Nelder-Mead simplex method

Define "norm" to measure length of vectors. Also set up routine to print given number of decimal places.

```
In[218]:= Clear[norm, nn, dp, x];
          norm[x_] = Sqrt[x.x]
          dp = 6;
          nn[x_] := NumberForm[N[x], {20, dp}];
```

Out[219]= $\sqrt{x.x}$

Our standard function, gradient, etc. (actually don't need the Hessian for steepest descent). Added constant 2 to f so values will be positive; makes it easier to compare them.

In[222]:=
```
Clear[f, g, h, x, x1, x2, x3, xi];
f[{x1_, x2_, x3_}] = x1^2 + 2 x2^2 + 3 x3^2 - 1 / (x3 ^2 + 1) + Sin[x1 + 0.9 * x2 + 0.8 * x3] + 2
x = {x1, x2, x3};
g[{x1_, x2_, x3_}] = Map[Function[xi, D[f[x], xi]], x] ;
g[x] // MatrixForm
h[{x1_, x2_, x3_}] = Map[Function[xi, D[g[x], xi]], x] ;
h[x] // MatrixForm
```

Out[223]= $2 + x1^2 + 2\,x2^2 + 3\,x3^2 - \frac{1}{1 + x3^2} + \text{Sin}[x1 + 0.9\,x2 + 0.8\,x3]$

Out[226]//MatrixForm=

$$\begin{pmatrix} 2\,x1 + \text{Cos}[x1 + 0.9\,x2 + 0.8\,x3] \\ 4\,x2 + 0.9\,\text{Cos}[x1 + 0.9\,x2 + 0.8\,x3] \\ 6\,x3 + \frac{2\,x3}{(1+x3^2)^2} + 0.8\,\text{Cos}[x1 + 0.9\,x2 + 0.8\,x3] \end{pmatrix}$$

Out[228]//MatrixForm=

$$\begin{pmatrix} 2 - \text{Sin}[x1 + 0.9\,x2 + 0.8\,x3] & -0.9\,\text{Sin}[x1 + 0.9\,x2 + 0.8\,x3] & -0.8\,\text{Sin}[x1 + 0.9\,x2 + 0.8\,x3] \\ -0.9\,\text{Sin}[x1 + 0.9\,x2 + 0.8\,x3] & 4 - 0.81\,\text{Sin}[x1 + 0.9\,x2 + 0.8\,x3] & -0.72\,\text{Sin}[x1 + 0.9\,x2 + 0.8\,x3] \\ -0.8\,\text{Sin}[x1 + 0.9\,x2 + 0.8\,x3] & -0.72\,\text{Sin}[x1 + 0.9\,x2 + 0.8\,x3] & 6 - \frac{8\,x3^2}{(1+x3^2)^3} + \frac{2}{(1+x3^2)^2} - 0.64\,\text{Sin}[x1 + 0.9 \end{pmatrix}$$

In[229]:=
```
Clear[alpha, beta, gamma, nminit, xinit, printxf, setlsh, ll, ss, hh];
Clear[xh, xc, xe, xi, xu, xl, reflect,
  expand, contractin, contractout, shrink, accept, xx];
Clear[h, s, l];

alpha = 1;
beta = 0.5;
gamma = 2;

nminit[xinit_] := Module[{},
      Clear[x, n, k];
      x = N[xinit];
      n = Length[x] - 1;
      k = 0; printxf;
 ]

printxf := Module[{i},
      Print[k];
      For[i = 1, i ≤ n + 1, i++,
       Print[i, "  ", x[[i]] // nn, "  ", f[x[[i]]] // nn ];
       ]
 ]

sethsl[hh_, ss_, ll_] := Module[{},
      h = hh; s = ss; l = ll;
      xh = x[[h]];
      Print["  xh=", xh // nn, "  fh=", f[ xh ] // nn];
      Print["  xs=", x[[s]] // nn, "  fs=", f[ x[[s]] ] // nn];
      Print["  xl=", x[[l]] // nn, "  fl=", f[ x[[l]] ] // nn];
      xc = (Sum[x[[i]], {i, 1, n + 1}] - xh) / n;
      Print["  xc=", xc // nn];
 ]
```

```
reflect := Module[{},
      xr = xc + alpha * (xc - xh);
       Print["  xr=", xr // nn, "  fr=", f[xr ] // nn];
 ]

expand := Module[{},
      xe = xc + gamma * (xr - xc);
       Print["  xe=", xe // nn, "  fe=", f[xe ] // nn];
 ]

contractout := Module[{},
      xu = xc + beta * (xr - xc);
       Print["  xu=", xu // nn, "  fu=", f[xu ] // nn];
 ]

contractin := Module[{},
      xi = xc + beta * (xh - xc);
       Print["  xi=", xi // nn, "  fi=", f[xi ] // nn];
 ]

shrink := Module[{i},
      xl = x[[l]];
      For[i = 1, i ≤ n + 1, i++,
       x[[i]] = xl + (x[[i]] - xl) / 2;
       ];
      k = k + 1; printxf;
 ]

accept[xx_] := Module[{},
      x[[h]] = xx;
      k = k + 1; printxf;
 ]
```

```
In[244]:= nminit[{ {0, 0, 0}, {1, 0, 0}, {0, 1, 0}, {0, 0, 1} }]
```

```
0

1  {0.000000, 0.000000, 0.000000}  1.000000

2  {1.000000, 0.000000, 0.000000}  2.841471

3  {0.000000, 1.000000, 0.000000}  3.783327

4  {0.000000, 0.000000, 1.000000}  5.217356
```

```
In[245]:= sethsl[4, 3, 1]
```

```
  xh={0.000000, 0.000000, 1.000000}  fh=5.217356

  xs={0.000000, 1.000000, 0.000000}  fs=3.783327

  xl={0.000000, 0.000000, 0.000000}  fl=1.000000

  xc={0.333333, 0.333333, 0.000000}
```

```
In[246]:= reflect
```

```
  xr={0.666667, 0.666667, -1.000000}  fr=6.283245
```

```
In[247]:= contractin

  xi={0.166667, 0.166667, 0.500000}  fi=2.690208

In[248]:= accept[xi]

1

1  {0.000000, 0.000000, 0.000000}  1.000000

2  {1.000000, 0.000000, 0.000000}  2.841471

3  {0.000000, 1.000000, 0.000000}  3.783327

4  {0.166667, 0.166667, 0.500000}  2.690208

In[249]:= sethsl[3, 2, 1]

  xh={0.000000, 1.000000, 0.000000}  fh=3.783327

  xs={1.000000, 0.000000, 0.000000}  fs=2.841471

  xl={0.000000, 0.000000, 0.000000}  fl=1.000000

  xc={0.388889, 0.055556, 0.166667}

In[250]:= reflect

  xr={0.777778, -0.888889, 0.333333}  fr=3.860536

In[251]:= contractin

  xi={0.194444, 0.527778, 0.083333}  fi=2.294048

In[252]:= accept[xi]

2

1  {0.000000, 0.000000, 0.000000}  1.000000

2  {1.000000, 0.000000, 0.000000}  2.841471

3  {0.194444, 0.527778, 0.083333}  2.294048

4  {0.166667, 0.166667, 0.500000}  2.690208

In[253]:= sethsl[2, 4, 1]

  xh={1.000000, 0.000000, 0.000000}  fh=2.841471

  xs={0.166667, 0.166667, 0.500000}  fs=2.690208

  xl={0.000000, 0.000000, 0.000000}  fl=1.000000

  xc={0.120370, 0.231481, 0.194444}

In[254]:= reflect

  xr={-0.759259, 0.462963, 0.388889}  fr=2.558739
```

In[255]:= **accept[xr]**

```
3
1  {0.000000, 0.000000, 0.000000}  1.000000
2  {-0.759259, 0.462963, 0.388889}  2.558739
3  {0.194444, 0.527778, 0.083333}  2.294048
4  {0.166667, 0.166667, 0.500000}  2.690208
```

In[256]:= **sethsl[4, 2, 1]**

```
  xh={0.166667, 0.166667, 0.500000}  fh=2.690208
  xs={-0.759259, 0.462963, 0.388889}  fs=2.558739
  xl={0.000000, 0.000000, 0.000000}  fl=1.000000
  xc={-0.188272, 0.330247, 0.157407}
```

In[257]:= **reflect**

```
  xr={-0.543210, 0.493827, -0.185185}  fr=1.674432
```

In[258]:= **accept[xr]**

```
4
1  {0.000000, 0.000000, 0.000000}  1.000000
2  {-0.759259, 0.462963, 0.388889}  2.558739
3  {0.194444, 0.527778, 0.083333}  2.294048
4  {-0.543210, 0.493827, -0.185185}  1.674432
```

In[259]:= **sethsl[2, 3, 1]**

```
  xh={-0.759259, 0.462963, 0.388889}  fh=2.558739
  xs={0.194444, 0.527778, 0.083333}  fs=2.294048
  xl={0.000000, 0.000000, 0.000000}  fl=1.000000
  xc={-0.116255, 0.340535, -0.033951}
```

In[260]:= **reflect**

```
  xr={0.526749, 0.218107, -0.456790}  fr=2.521252
```

In[261]:= **contractout**

```
  xu={0.205247, 0.279321, -0.245370}  fu=1.692983
```

In[262]:= **accept[xu]**

```
5
1  {0.000000, 0.000000, 0.000000}  1.000000
2  {0.205247, 0.279321, -0.245370}  1.692983
3  {0.194444, 0.527778, 0.083333}  2.294048
4  {-0.543210, 0.493827, -0.185185}  1.674432
```

In[263]:= **sethsl[3, 2, 1]**

```
xh={0.194444, 0.527778, 0.083333}  fh=2.294048
xs={0.205247, 0.279321, -0.245370}  fs=1.692983
xl={0.000000, 0.000000, 0.000000}  fl=1.000000
xc={-0.112654, 0.257716, -0.143519}
```

In[264]:= **reflect**

```
xr={-0.419753, -0.012346, -0.370370}  fr=1.043896
```

In[265]:= **accept[xr]**

```
6
1  {0.000000, 0.000000, 0.000000}  1.000000
2  {0.205247, 0.279321, -0.245370}  1.692983
3  {-0.419753, -0.012346, -0.370370}  1.043896
4  {-0.543210, 0.493827, -0.185185}  1.674432
```

In[266]:= **sethsl[2, 4, 1]**

```
xh={0.205247, 0.279321, -0.245370}  fh=1.692983
xs={-0.543210, 0.493827, -0.185185}  fs=1.674432
xl={0.000000, 0.000000, 0.000000}  fl=1.000000
xc={-0.320988, 0.160494, -0.185185}
```

In[267]:= **reflect**

```
xr={-0.847222, 0.041667, -0.125000}  fr=0.994184
```

In[268]:= **expand**

```
xe={-1.373457, -0.077160, -0.064815}  fe=1.917967
```

In[269]:= **accept[xr]**

```
7
1  {0.000000, 0.000000, 0.000000}  1.000000
2  {-0.847222, 0.041667, -0.125000}  0.994184
3  {-0.419753, -0.012346, -0.370370}  1.043896
4  {-0.543210, 0.493827, -0.185185}  1.674432
```

In[270]:= **sethsl[4, 3, 2]**

```
xh={-0.543210, 0.493827, -0.185185}  fh=1.674432
xs={-0.419753, -0.012346, -0.370370}  fs=1.043896
xl={-0.847222, 0.041667, -0.125000}  fl=0.994184
xc={-0.422325, 0.009774, -0.165123}
```

In[271]:= **reflect**

```
xr={-0.301440, -0.474280, -0.145062}  fr=0.876953
```

In[272]:= **expand**

```
xe={-0.180556, -0.958333, -0.125000}  fe=2.021760
```

In[273]:= **accept[xr]**

```
8

1  {0.000000, 0.000000, 0.000000}  1.000000

2  {-0.847222, 0.041667, -0.125000}  0.994184

3  {-0.419753, -0.012346, -0.370370}  1.043896

4  {-0.301440, -0.474280, -0.145062}  0.876953
```

In[274]:= **sethsl[3, 1, 4]**

```
xh={-0.419753, -0.012346, -0.370370}  fh=1.043896

xs={0.000000, 0.000000, 0.000000}  fs=1.000000

xl={-0.301440, -0.474280, -0.145062}  fl=0.876953

xc={-0.382888, -0.144204, -0.090021}
```

In[275]:= **reflect**

```
xr={-0.346022, -0.276063, 0.190329}  fr=0.987845
```

In[276]:= **accept[xr]**

```
9

1  {0.000000, 0.000000, 0.000000}  1.000000

2  {-0.847222, 0.041667, -0.125000}  0.994184

3  {-0.346022, -0.276063, 0.190329}  0.987845

4  {-0.301440, -0.474280, -0.145062}  0.876953
```

In[277]:= **sethsl[1, 2, 4]**

```
xh={0.000000, 0.000000, 0.000000}  fh=1.000000

xs={-0.847222, 0.041667, -0.125000}  fs=0.994184

xl={-0.301440, -0.474280, -0.145062}  fl=0.876953

xc={-0.498228, -0.236225, -0.026578}
```

In[278]:= **reflect**

```
xr={-0.996456, -0.472451, -0.053155}  fr=1.456316
```

In[279]:= **contractin**

```
xi={-0.249114, -0.118113, -0.013289}  fi=0.732739
```

In[280]:=
```
accept[xi]
```

```
10

1  {-0.249114, -0.118113, -0.013289}  0.732739

2  {-0.847222, 0.041667, -0.125000}  0.994184

3  {-0.346022, -0.276063, 0.190329}  0.987845

4  {-0.301440, -0.474280, -0.145062}  0.876953
```

Best point here is x1. From Newton's method,best point was {-0.403510957,-0.181579931,-0.080964981}. We are sort of in the right neighbourhood, but we have a long way to go!