Chapter 5 Project: Apply Nelder-Mead to the Rheology Problem

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The Rheology Problem

Viscosity of a system

$$\eta(\dot{\gamma}) = \eta_0(1+\lambda^2\dot{\gamma}^2)^{\frac{\beta-1}{2}}$$

A function of the strain rate, $\dot{\gamma}$, with parameters η_0, λ, and β.

TABLE 1.1. Observed data in rheology of polymeric systems

Observation i	Strain rate $\dot{\gamma}_i$ (s^{-1})	Viscosity η_i $(Pa \cdot s)$
1	0.0137	3220
2	0.0274	2190
3	0.0434	1640
4	0.0866	1050
5	0.137	766
6	0.274	490
7	0.434	348
8	0.866	223
9	1.37	163
10	2.74	104
11	4.34	76.7
12	5.46	68.1
13	6.88	58.2

Absolute Error:

$$\epsilon_i(\eta_0,\lambda,\beta) = |\eta_0(1+\lambda^2\dot{\gamma}^2)^{\frac{\beta-1}{2}} - \eta_i|$$

Non-smooth optimization problem:

$$\hat{g}(\eta_0,\lambda,\beta) = \sum_{i=1}^{13} \epsilon_i(\eta_0,\lambda,\beta)$$

Table 1.1 from textbook

Nelder-Mead Algorithm

Given $f : \mathbb{R}^n \mapsto \mathbb{R}$ and the vertices of an initial simplex $\mathrm{Y}^0 = \{\mathrm{y}^0, \mathrm{y}^1, \ldots, \mathrm{y}^n\}$

0. Initialize:
   - $\delta^e, \delta^{oc}, \delta^{ic}, \gamma$ — parameters
   - $k \leftarrow 0$ — iteration counter
1. Order and create centroid:
   - reorder Y^k so $f(y^0) \leq f(y^1) \leq \ldots \leq f(y^n)$
   - set $x^c = \frac{1}{n}\sum_{i=0}^{n-1} y^i$, the centroid of all except the worst point
2. Reflect:
   - test reflection point $x^r = x^c + (x^c - y^n)$
     - if $f(y^0) \leq f(x^r) < f(y^{n-1})$, then accept x^r and goto 1
3. Expand:
   - if $f(x^r) < f(y^0)$, then test expansion point $x^e = x^c + \delta^e(x^c - y^n)$

4a). Outside Contraction:
   - if $f(y^{n-1}) \leq f(x^r) < f(y^n)$, then test outside contraction $x^{oc} = x^c + \delta^{oc}(x^c - y^n)$

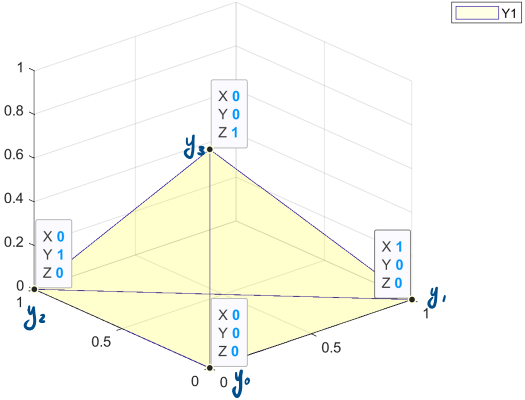
4b). Inside Contraction:
   - if $f(x^r) \geq f(y^n)$, then test inside contraction point $x^{ic} = x^c + \delta^{ic}(x^c - y^n)$

5. Shrink:
   - if all tests fail, then shrink
     $\mathrm{Y}^{k+1} = \{\mathrm{y}^0, \mathrm{y}^0 + \gamma(\mathrm{y}^1 - \mathrm{y}^0), \mathrm{y}^0 + \gamma(\mathrm{y}^2 - \mathrm{y}^0), \ldots, \mathrm{y}^0 + \gamma(\mathrm{y}^n - \mathrm{y}^0)\}$

Algorithm from lecture slides

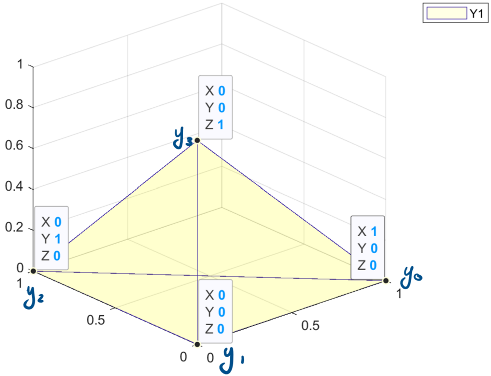
0. Initialize

```
% Question 1a)
Y0a = [0 1 0 0;
       0 0 1 0;
       0 0 0 1];

del_e_s = 2;
del_oc_s = 1/2;
del_ic_s = -1/2;
gamma_s = 0.1;
```



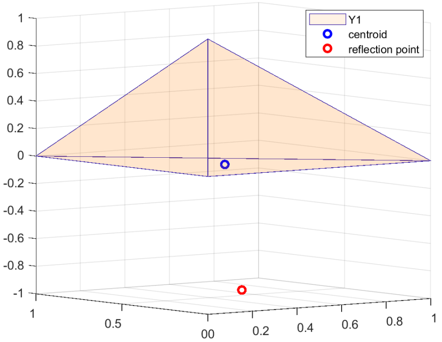
1. Order

```
case 'nonshrink'
    k = length(Yi(1,:));
    for i = k:-1:2
        if fYi(i)< fYi(i-1)
            temp = Yi(:,i-1);
            Yi(:,i-1) = Yi(:,i);
            Yi(:,i) = temp;

            tempf = fYi(i-1);
            fYi(i-1) = fYi(i);
            fYi(i) = tempf;
        else
            break;
        end
    end
case 'shrink'
    for i = 2:k
        key = Yi(:,i);
        fkey = fYi(i);
        j = i-1;
        while ((j>= 1) && (fkey < fYi(j)))
            Yi(:,j+1) = Yi(:,j);
            fYi(j+1) = fYi(j);
            j = j -1;
        end
        Yi(:,j+1) = key;
        fYi(j+1) = fkey;
    end
```



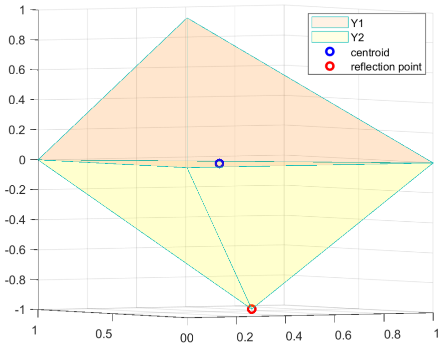
1 and 2. Calculate centroid and x^r

```
%CALCULATE CENTROID%
xc = zeros(k - 1,1);
for i = 1:k-1
    xc = xc + Yk(:,i);
end
xc = (1/(k-1)).*xc;

%CALCULATE REFLECTION POINT%
xr = xc + (xc - Yk(:,k));
fr = f(xr);
feval = feval + 1;
```



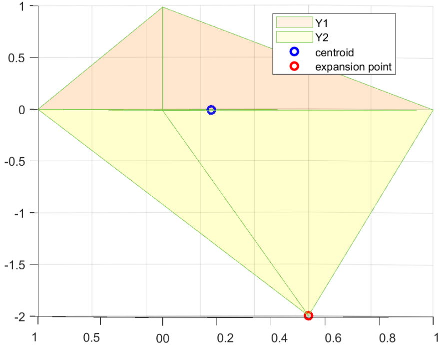
2. Reflect

```
%REFLECTION STEP%
if (f_store(1) <= fr)&&(fr < f_store(k-1))
    %disp("ref")
    Yk(:,k) = xr;
    f_store(k) = fr;
    stepComputed = "nonshrink";
```



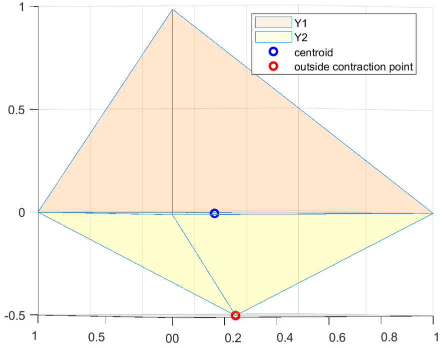
3. Expand

```
%EXPANSION%
elseif (fr < f_store(1))
    %disp("exp")
    xe = xc + del_e*(xc - Yk(:,k));
    fe = f(xe);
    feval = feval + 1;
    if fe < fr
        Yk(:,k) = xe;
        f_store(k) = fe;
    else
        Yk(:,k) = xr;
        f_store(k) = fr;
    end
    stepComputed = "nonshrink";
```



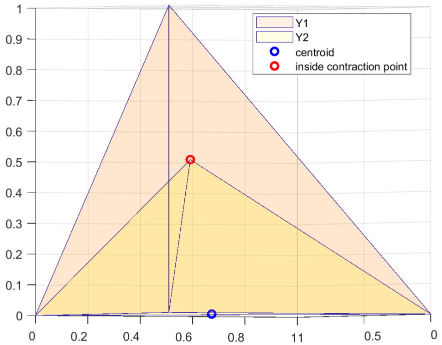
4.a) Outside Contraction

```
%OUTSIDE CONTRACTION%
elseif (f_store(k-1) <= fr)&&(fr < f_store(k))
    xoc = xc + del_oc*(xc - Yk(:,k));
    foc = f(xoc);
    feval = feval + 1;
    stepComputed = "nonshrink";
    if foc < fr
       % disp("oc")
        Yk(:,k) = xoc;
        f_store(k) = foc;
        stepComputed = "nonshrink";
    else
        %disp("ocref")
        Yk(:,k) = xr;
        f_store(k) = fr;
        stepComputed = "nonshrink" ;
    end
```



4.b) Inside Contraction

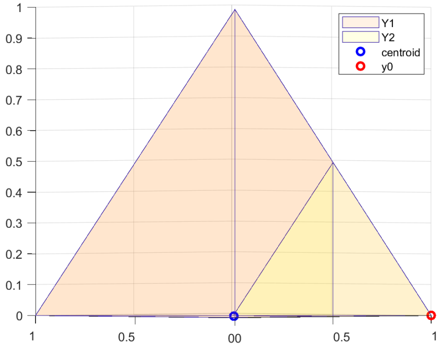
```
%INSIDE CONTRACTION%
elseif (fr >= f_store(k))
    xic = xc + del_ic.*(xc - Yk(:,k));
    fic = f(xic);
    feval = feval + 1;
    if fic < f_store(k)
       % disp("ic")
        Yk(:,k) = xic;
        f_store(k) = fic;
        stepComputed = "nonshrink";
```



5. Shrink

```
%SHRINK%
else
    % disp("shrink")
    for i = 2:k
        Yk(:,i) = (1-gamma).*Yk(:,1) + gamma.*Yk(:,i);
        f_store(i) = f(Yk(:,i));
        feval = feval + 1;
    end
    stepComputed = "shrink";
    [Yk,f_store] = sortSimplex(Yk,f_store,stepComputed);
end
```

```
    case 'shrink'
        for i = 2:k
            key = Yi(:,i);
            fkey = fYi(i);
            j = i-1;
            while ((j>= 1) && (fkey < fYi(j)))
                Yi(:,j+1) = Yi(:,j);
                fYi(j+1) = fYi(j);
                j = j -1;
            end
            Yi(:,j+1) = key;
            fYi(j+1) = fkey;
        end
```



Examples of Nelder-Mead at work

The Rheology Problem: Revisited

1. Standard parameters

Here is the code we gave to NM to run the standard parameters

Here is the simplex and function values we obtained by running NM on the standard parameters

2. New parameters

We proposed new parameters using grid search on the parameter space

Here is the code we gave to NM to run the new parameters

Here is the simplex and function values we obtained by running NM on our new parameters

The Rheology Problem: Revisited

Here is our convergence plot code

Here is our convergence plot of all the cases