

Survey of Applied Mathematics Techniques

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Lecture 3

Modelling, Scaling, and Nonlinear Problems

3.1 Introduction

We have seen the problem A in the previous two lectures: to find $u(x)$ that satisfies

$$-u'' + au = f(x) \tag{3.1}$$

when f and $a \geq 0$ are given. Notice that there are no units in the equation above, all quantities are dimensionless. This type of boundary value problem can come from many types of applications and we will see two examples below. We will start with simple descriptions of the basic Physics behind the models, write down equations that describe the Physics, scale the independent and dependent variables to derive dimensionless equations, and then use the relative size of terms to simplify the equations to the form of problem A above.

In a final section of the notes for this lecture, we will review Newton's method for solving nonlinear systems of equations and apply the ideas to Finite Difference approximation of a simple nonlinear variant of Problem A.

3.2 Thermal Model

3.2.1 Physics I: temperature variations in time

Consider thermal energy (heat) applied to an object and its resulting temperature increase. Some quantities that will come into play in the model are

Volume V : of the object in m^3 .

Density ρ : of the material the object is made of in kg m^{-3} .

Specific Heat Capacity c : of the material the object is made of in $\text{J kg}^{-1} \text{K}^{-1}$

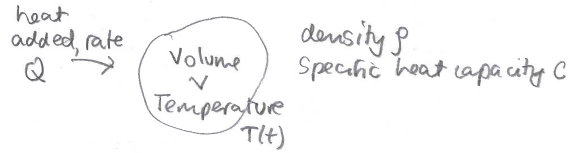


Figure 3.1: Heating up a rock.

K: degrees Kelvin

J: Joule, unit of energy $\text{kg m}^2 \text{s}^{-2}$

Rate of Heat Energy Applied Q : in W.

W: Watt, unit of power J s^{-1}

Temperature $T(t)$: of the object in K.

Time t : in s.

Here ρ and c are material parameters that you can find values of in the literature for your material, V is from the size of your object and Q is the heat you are applying. Assuming $Q > 0$ the object should be increasing in temperature according to the relationship

$$\rho c V \frac{dT}{dt} = Q. \quad (3.2)$$

Note that an important check when writing down a model equation is to *check that the units match*. On the right we have Watts. On the left we have

$$\frac{\text{kg}}{\text{m}^3} \frac{\text{J}}{\text{kgK}} \text{m}^3 \frac{\text{K}}{\text{s}} = \frac{\text{J}}{\text{s}} = \text{W} \quad \text{check!}$$

Checking units is the easiest way to find errors in your model equations. Looking at the units also helps you somewhat in the understanding of the processes you are modelling. Equation (3.2) is often written as

$$\rho c \frac{dT}{dt} = Q/V := q \quad (3.3)$$

where q is the volumetric applied heating, with units W/m^3 .

3.2.2 Physics II: internal heat flux

If a flat object with area A and thickness L has a temperature T_0 applied on the left and $T_1 < 0$ on the right, and left to come to equilibrium, the temperature

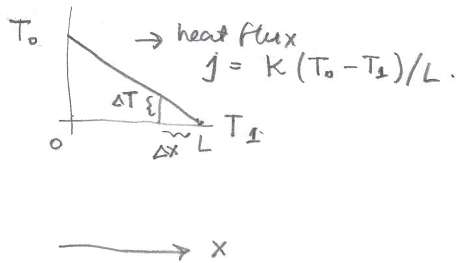


Figure 3.2: Heat flux due to temperature differences.

will vary linearly through the object from one side to the other and there will be a heat transfer of

$$Q = \kappa A(T_0 - T_1)/L$$

to the right, where κ is a material parameter called the thermal conductivity, with units of $W/(mK)$, giving Q with units of W (check!). Taking limits as $\Delta x \rightarrow 0$ as shown in Figure 3.2 gives

$$-\kappa \frac{\partial T}{\partial x} = Q/A := j \quad (3.4)$$

where j is the heat flux (heat transfer per unit area). If $T(x, y, z)$ then \mathbf{j} is a vector given by

$$\mathbf{j} = -\kappa \nabla T.$$

The interpretation of \mathbf{j} is that if you chose a unit vector \hat{n} and a point \mathbf{x} , then $\mathbf{j} \cdot \hat{n}$ is the local heat flux at that point in the direction \hat{n} .

At this stage look back and make sure you understand the difference between *heat* (units of W , Watt), *volumetric heating* (W/m^3), and *heat flux* (W/m^2).

3.2.3 Physics III = I+II

Now let us consider an object that has temperature that varies in time and space. For simplicity, let us consider one dimensional variations $T(x, t)$. Consider Figure 3.3. The volume of the slab depicted is $A\Delta x$. The net heat transfer into the slab is

$$A(j(x) - j(x + \Delta x))$$

which when converted into a volumetric heat flux is

$$(j(x) - j(x + \Delta x))/\Delta x.$$

This heating can be put into (3.3) to give

$$\rho c \frac{\partial T}{\partial t} = (j(x) - j(x + \Delta x))/\Delta x + f(x, t)$$

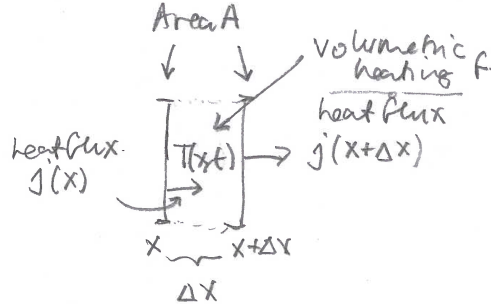


Figure 3.3: Derivation of the one dimensional heat equation.

where f is a true volumetric heating term. Taking the limit as $\Delta x \rightarrow 0$ in the equation above and using (3.4) gives

$$\rho c \frac{\partial T}{\partial t} = \kappa T_{xx} + f$$

known as *the heat equation*. Note that if $\kappa(x)$ then if we look back through the argument we will find that

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}(\kappa T_x) + f$$

In three spatial dimensions, the same type of argument (using a little cube instead of a thin slab) gives

$$\rho c \frac{\partial T}{\partial t} = \kappa \Delta T + f \quad (3.5)$$

where here we have taken κ constant again and Δ here is the Laplacian operator, $\Delta T = T_{xx} + T_{yy} + T_{zz}$.

3.2.4 Heat transfer in a rod: scaling and reduced problem

Consider heat transfer in the rod shown in Figure 3.4. It is described by the equation we derived above (3.5)

$$\rho c \frac{\partial T}{\partial t} = \kappa(T_{xx} + \Delta_r T) + f(x, r, \theta) \quad (3.6)$$

where we have written the Laplacian in cylindrical coordinates,

$$\Delta_r T = \frac{1}{r^2} T_{\theta\theta} + \frac{1}{r} (r T_r)_r.$$

The rod is in an environment with ambient temperature T_{AMB} . Heat is exchanged to the environment at the boundary of the rod according to the relationship

$$\kappa T_r |_{r=R} = N(T_{\text{AMB}} - T |_{r=R}) \quad (3.7)$$

where N is a given parameter determined experimentally, with units of $\text{W}/(\text{m}^2\text{K})$. The relationship (3.7) is a crude approximation to the transfer of heat to the external environment, but can be justified in some situations. For this example, I will ignore what happens at the $x = 0$ and $x = L$ boundaries.

Assume that the system reaches steady state with T independent of t and then

$$-\kappa(T_{xx} + \Delta_r T) = f(x, r, \theta). \quad (3.8)$$

We will non-dimensionalize the equation (3.8) and boundary condition (3.7) in a series of steps. First, we shift the temperature to be relative to ambient:

$$v = T - T_{\text{AMB}}$$

which still satisfies (3.8) but now the boundary condition (3.7) is homogeneous for v :

$$\kappa v_r |_{r=R} = -Nv |_{r=R} \quad (3.9)$$

Then we will scale x and r in the natural way by L and R respectively, giving non-dimensional variables X and s both in $[0,1]$ with

$$x = XL \quad \text{and} \quad r = sR$$

Putting these into (3.8) and (3.9) gives

$$\begin{aligned} -\left(v_{XX} + \frac{L^2}{R^2} \Delta_s v\right) &= \frac{L^2}{\kappa} f(x, r, \theta) \\ v_s &= -\frac{NR}{\kappa} v \quad \text{at } s = 1 \end{aligned}$$

For linear problems, scaling for the unknown is a bit arbitrary, but here it makes sense to take the non-dimensional temperature u with $v = \tau u$ with temperature scale

$$\tau = \frac{L^2}{\kappa} \|f\|_{\infty}$$

(check that τ has units of K!). Now the scaled equations are

$$\begin{aligned} -\left(u_{XX} + \frac{L^2}{R^2} \Delta_s u\right) &= f(X, s, \theta) / \|f\|_{\infty} \\ u_s &= -\frac{NR}{\kappa} u \quad \text{at } s = 1 \end{aligned}$$

and we see that there are two dimensionless parameters $\epsilon = R/L$, the aspect ratio of the rod, and $\frac{NR}{\kappa}$, the ratio of surface to internal heat transfer effects.

We are writing things this way under the assumption that $R \ll L$ so that $\epsilon \ll 1$. We will assume a special scaling for the surface term, that

$$\frac{NR}{\kappa} = A\epsilon^2$$

which says that the surface heat transfer effects are small. Note that this equation defines A in terms of the other parameters, but by writing it this way we are implying that the scaling makes A of “reasonable” size (like “between 0.1 and 10”). We now have the final, scaled equations

$$-(u_{xx} + \frac{1}{\epsilon^2}\Delta_r u) = f(x, r, \theta)/\|f\|_\infty \quad (3.10)$$

$$\frac{1}{\epsilon^2}u_r = -Au \text{ at } r = 1 \quad (3.11)$$

Note that we have gone back to the original coordinate names x and r , which is typically done. We just have to remember these are scaled variables now. We can now do some simplifications based on the size of the terms above. At order $1/\epsilon^2$ we have

$$\Delta_r u = 0 \text{ with } u_r = 0 \text{ on the boundary}$$

which means that at each x , to highest order u is a constant in the (r, θ) plane, that is $u(x)$. To proceed, we integrate (3.10) over the unit circle C at each x , using Gauss’ theorem:

$$\int_C \Delta_r u = \int_\Gamma u_r$$

where Γ is the boundary of C , and (3.11) in the right hand side above to obtain

$$-\pi u'' + 2\pi Au = \frac{1}{\|f\|_\infty} \int_C f(x, r, \theta)$$

or

$$-u'' + 2Au = \frac{1}{\pi\|f\|_\infty} \int_C f(x, r, \theta) := g(x) \quad (3.12)$$

This approximate equation has the form (3.1). Solutions of this equation will differ to those of the original equations (3.10) and (3.11) by terms of size ϵ^2 . Note that the factor of “2” on the left hand side of the equation above is the ratio of the perimeter of the rod cross section to the area in the scaled coordinates. It is only this ratio that determines how changes in cross-section affect this parameter, at leading order.

Note 1 After you solve the problem analytically or numerically do not forget to scale back to the original variables to answer application questions.

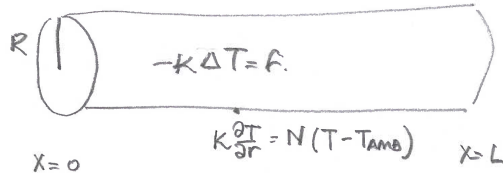


Figure 3.4: Heat transport in a rod.

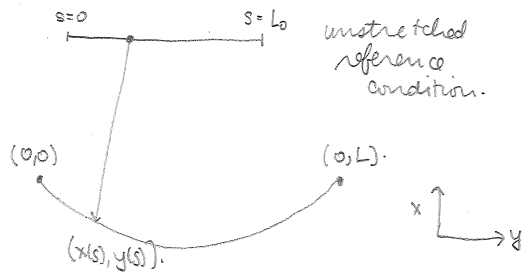


Figure 3.5: Un-stretched reference frame s and stretched frame $(x(s), y(s))$.

3.3 Weighted String Model

3.3.1 Physics

Consider a wire idealized to be infinitely thin. We assume the following material property of the wire, that relative extension varies linearly with tension. That is, if a wire of length l_0 experiences a tension T uniformly along its length and extends to length l , that

$$\frac{l - l_0}{l_0} = \frac{T}{k} \quad (3.13)$$

for some constant material parameter k (units of Newton $N = \text{kg m/s}^2$). This is true for fibreglass fibres for a large range of T , for example.

We consider a wire of un-stretched length L_0 stretched into a curve $(x(s), y(s))$ where s is a material point in the reference frame of the un-stretched curve $s \in [0, L_0]$ as shown in Figure 3.5.

Consider now a small segment of the wire of un-stretched length Δs , $s \in [s_0, s_0 + \Delta s]$. It will have stretched length approximately

$$\sqrt{(x')^2 + (y')^2} \Delta s$$

and so using (3.13) and taking $\Delta s \rightarrow 0$, the tension in the wire at that point is

$$k \left(\sqrt{(x')^2 + (y')^2} - 1 \right)$$

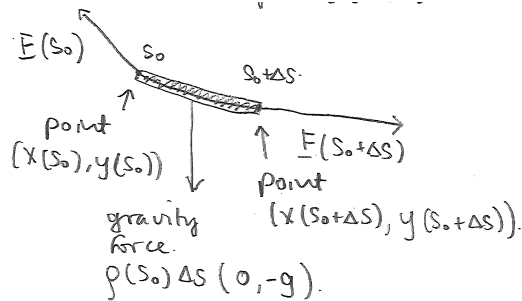


Figure 3.6: Local net force per unit un-stretched length of the wire

in the direction of the tangent of the curve with unit vector

$$\pm(x', y')/\sqrt{(x')^2 + (y')^2}.$$

Taking \mathbf{F} to be the tension vector with positive sign above we have

$$\mathbf{F} = k \frac{(\sqrt{(x')^2 + (y')^2} - 1)}{\sqrt{(x')^2 + (y')^2}}(x', y').$$

Considering Figure 3.6 now, we see that the net force on the segment of wire with un-stretched length Δs is

$$\mathbf{F}(s + \Delta s) - \mathbf{F}(s).$$

Dividing by Δs and taking $\Delta s \rightarrow 0$ we get the force per unit un-stretched length of

$$k \left[\frac{(\sqrt{(x')^2 + (y')^2} - 1)}{\sqrt{(x')^2 + (y')^2}}(x', y') \right]' \quad (3.14)$$

3.3.2 Steady solution wire under gravity

As suggested by the Figures, we will be considering a wire with added mass per unit un-stretched length $\rho(s)$ (units kg/m) and then stretched to hang between two points a distance $L > L_0$ apart: $(x(0), y(0)) = (0, 0)$ and $(x(L_0), y(L_0)) = (0, L)$ and left to come to steady state. The force per unit un-stretched length (3.14) must balance the gravitational force on the density per unit un-stretched length, leading to

$$\left[\frac{(\sqrt{(x')^2 + (y')^2} - 1)}{\sqrt{(x')^2 + (y')^2}}(x', y') \right]' = (0, \frac{g\rho(s)}{k})$$

We scale s by L_0 , x by L , y by Y to be determined later, and obtain the scaled equations

$$\left[\frac{\left(\sqrt{(x')^2 + (y'Y/L)^2} - L_0/L \right)}{\sqrt{(x')^2 + (y'Y/L)^2}} (x', y'Y/L) \right]' = \left(0, \frac{L_0^2}{L} \frac{g\rho(s)}{k} \right)$$

It is now clear that the right scale for Y is

$$Y = L_0^2 \frac{g\|\rho\|_\infty}{k}$$

(units of m, check!) and to proceed we will assume now that

$$Y/L := \epsilon \ll 1$$

leading to

$$\left[\frac{\left(\sqrt{(x')^2 + (\epsilon y')^2} - L_0/L \right)}{\sqrt{(x')^2 + (\epsilon y')^2}} (x', y') \right]' = (0, \rho(s)/\|\rho\|_\infty)$$

At highest order (neglecting the terms of size ϵ) the equations decouple. The first component is satisfied if x' is constant and to match the scaled end conditions we have $x \equiv s$. For y we have

$$y'' = \rho(s)/\|\rho\|_\infty \frac{1}{1 - L_0/L}$$

with $y(0) = 0$ and $y(1) = 0$ and we can think of the independent variable as x instead of s .

3.4 Solving Nonlinear Systems with Newton's Method

3.4.1 Review of scalar Newton's method

Consider solving for the root x_* of a scalar equation:

$$f(x_*) = 0.$$

Begin with a relatively accurate estimate x_0 of the root, and the linear (tangent line) approximation of $f(x)$ based at x_0 as shown in Figure 3.7. We take as the next approximation x_1 , the root of the tangent line. That is, x_1 satisfies

$$f(x_0) + f'(x_0)(x_1 - x_0) = 0$$

which can be solved for

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

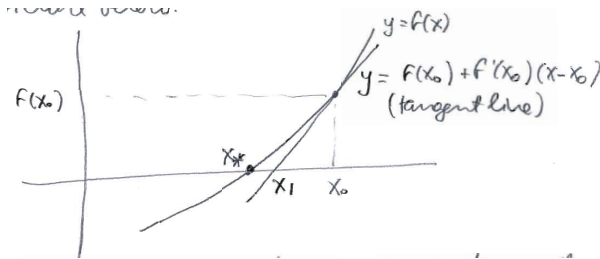


Figure 3.7: Diagram of the iterations to approximate x_* for scalar Newton's method

and then continued iteratively,

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}.$$

Theorem 1 *If f is C_2 , $f'(x_*) \neq 0$, x_0 is sufficiently close to x_* (depends on the size of $f'(x_*)$ and f'' in a neighbourhood of x_*) then $\{x_n\}$ converges to x_* quadratically. That is*

$$\lim_{n \rightarrow \infty} x_n = x_*$$

and

$$|x_{n+1} - x_*| \leq c|x_n - x_*|^2$$

where c depends on the size of f' and f'' .

Note 2 *If x_0 is not "sufficiently close" to x_* then $\{x_n\}$ may not converge or may converge to a different root.*

3.4.2 Newton's method for multi-component vector systems

Let us consider the simplest case of roots (x_*, y_*) of two equations

$$f(x_*, y_*) = 0 \quad \text{and} \quad g(x_*, y_*) = 0. \quad (3.15)$$

This can be put into vector notation $\mathbf{x} = (x, y)$, $\mathbf{f} = (f, g)$ so (3.15) becomes

$$\mathbf{f}(\mathbf{x}) = \mathbf{0}.$$

The two component case has the graphical interpretation of (x_*, y_*) being the intersection of the zero level set of f with the zero level set of g . The level sets would have the generic character of non-parallel curves at the root if $\nabla f(x_*, y_*)$ and $\nabla g(x_*, y_*)$ were not parallel, as shown in Figure 3.8. We assume this condition of the roots we will approximate below.

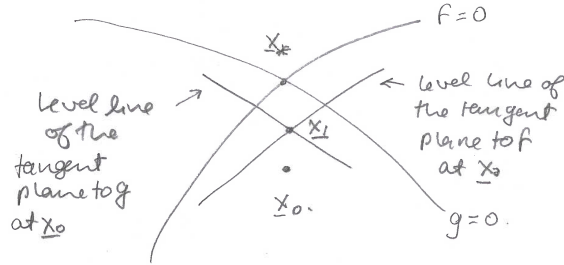


Figure 3.8: Diagram of the geometry of roots of two component systems. I forgot to add the gradients to this picture: recall that the gradient of a function is perpendicular to its level lines.

Newton's method can be extended to the vector case. Considering the two component system and starting at a point (x_0, y_0) near the root, we can approximate f and g by their tangent planes at (x_0, y_0) :

$$f(x, y) \approx f(x_0, y_0) + \frac{\partial f}{\partial x}(x_0, y_0)(x - x_0) + \frac{\partial f}{\partial y}(x_0, y_0)(y - y_0)$$

$$g(x, y) \approx g(x_0, y_0) + \frac{\partial g}{\partial x}(x_0, y_0)(x - x_0) + \frac{\partial g}{\partial y}(x_0, y_0)(y - y_0)$$

As in the scalar case, the next approximation for the root (x_1, y_1) is chosen as the root of the tangent plane approximations, which results in the linear system:

$$\begin{bmatrix} f_x & f_y \\ g_x & g_y \end{bmatrix} \begin{bmatrix} x_1 - x_0 \\ y_1 - y_0 \end{bmatrix} = - \begin{bmatrix} f(x_0, y_0) \\ g(x_0, y_0) \end{bmatrix} \quad (3.16)$$

where the matrix of partial derivatives on the LHS above is called the Jacobian matrix \mathcal{J} and is evaluated at (x_0, y_0) . It is nonsingular at the root (x_*, y_*) by the geometric condition on the gradients of f and g discussed above, and by continuity will be nonsingular for (x_0, y_0) sufficiently close to (x_*, y_*) . We can write (3.16) in vector form:

$$\mathcal{J}(\mathbf{x}_0)(\mathbf{x}_1 - \mathbf{x}_0) = -\mathbf{f}(\mathbf{x}_0)$$

which can be solved for

$$\mathbf{x}_1 = \mathbf{x}_0 - [\mathcal{J}(\mathbf{x}_0)]^{-1}\mathbf{f}(\mathbf{x}_0)$$

and then repeated iteratively

$$\mathbf{x}_{n+1} = \mathbf{x}_n - [\mathcal{J}(\mathbf{x}_n)]^{-1}\mathbf{f}(\mathbf{x}_n) \quad (3.17)$$

Note 3 The iterations (3.17) are in the form of a residual correction since $\mathbf{f}(\mathbf{x}_n)$ is the residual in the equations $\mathbf{f}(\mathbf{x}) = \mathbf{0}$.

Remember that we never compute matrix inverses, so although (3.17) is a nice form for the iterations, we actually compute

$$\begin{aligned}\mathcal{J}_n \mathbf{u}_n &= -\mathbf{f}(\mathbf{x}_n) \\ \mathbf{x}_{n+1} &= \mathbf{x}_n + \mathbf{u}_n.\end{aligned}$$

The methods extend to the N vector case $\mathbf{f}(\mathbf{x}) = \mathbf{0}$ with the Jacobian matrix $N \times N$ with entries

$$J_{i,j} = \frac{\partial f_i}{\partial x_j}.$$

An important example of nonlinear systems comes in the optimization (maximization or minimization) of functions of many variables $f(\mathbf{x})$ (scalar f). The optimal value occurs at critical points that satisfy $\nabla f = \mathbf{0}$, which is a nonlinear system of N equations in N unknowns. In this case, the Jacobian matrix of ∇f is the Hessian matrix of f ,

$$J_{i,j} = \frac{\partial^2 f}{\partial x_i \partial x_j}.$$

Note that in this case \mathcal{J} is symmetric, and near a generic local minimum it is positive definite, so there are good solver options for the Newton updates.

3.4.3 Application to finite difference methods

We have seen in section 3.3 that physical models can be nonlinear. Let us consider the simplest nonlinear model relative of problem A, with nonlinearity in u but not in derivatives. An example is given below, for $u(x)$ 1-periodic in x :

$$-u'' + u + u^3 = f(x). \quad (3.18)$$

We could make a finite difference discretization as usual including the nonlinearity:

$$-(U_{j-1} - 2U_j + U_{j+1})/h^2 + U_j + U_j^3 - F_j = 0$$

which is a nonlinear system. We can do Newton iterations $\mathbf{U}^{(m)}$ to approximate the solution to the system. The Jacobian matrix \mathcal{J} at the m 'th update has entries

$$J_{i,j} = \begin{cases} -1/h^2 & \text{if } j = i - 1 \text{ or } j = i + 1 \\ 2/h^2 + 1 + 3[U_j^{(m)}]^2 & \text{if } j = i \\ 0 & \text{otherwise} \end{cases}$$

where the indices are taken mod N . We see that $\mathcal{J} = \mathcal{A} + \text{diag}\{3[U_j^{(m)}]^2\}$ where \mathcal{A} is the matrix from the linear problem A. A MATLAB implementation for this problem will be provided.

Note 4 *Iterates converge to the exact solution \mathbf{U} of the discrete problem, but not to the exact solution to the continuum problem (3.18). We will want the iteration error to be smaller than the discretization error so as not to confuse the*

accuracy of the result. On the other hand, we should not spend too many computational resources on making this much more accurate than the discretization error. If you really understand the properties of the method, you would balance the accuracy to computational cost benefit.

For some nonlinear problems, finding an initial vector $\mathbf{U}^{(0)}$ close enough to the exact solution so that Newton iterations converge can be very difficult. That is not true for the problem (3.18) for which it can be proved that the iterations converge for any initial guess (it is a convex problem). However, let us use this as an example, and explain a technique that can solve the issue of having a good initial vector. Consider (3.18) as a family of problems indexed by the scalar $\theta \in [0, 1]$:

$$-D_2U_j + U_j + \theta U_j^3 = F_j.$$

There is a continuous family of solutions $\mathbf{U}(\theta)$ and we want $\mathbf{U}(1)$. The solution $\mathbf{U}(0)$ is easy to find, it is just the discretization of the original, linear problem A. If we had the solution $\mathbf{U}(\theta)$ for $\theta \in (0, 1)$ it would be a good initial guess for Newton's method for $\mathbf{U}(\theta + \Delta\theta)$ for $\Delta\theta$ sufficiently small. Thus we could move from $\theta = 0$ to $\theta = 1$ with $\Delta\theta$ adaptively reduced as needed to guarantee convergence of the Newton iterations at each step. This technique is called *continuation*.

3.5 Problems

Problem 1 Consider the heat conduction problem in Section 3.2. If the surface heat transfer term has a different scaling, that is

$$\frac{NR}{\kappa} = O(1)$$

derive the leading order behaviour in this case.

Problem 2 Identify the problem for the next order correction in the heat conduction problem in Section 3.2. That is, consider the scaled equations (3.10, 3.11). Assume that the solution has the asymptotic expansion

$$u(x, r, \theta) = u(x) + \epsilon^2 v(x, r, \theta) + O(\epsilon^4)$$

where $u(x)$ is the solution to the problem (3.12) we identified as describing the dominant effects. Find the equations for v . Often, u above is denoted by $u^{(0)}$ and v by $u^{(2)}$ to denote the orders that they appear in the expansion.

Problem 3 Identify the next order correction in the weighted string model equations.

Problem 4 Consider the nonlinear boundary value problem (3.18). Show existence and uniqueness of solutions and the regularity of solutions in terms of the

data f . If you want a harder equation to prove things about, try the nonlinear weighted string model equations. Note that negative tension is not physical (leads to ill-posedness), so show that this does not occur in the solutions to the model.

Problem 5 Write a Finite Difference discretization of the nonlinear string problem. Find solutions using Newton's method. Show numerically that as $\epsilon \rightarrow 0$ the solutions tend those of the linear problem.