Boundary value problems

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Today's outline

1. Solution techniques in Excel
   - Solver and goal-seek
2. Boundary value problems

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Solver and goal-seek

Excel comes with a goal-seek and solver function. For Excel 2010:

- Install via Excel ⇒ File ⇒ Options ⇒ Add-Ins ⇒ Go (at the bottom) ⇒ Select solver add-in. You can now call the solver screen on the 'data' menu ('Oplosser' in Dutch)
- Select the goal-cell, and whether you want to minimize, maximize or set a certain value
- Enter the variable cells; Excel is going to change the values in these cells to get to the desired solution
- Specify the boundary conditions (e.g. to keep certain cells above zero)
- Click 'solve' (possibly after setting the advanced options).

Goal-seek: a simple example

Goal-Seek can be used to make the goal-cell to a specified value by changing another cell:

- Open Excel and type the following:

	A	B
1	x	3
2	f(x)	=–3*B1^2–5*B1+2
3		

- Go to Data ⇒ What-If Analysis ⇒ Goal Seek...
  - Set cell: B2
  - To value: 0
  - By changing cell: B1
- OK. You find a solution of 0.333 . . ..

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Solver: a simple example

The solver is used to change the value in a goal-cell, by changing the values in 1 or more other cells while keeping boundary conditions:

- Use the following sheet:

	A	B	C
1		x	f(x)
2	x1	3	=2*B2*B3–B3+2
3	x2	4	=2*B3–4*B2-4

- Go to Data ⇒ Solver
  - Goalfunction: C1 (value of: 0)
  - Add boundary condition: C2 = 0
  - By changing cells: $B$1:$B$2 (you can just select the cells)
- Solve. You will find B1=0 and B2=2.

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Exercise

Use Excel functions to obtain the Antoine coefficients A, B and C for carbon monoxide following the equation:

$$\ln P = A - \frac{B}{T + C}$$

P in Pa, T in K. Experimental data is given:

P [mmHg]	T [°C]
1	-222.0
5	-217.2
10	-215.0
20	-212.8
40	-210.0
60	-208.1
100	-205.7
200	-201.3
400	-196.3
760	-191.3

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2. Convert all values to proper units (hint: use e.g. =CONVERT(A2,"mmHg","Pa"))

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What is an ODE?

- Algebraic equation:

$$f(y(x), x) = 0 \qquad \text{e.g.} \; -\ln(K_{eq}) = (1-\zeta)$$

- First order ODE:

$$f\left(\frac{dy}{dx}(x), y(x), x\right) = 0 \quad \text{e.g.} \; \frac{dc}{dt} = -kc^n$$

- Second order ODE:

$$f\left(\frac{d^2y}{dx^2}(x), \frac{dy}{dx}(x), y(x), x\right) = 0 \quad \text{e.g.} \quad \mathcal{D}\frac{d^2c}{dx^2} = -\frac{kc}{1+Kc}$$

About second order ODEs

Very often a second order ODE can be rewritten into a system of first order ODEs (whether it is handy depends on the boundary conditions!)

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In general

Consider the second order ODE:

$$\frac{d^2y}{dx^2} + q(x)\frac{dy}{dx} = r(x)$$

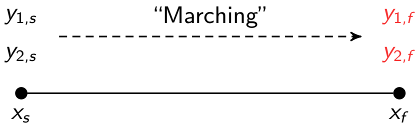
Now define and solve using z as a new variable:

$$\frac{dy}{dx} = z(x)$$
$$\frac{dz}{dx} = r(x) - q(x)z(x)$$

Importance of boundary conditions

The nature of boundary conditions determines the appropriate numerical method. Classification into 2 main categories:

- *Initial value problems (IVP)*
  We know the values of all y_i at some starting position x_s, and it is desired to find the values of y_i at some final point x_f.



- *Boundary value problems (BVP)*
  Boundary conditions are specified at more than one x. Typically, some of the BC are specified at x_s and the remainder at x_f.