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:

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

(Audet and Hare, 2017)

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 $x^{oc} = x^c + \delta^{oc}(x^c - y^n)$

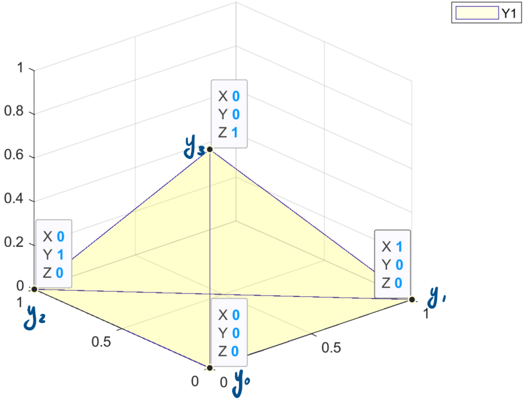
4b). Inside Contraction:
   - if $f(x^r) \geq f(y^n)$, then test inside contraction point $x^{ic} = x^c + \delta^{ic}(x^c - y^n)$

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

(Math 462, UBCO, 2020)

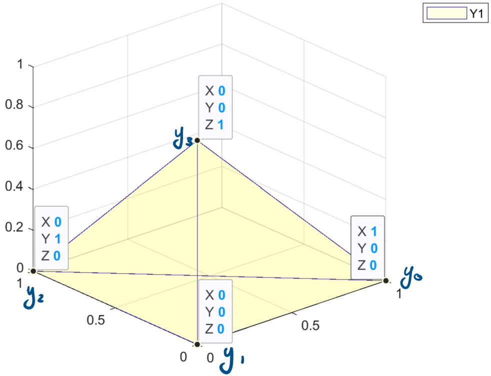
0. Initialize

```
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 = 1/2;
```



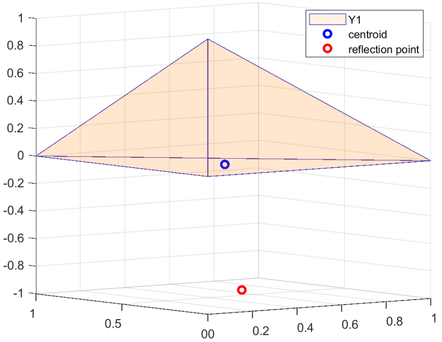
1. Order

```
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
```



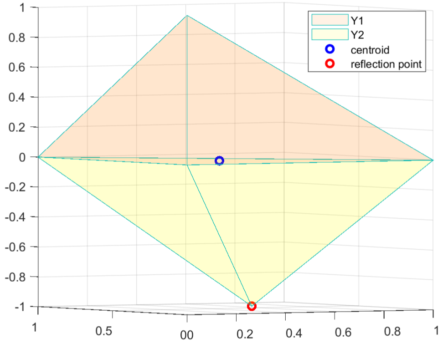
1 and 2. Calculate centroid and x^r

```
%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;
```



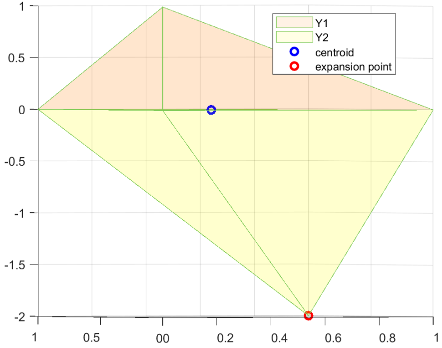
2. Reflect

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



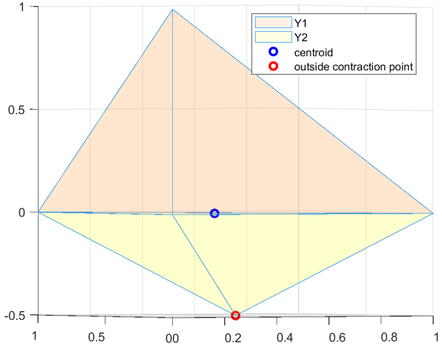
3. Expand

```
%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";
```



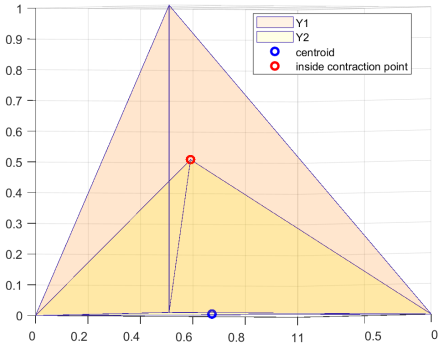
4.a) Outside Contraction

```
%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

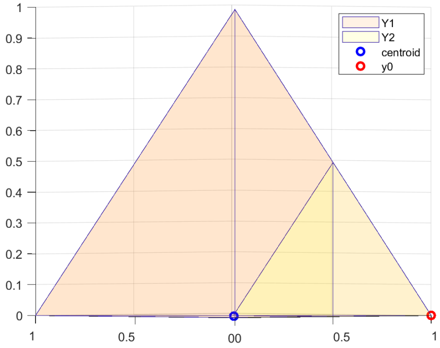
```
%INSIDE CONTRACTION%
elseif (fr >= f_store(k))
    xic = xc + del_ic.*(xc - Yk(:,k));
    fic = f(xic);
    feval = feval + 1;
    if fic < f_store(k)
       % disp("ic")
        Yk(:,k) = xic;
        f_store(k) = fic;
        stepComputed = "nonshrink";
```



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
```

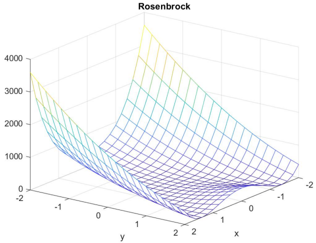


Examples of Nelder-Mead at work: A nice example

plot of a nice function goes here

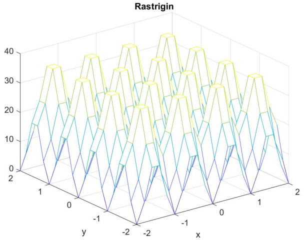
put a convergence plot here and the min that we observe vs what our NM code takes us to

Examples of Nelder-Mead at work: Rosenbrock function



put a convergence plot here and the min that we observe vs what our NM code takes us to

Examples of Nelder-Mead at work: Rastrigin function



put a convergence plot here and the min that we observe vs what our NM code takes us to

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