: 0
    message: [1x777 char]
```

In this run the number of function evaluations (in output2.funcCount) is 2745, compared to 28 (in output.funcCount) when using gradients and Hessian.

Clear the Symbolic Variable Assumptions

The symbolic variables in this example have the assumption, in the symbolic engine workspace, that they are real. To clear this assumption from the symbolic engine workspace, it is not sufficient to delete the variables. You must clear the variables using the syntax

```
syms x11 x12 x13 clear
```

or reset the symbolic engine using the command

```
reset(symengine)
```

After resetting the symbolic engine you should clear all symbolic variables from the MATLAB workspace with the clear command, or clear variable list.

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Example: One-Dimensional Semi-Infinite Constraints

Find values of x that minimize

$$f(x) = (x_1 - 0.5)^2 + (x_2 - 0.5)^2 + (x_3 - 0.5)^2$$

where

$$\begin{split} K_1(x,w_1) &= \sin(w_1x_1)\cos(w_1x_2) - \frac{1}{1000}(w_1 - 50)^2 - \sin(w_1x_3) - x_3 \le 1, \\ K_2(x,w_2) &= \sin(w_2x_2)\cos(w_2x_1) - \frac{1}{1000}(w_2 - 50)^2 - \sin(w_2x_3) - x_3 \le 1, \end{split}$$

for all values of w_1 and w_2 over the ranges

$$1 \le w_1 \le 100,$$

 $1 \le w_2 \le 100.$

Note that the semi-infinite constraints are one-dimensional, that is, vectors. Because the constraints must be in the form $K_i(x, w_i) \le 0$, you need to compute the constraints as

$$K_1(x,w_1) = \sin(w_1x_1)\cos(w_1x_2) - \frac{1}{1000}(w_1 - 50)^2 - \sin(w_1x_3) - x_3 - 1 \le 0,$$

$$K_2(x,w_2) = \sin(w_2x_2)\cos(w_2x_1) - \frac{1}{1000}(w_2 - 50)^2 - \sin(w_2x_3) - x_3 - 1 \le 0.$$

First, write a file that computes the objective function.

```
function f = myfun(x,s)
% Objective function
```

```
f = sum((x-0.5).^2);
```

Second, write a file mycon.m that computes the nonlinear equality and inequality constraints and the semi-infinite constraints.

```
function [c, ceq, K1, K2, s] = mycon(X, s)
% Initial sampling interval
if isnan(s(1,1)),
   s = [0.2 0; 0.2 0];
end
% Sample set
w1 = 1:s(1,1):100;
w2 = 1:s(2,1):100;
% Semi-infinite constraints
K1 = \sin(w1*X(1)).*\cos(w1*X(2)) - 1/1000*(w1-50).^2 - ...
       sin(w1*X(3))-X(3)-1;
K2 = \sin(w2*X(2)).*\cos(w2*X(1)) - 1/1000*(w2-50).^2 - ...
       sin(w2*X(3))-X(3)-1;
% No finite nonlinear constraints
c = []; ceq=[];
% Plot a graph of semi-infinite constraints
plot(w1,K1,'-',w2,K2,':')
title('Semi-infinite constraints')
drawnow
```

Then, invoke an optimization routine.

After eight iterations, the solution is

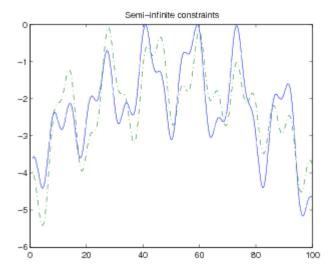
```
x
x =
0.6675
0.3012
0.4022
```

The function value and the maximum values of the semi-infinite constraints at the solution \mathbf{x} are

```
fval
fval =
    0.0771

[c,ceq,K1,K2] = mycon(x,NaN); % Initial sampling interval
max(K1)
ans =
    -0.0077
max(K2)
ans =
    -0.0812
```

A plot of the semi-infinite constraints is produced.



This plot shows how peaks in both constraints are on the constraint boundary.

The plot command inside mycon.m slows down the computation. Remove this line to improve the speed.

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Example: Two-Dimensional Semi-Infinite Constraint

Find values of x that minimize

$$f(x) = (x_1 - 0.2)^2 + (x_2 - 0.2)^2 + (x_3 - 0.2)^2,$$

where

$$K_1(x,w) = \sin(w_1x_1)\cos(w_2x_2) - \frac{1}{1000}(w_1 - 50)^2 - \sin(w_1x_3) - x_3 + \dots$$

$$\sin(w_2x_2)\cos(w_1x_1) - \frac{1}{1000}(w_2 - 50)^2 - \sin(w_2x_3) - x_3 \le 1.5,$$

for all values of w_1 and w_2 over the ranges

```
\begin{array}{l} 1 \leq w_{_{1}} \leq 100, \\ 1 \leq w_{_{2}} \leq 100, \end{array}
```

starting at the point x = [0.25, 0.25, 0.25].

Note that the semi-infinite constraint is two-dimensional, that is, a matrix.

First, write a file that computes the objective function.

```
function f = myfun(x,s)
% Objective function
f = sum((x-0.2).^2);
```

Second, write a file for the constraints, called mycon.m. Include code to draw the surface plot of the semi-infinite constraint each time mycon is called. This enables you to see how the constraint changes as x is being minimized.

```
function [c,ceq,K1,s] = mycon(X,s)
% Initial sampling interval
if isnan(s(1,1)),
    s = [2 2];
```

Next, invoke an optimization routine.

```
x0 = [0.25, 0.25, 0.25];  % Starting guess
[x,fval] = fseminf(@myfun,x0,1,@mycon)
```

After nine iterations, the solution is

```
x
x =
0.2522 0.1714 0.1936
```

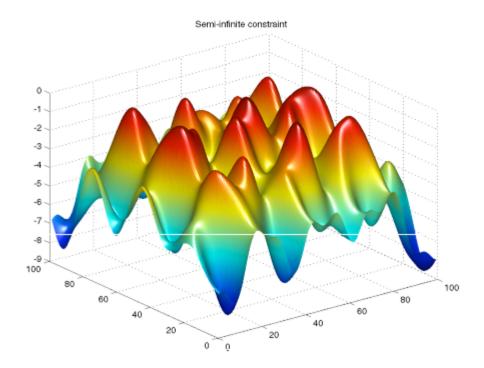
and the function value at the solution is

```
fval
fval =
    0.0036
```

The goal was to minimize the objective f(x) such that the semi-infinite constraint satisfied $K_1(x,w) \le 1.5$. Evaluating mycon at the solution x and looking at the maximum element of the matrix K1 shows the constraint is easily satisfied.

```
[c,ceq,K1] = mycon(x,[0.5,0.5]); % Sampling interval 0.5
max(max(K1))
ans =
    -0.0333
```

This call to mycon produces the following surf plot, which shows the semi-infinite constraint at x.



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Was this topic helpful?

Constrained Nonlinear Optimization Algorithms

Linear Programming Algorithms

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