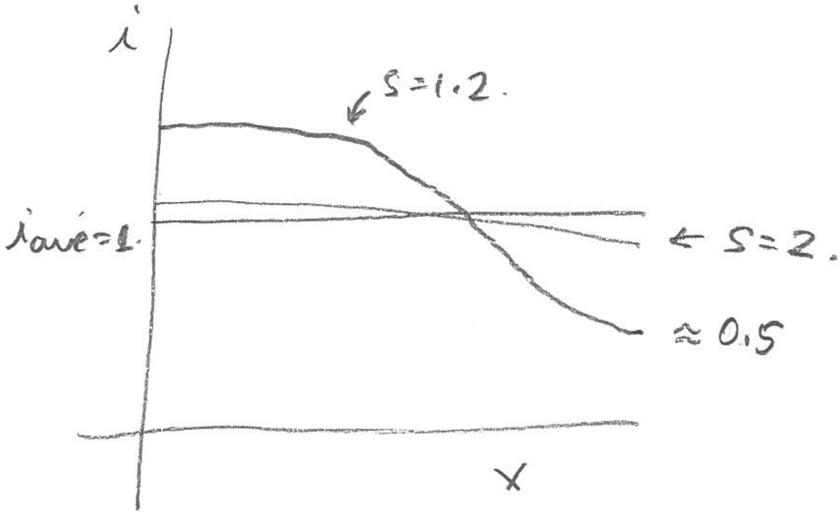
Mathematical Modelling of Fuel Cells
Mini-course, part III.

Unit cell model implemented - code will be posted. Results of Exercise 4:

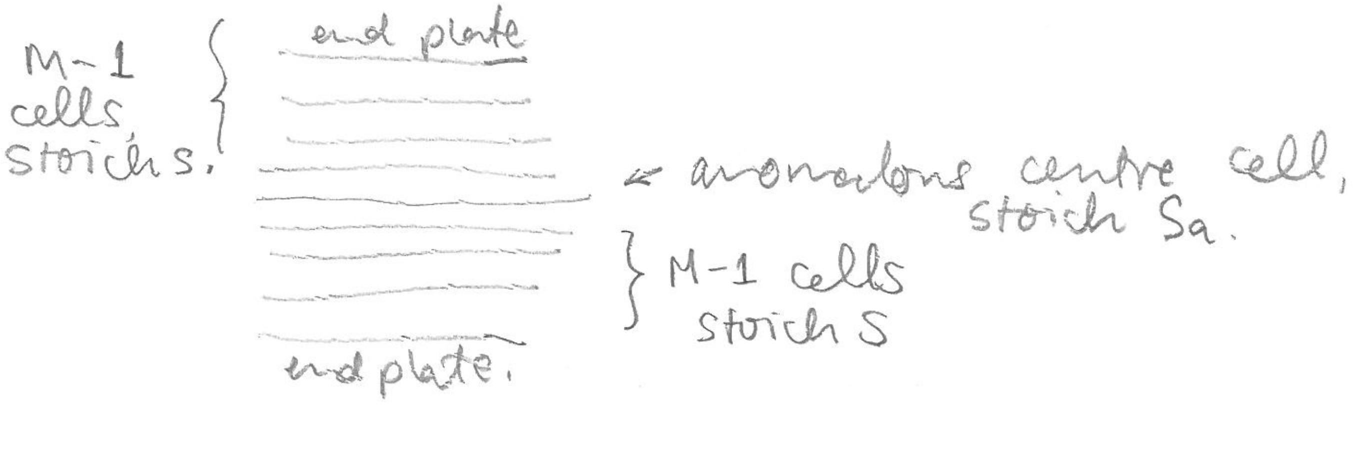
S	U
2.0	0.6450
1.5	0.6351
1.2	0.6105
1.1	0.5660



Solution exists for $S=1.06$ but not for $S=1.05$
Computational picture next page.

Further notes on the stack level model described in part II of the notes:

- The larger value $\lambda=100$ is consistent with the rest of the units in the model.
- In order to make sense of the stack model results, let us consider the effect of one anomalous cell in the stack. For simplicity, let's consider $2M-1$ cells with an anomalous centre cell



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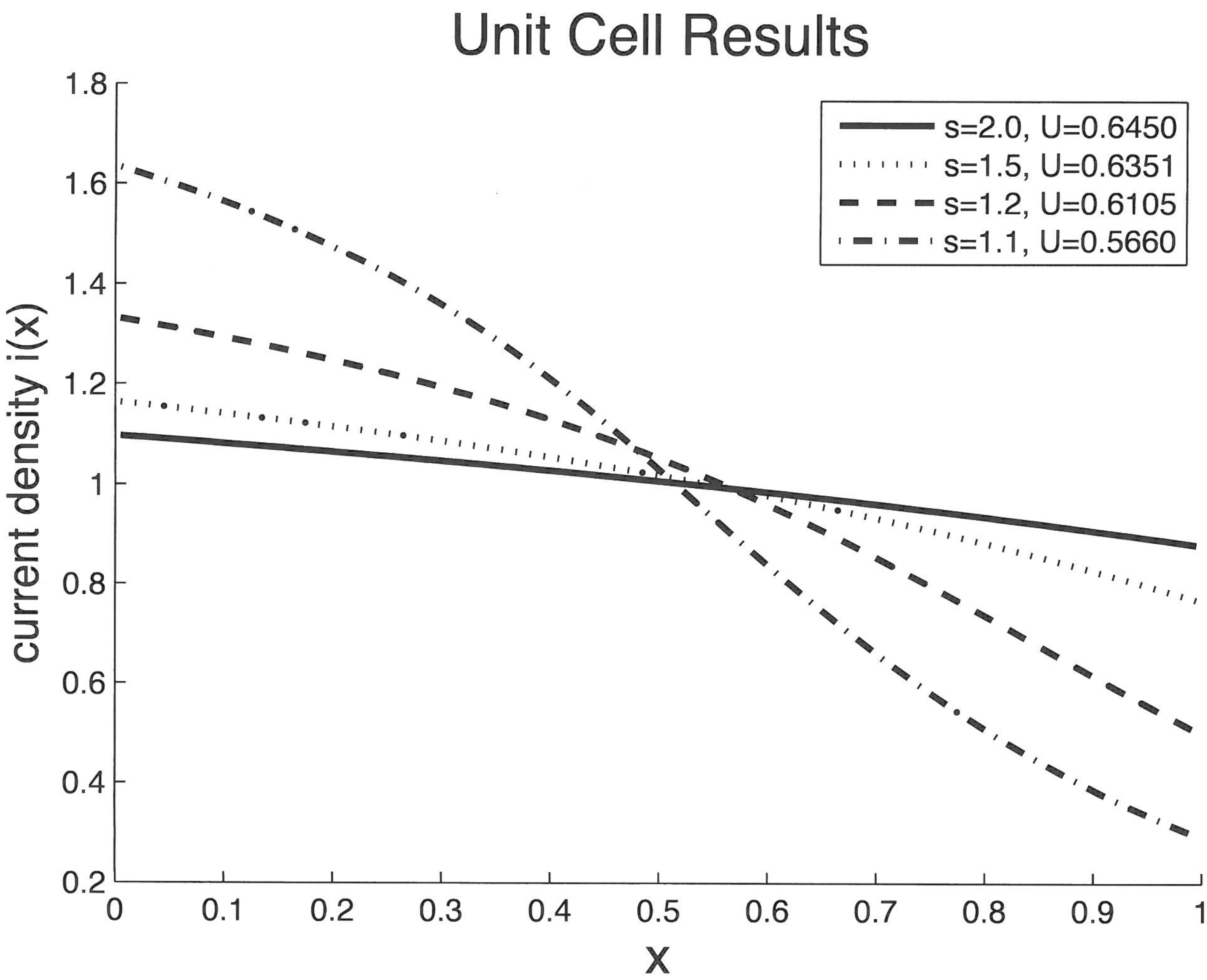

Unit Cell Results
s=2.0, U=0.6450
s=1.5, U=0.6351
s=1.2, U=0.6105
s=1.1, U=0.5660
current density i(x)
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
X

In this situation, symmetry can reduce the computation to M cells with a symmetry condition on the anomalous cell instead of an end-plate one.

- Starting with the base unit cell solution with stoich s obtained with the unit cell code, we could do continuation in the anomalous stoich $s + \theta(s_a - s)$.

<u>Exercise 15</u> Derive the symmetry condition for the anomalous centre cell stack model.

<u>Anomalous centre cell stack model results:</u>

Stack model implemented - code will be posted. Some results for $M = 7$, $s = 2$, $s_a = 1.2$ are shown on the next pages for $\lambda = 100$.

Note that as $M \to \infty$ or $\lambda \to 0$, $i_M(x)$ will approach $i(x)$, the unit cell current of the unit cell at base conditions s.

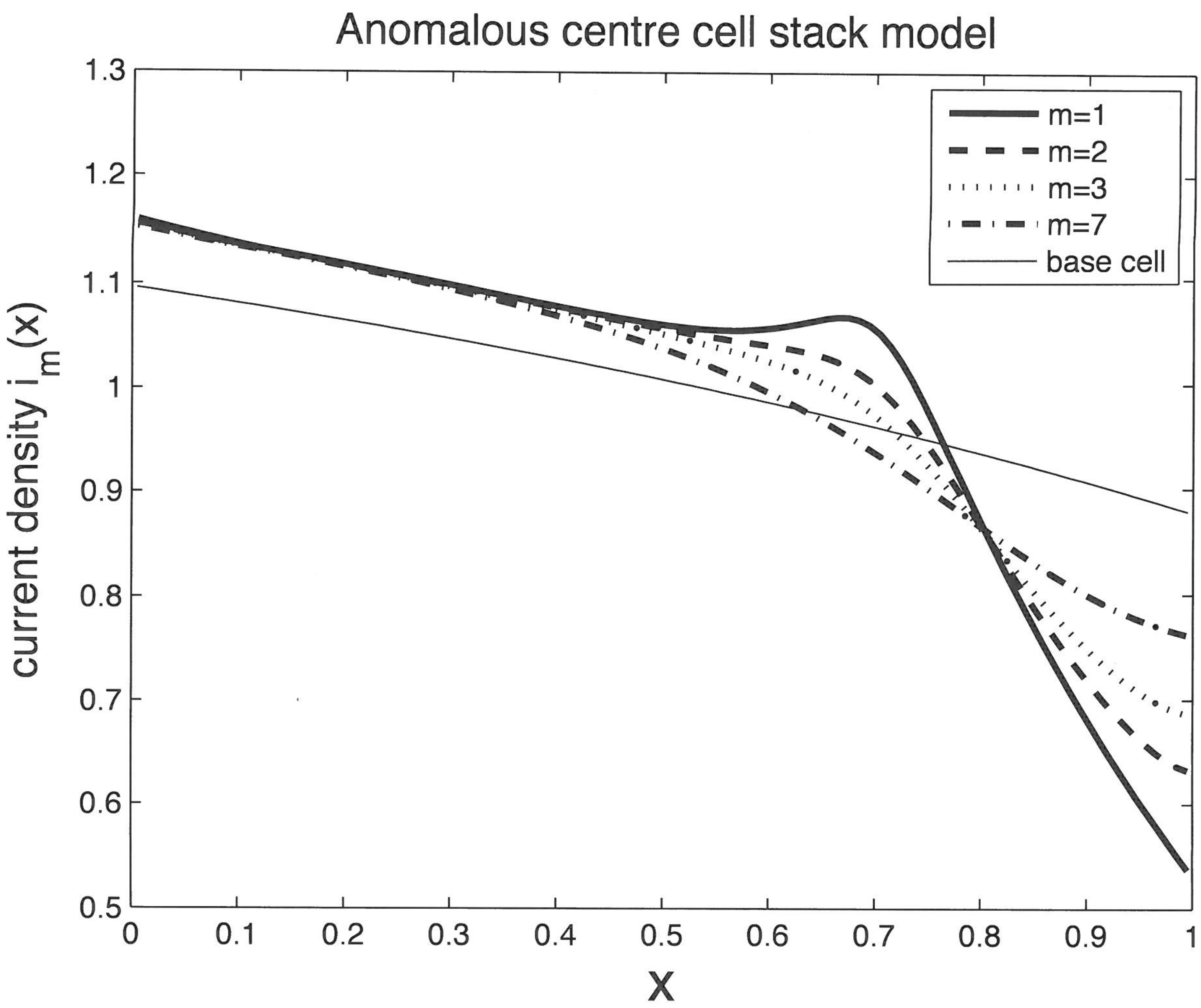
For $\lambda = 0$, stack voltage is

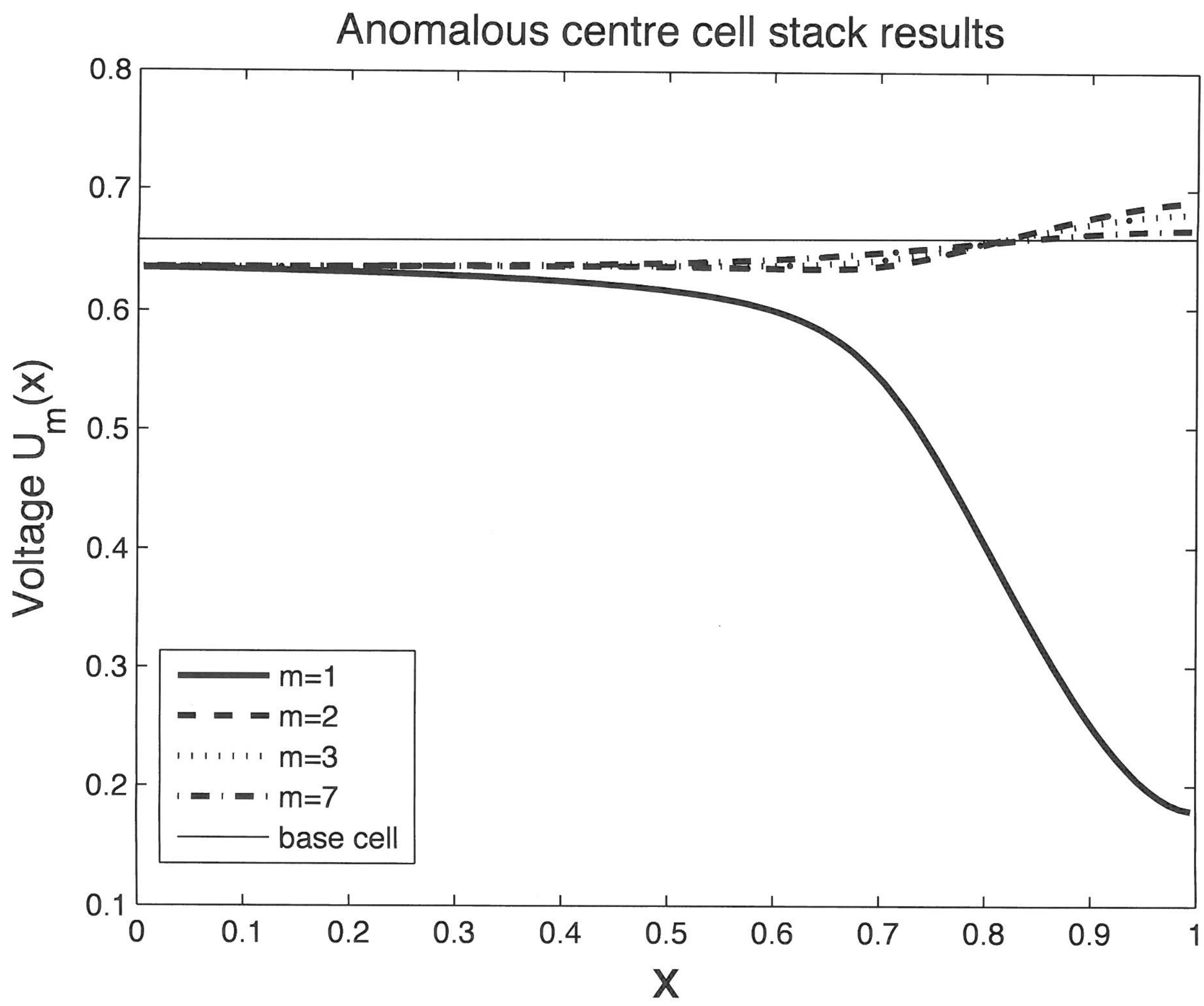
$$V = \underset{\substack{\uparrow \\ \text{anomalous conditions} \\ \text{in unit cell}}}{U(s_a)} + 2(M-1)\,U(s) \quad \nwarrow \text{base cell results}$$

With $M = 7$, $s = 2$, $s_a = 1.2$,

	$V = 8.3505$	$\lambda = 0$
bipolar plate resistance $\longrightarrow$	$V = 8.3451$	$\lambda = 1$
increases losses due to	$V = 8.3253$	$\lambda = 10$
anomalous cells.	$V = 8.2746$	$\lambda = 100$

<u>Exercise 16</u> Show analytically that the stack voltage in the anomalous centre cell stack model decreases with λ.


Anomalous centre cell stack model
current density $i_m(x)$
x
m=1
m=2
m=3
m=7
base cell
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1.1
1.2
1.3



Anomalous centre cell stack results
Voltage U_m(x)
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
X
m=1
m=2
m=3
m=7
base cell

Consider now the anomalous centre cell stack model in an idealized setting to try and gain some analytical understanding.

$$\frac{d^2 U_m}{dx^2} - \lambda \left(i_{m-1} - 2 i_m + i_{m+1} \right) = 0 \qquad (1).$$

Consider a linearized version of $i(U)$, neglecting channel concentration variations.

$$-A \left(i_m - i_{ave} \right) = U_m - U \qquad (2)$$

base cell voltage

Resistivity, $A = R_m = 0.1\ \Omega\text{-cm}^2$ if we ignore electrochemical effects. Now make the Ansatz

$$U_m - U = \sum_{n=1}^{\infty} f_n \phi_n(x)\, G_n^m$$

$$\phi_n'' + W\left(G_n - 2 + \frac{1}{G_n}\right)\phi_n, \quad W = \frac{\lambda}{A} \text{ Wagner number.}$$

$$\phi_n'(0) = \phi_n'(1) = 0.$$

$$\phi_n(x) = \cos n\pi x.$$

$$W\left(G_n - 2 + \frac{1}{G_n} \right) = n^2 \pi^2 \qquad (3)$$

$$G_n = \frac{b \pm \sqrt{b^2 - 4}}{2} \quad \text{where} \quad b = 2 + \frac{n^2\pi^2}{W}.$$

Note from (3) that roots come in reciprocal pairs. Consider $m > 0$, we would want $G_n^m \to 0$ as $m \to \infty$, so take the root of (3) with $|G_n| < 1$. Consider the $n = 1$ root, this will have the slowest decay with m.

$$G = 1 + \frac{\pi^2}{2W} - \sqrt{\left(1 + \frac{\pi^2}{2W}\right)^2 - 1}$$

For $A = 0.1$, $\lambda = 100$, $(W = 1000)$

$G \approx 0.90$, $G^7 \approx 0.50$.

$\lambda = 10$, $G \approx 0.73$, $G^7 \approx 0.11$.

This does not solve the linearized anomalous centre cell stack problem (c_n not determined) but does give an estimate on the characteristic number of adjacent cells affected by an anomaly.