MATH604 - Assignment 4 - Deepak Kumar, 73217151

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Q 5.2→ Provide a breakdown of how many function evaluations Nelder-mead will use during a given iteration.

Ans 5.2→ For reordering, we will have n(number of dimensions)+1 function evaluations (which can be reduced to just one/zero if we use function values from last iteration). After this we have one more evaluation at the reflected point and then upon comparing with f^k_{best}, f^{y-1} & f^k_{worst}, the following cases will give rise to following number of function evaluations.

if $f^k_{best} \le f^r < f(y^{n-1})$, no more evaluation

if (expansion, inside and outside contraction), one more function evaluation.

if shrink step occurs and we are not computing at the time of reordering then n more function evaluation.

Q 5.3→

Sol. 5.3 → let $Y^k = \{y^0, y^1, y^2\}$ such that $y^i \in \mathbb{R}^2$, then the Centroid point x^c would be,

$$x^c = \frac{1}{2}(y^0 + y^1),$$

Now, if $f(x^c)$ lies between $f(y^0)$ and $f(y^1)$ then $Y^{k+1} = \{y^0, x^c, y^1\}$, which is not a simplex as y^0, x^c, y^1 lie on the same line.

Q 5.6

Sol. 5.6 → $Y^k = \{y^0, y^1, \ldots, y^3\} \subseteq \mathbb{R}^n$, where

$$y^0 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \quad y^1 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad y^2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \quad y^3 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

If non shrink step occurs,

$y^{0+} = y^0$, $y^{1+} = y^1$, $y^{2+} = y^2$, $y^{3+} = x^c + \delta(x^c - y^3)$ where $\delta \in \{\delta^r, \delta^e, \delta^{ic}, \delta^{oc}\}$,

$x^c = \frac{1}{n}\sum_{1}^{n-1} y^i$, $y^i \in Y$ and, $\delta^r = 1$, $\delta^e \in (1, \infty)$

$x^c = \frac{1}{n}\sum_i y^i$, $y^i \in Y$ and $\delta^r = 1$, $\delta^e \in (1,\infty)$

$\delta^{ic} \in (-1,0)$, $\delta^{oc} \in (0,1)$

Now, $x^c = \frac{1}{3} \times \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}$

So, $$y^{3t} = \frac{1}{3}\begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} + \delta\left(\frac{1}{3}\begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} - \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}\right)$$

$$= \begin{bmatrix} 0 \\ 1/3 \\ 1/3 \end{bmatrix} + \delta\begin{bmatrix} -1 \\ -2/3 \\ -2/3 \end{bmatrix}$$

If shrink step occurs,

$y^{0t} = y^0$, $y^{1t} = y^0 + \gamma(y^1 - y^0)$, $y^{2t} = y^0 + \gamma(y^2 - y^0)$, $y^{3t} = y^0 + \gamma(y^3 - y^0)$

where $\gamma \in (0,1)$

So,

$$Y^{k+1} = \left\{ \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \gamma\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \gamma\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \gamma\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \right\}.$$

Q 5.7 →

Ans 5.7 → $Y^k = \{$ [illegible]

Ans 5.7 → $Y^k = \{ y^0, y^1, y^2, y^3 \} \subseteq \mathbb{R}^3$,

$$y^0 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \quad y^1 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad y^2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \quad y^3 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

For reflection,

$$y^{3t} = x^c + (x^c - y^3)$$

$$= \frac{1}{3} \cdot \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} + \begin{bmatrix} 0 \\ 1/3 \\ 1/3 \end{bmatrix} - \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$= \begin{bmatrix} -1 \\ -1/3 \\ -1/3 \end{bmatrix}$$

hence,

$$Y^{k+1} = \left\{ y^0, y^1, y^2, \begin{bmatrix} -1 \\ -1/3 \\ -1/3 \end{bmatrix} \right\}$$

Now, for $\mathrm{Vol}(Y^k)$,

$$\det(L) = \begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \end{vmatrix}$$

$$\det(C) = \begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{vmatrix}$$

$$= -1.$$

$$\mathrm{Vol}(\gamma) = \frac{|-1|}{3!} = 1/6$$

$$\mathrm{diam}(\gamma) = \sqrt{1^2+1^2} = \sqrt{2}$$

hence, $\mathrm{Von}(\gamma) = \dfrac{\mathrm{Vol}(\gamma)}{(\mathrm{diam}(\gamma))^n} = \dfrac{1}{6} \times \dfrac{1}{2\sqrt{2}}$

for $\mathrm{Von}(\gamma^{k+1})$ after reflection step,

$$\det(C^+) = \begin{vmatrix} 0 & 0 & -1 \\ 0 & 1 & -1/3 \\ 1 & 0 & -1/3 \end{vmatrix} = 1$$

$$\mathrm{Vol}(\gamma^{k+1}) = \frac{|1|}{3!} = 1/6$$

$$\mathrm{diam}(\gamma^{k+1}) = \sqrt{1^2+1^2} = \sqrt{2}$$

hence, $\text{Von}(\gamma^{k+1}) = \dfrac{\text{Vol}(\gamma^{k+1})}{(\text{diam}(\gamma^{k+1}))^n} = \dfrac{1}{6} \times \dfrac{1}{2\sqrt{2}}$

hence, After reflection step, $\text{Von}(\gamma^k)$ is same as $\text{Von}(\gamma^{k+1})$.

Q2.15→

2.15→ (a) $\text{Conv}(\{(0,0,0), (0,0,1), (0,1,0), (1,0,0)\})$

Sol. (a)

$$L = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

$\det(L) = -1$, $\quad \text{vol}(\gamma) = \dfrac{|-1|}{3!} = 1/6$, hence a normal simplex.

$\text{diam}(\gamma) = \sqrt{1+1} = \sqrt{2}$

$\text{Von}(\gamma) = \dfrac{\text{Vol}(\gamma)}{(\text{diam}(\gamma))^n} = \dfrac{1}{6} \times \dfrac{1}{2\sqrt{2}}$

(b) $\text{Conv}(\{(4,0,1), (0,0,1), (0,0,5), (0,4,1)\})$.

Sol. (b) $L = \begin{bmatrix} -4 & -4 & -4 \end{bmatrix}$

Sol.(b) $L = \begin{bmatrix} -4 & -4 & -4 \\ 0 & 0 & 4 \\ 0 & +4 & 0 \end{bmatrix}$

$\det(L) = 64$

$\text{Vol}(\gamma) = \frac{64}{6} = \frac{32}{3}$, hence a simplex.

$\text{diam}(\gamma) = \sqrt{16+16+0} = \sqrt{32} = 4\sqrt{2}$

$\text{Von}(\gamma) = \frac{\text{Vol}(\gamma)}{(\text{diam}(\gamma))^n} = \frac{32}{3} \times \frac{1}{(4\sqrt{2})^3}$

(c) $\text{Conv}(\{(2,2,2),(3,1,4),(2,4,-6),(4,-1,6)\})$

Sol. (c) $L = \begin{bmatrix} 1 & 0 & 2 \\ -1 & 2 & -3 \\ 2 & -8 & 4 \end{bmatrix}$

$$\det(L) = 1(8-24) + 2(8-4)$$
$$= -16 + 2(4)$$
$$= -8$$

$\text{Vol}(\gamma) = \frac{|-8|}{6} = \frac{8}{6} = \frac{4}{3}$, hence a simplex.

$$\mathrm{Vol}(Y) = \frac{|-8|}{3!} = \frac{8}{6} = \frac{4}{3}$$, hence a simplex.

$$\mathrm{diam}(Y) = \sqrt{(4-2)^2 + (4+1)^2 + (6-(-6))^2} = 13.1529$$

$$\mathrm{Von}(Y) = \frac{\mathrm{Vol}(Y)}{(\mathrm{diam}(Y))^n} = \frac{4}{3} \times \frac{1}{(13.1529)^3}$$

Q2.16 → Let $Y = \{y^0, y^1, \dots, y^n\}$ form a simplex. Prove $\overline{\mathrm{diam}}(Y) \le \mathrm{diam}(Y) \le 2\,\overline{\mathrm{diam}}(Y)$

Sol. 2.16 → Since,

$$\overline{\mathrm{diam}}(Y) = \max\{\, \|y^i - y^0\| \mid y^i \in Y \}$$

$$\mathrm{diam}(Y) = \max_{i \ne j}\{\, \|y^i - y^j\| \mid y^i \in Y \}$$

let p, q be the farthest points, then

$\overline{\mathrm{diam}}(Y)$ will be either $\|p - y^0\|$ or $\|q - y^0\|$, hence,

$$\overline{\mathrm{diam}}(Y) \le \mathrm{diam}(Y)$$ [Equality arises when either p or q is y^0]

Now, we need to verify the inequality,

Now, we need to verify the inequality,

$$\operatorname{diam}(\gamma) \leq 2\, \overline{\operatorname{diam}(\gamma)}$$

$\Rightarrow \|p - q\| \leq 2\, \|p - y^0\|$ [let p be the point farthest to y^0]

$\Rightarrow \|2(p - y^0)\| - \|p - q\| \geq 0$

By using triangular inequality, we get

$\Rightarrow \|2(p - y^0) - (p - q)\| \geq \|2(p - y^0)\| - \|p - q\| \geq 0$

$\Rightarrow \|2p - 2y^0 - p + q\| \geq 0$

$\Rightarrow \|p + q - 2y^0\| \geq 0$

hence proved (equality occurs when $y^0 = \frac{1}{2}(p+q)$).