Chapter 6
Numerical techniques

The differential equations (4.61), (4.62) and (4.64), in combination with boundary conditions such as equations (4.65) – (4.68), constitute a two point boundary value problem. Non-trivial solutions to the problem can be obtained only at selected values of the frequency \( \omega \), which is therefore an eigenvalue of the problem. Problems of this nature are extremely common in theoretical physics, and hence there exists a variety of techniques for solving them. Nevertheless, the computation of solar adiabatic oscillations possesses special features, which merit discussion. In particular, we typically need to determine a large number of frequencies very accurately, to match the volume and precision of the observed data.

Specific numerical techniques are discussed in considerable detail by, for example, Unno et al. (1989) and Cox (1980). Here I concentrate more on general properties of the solution method. The choice of techniques and examples is unavoidably biased by my personal experience, but should at least give an impression of what can be achieved, and how to achieve it.

I note that a self-contained package for computing stellar adiabatic oscillations, with documentation and further notes on the numerical techniques, is available on the WWW at http://astro.phys.au.dk/~jcd/adipack.n/.

6.1 Difference equations

The numerical problem can be formulated generally as that of solving

\[
\frac{dy_i}{dx} = \sum_{j=1}^{I} a_{ij}(x)y_j(x), \quad \text{for} \quad i = 1, \ldots, I,
\]

with suitable boundary conditions at \( x = x_1 \) and \( x_2 \), say. Here the order \( I \) of the system is four for the full nonradial case, and two for radial oscillations or nonradial oscillations in the Cowling approximation.

To handle these equations numerically, I introduce a mesh \( x_1 = x^{(1)} < x^{(2)} < \ldots < x^{(N_{\text{me}})} = x_2 \) in \( x \), where \( N_{\text{me}} \) is the total number of mesh points. Similarly I introduce \( \tilde{y}_i^{(n)} \equiv y_i(x^{(n)}) \), and \( \tilde{a}_{ij}^{(n)} \equiv a_{ij}(x^{(n)}) \). A commonly used, very simple representation of the differential equations is in terms of second-order centred differences, where the differential
equations are replaced by the difference equations

\[
\frac{y_i^{(n+1)} - y_i^{(n)}}{x^{(n+1)} - x^{(n)}} = \frac{1}{2} \sum_{j=1}^{I} \left[ a_{ij}^{(n)} y_j^{(n)} + a_{ij}^{(n+1)} y_j^{(n+1)} \right], \quad i = 1, \ldots, I. \tag{6.2}
\]

These equations allow the solution at \( x = x^{(n+1)} \) to be determined from the solution at \( x = x^{(n)} \).

More elaborate and accurate difference schemes (e.g. Press et al. 1986; Cash & Moore 1980), can be set up which allow the rapid variation in high-order eigenfunctions to be represented with adequate accuracy on a relatively modest number of meshpoints. Alternatively one may approximate the differential equations on each mesh interval \((x^{(n)}, x^{(n+1)})\) by a set of equations with constant coefficients, given by

\[
\frac{dn_i^{(n)}}{dx} = \sum_{j=1}^{I} a_{ij}^{(n)} n_j^{(n)}(x), \quad \text{for} \quad i = 1, \ldots, I, \tag{6.3}
\]

where \( a_{ij}^{(n)} \equiv \frac{1}{2}(a_{ij}^{(n)} + a_{ij}^{(n+1)}) \) (Gabriel & Noels 1976). These equations may be solved analytically on the mesh intervals, and the complete solution is obtained by continuous matching at the mesh points. This technique clearly permits the computation of modes of arbitrarily high order. I have considered its use only for systems of order two, i.e., for radial oscillations or non-radial oscillations in the Cowling approximation.

### 6.2 Shooting techniques

Perhaps the conceptually simplest technique for handling a boundary value problem is the shooting technique. For simplicity, I consider first the case of a second-order system, such as results from making the Cowling approximation. Then there is one boundary condition, namely equation (4.65), at the centre, and one condition, equation (4.68), at the surface. For any value of \( \omega \) the equations may be integrated numerically, imposing the central boundary condition on \( \xi_r \) and \( \xi_h \), and the quantity

\[
\Delta(\omega) \equiv \left( p' + \frac{dp}{d\xi_r} \right) \bigg|_{r=R}. \tag{6.4}
\]

may be evaluated. The eigenfrequencies are obviously the zeros of \( \Delta(\omega) \). A convenient method of locating them is to evaluate \( \Delta(\omega) \) at a sequence of points \( \omega_1, \omega_2, \ldots \); once an interval has been found where \( \Delta \) changes sign the zero can be found, for instance, by applying the secant method. An attractive feature of the method is precisely this ability to search automatically for all modes in a given frequency range, particularly when it is combined with a method for determining the order of a given mode, so that a check can be made that no modes have been skipped.

A slight elaboration of this basic technique is required to make it computationally efficient. Due to the rapid decrease of temperature near the solar surface, the equations are almost singular there. Far from the eigenfrequencies the solution therefore generally increases rapidly towards the surface; this translates into a dramatic variation of \( \Delta \) with \( \omega \), which complicates the determination of the zeros. To avoid this problem, one may compute solutions \((\xi_r^{(i)}, \xi_h^{(i)})\) and \((\xi_r^{(s)}, \xi_h^{(s)})\) satisfying the inner and the surface boundary conditions,
respectively. A continuous match of the interior and exterior solutions requires the existence of non-zero constants $C^{(i)}$ and $C^{(s)}$ such that

$$C^{(i)} \xi^{(i)}_r (r_f) = C^{(s)} \xi^{(s)}_r (r_f)$$
$$C^{(i)} \xi^{(i)}_h (r_f) = C^{(s)} \xi^{(s)}_h (r_f),$$

(6.5)

where $r_f$ is an appropriately chosen fitting point. This set of equations has a solution only if the determinant

$$\Delta_f (\omega) = \xi^{(i)}_r (r_f) \xi^{(s)}_h (r_f) - \xi^{(i)}_h (r_f) \xi^{(s)}_r (r_f)$$

vanishes. Hence the eigenfrequencies are determined as the zeros of $\Delta_f$, as before.

The choice of fitting point should be guided by the expected behaviour of the eigenfunction, in such a way that the integration of the differential equations proceeds in a stable fashion. Thus, for instance, when solving for a strongly trapped g mode of high degree, $r_f$ should be near the maximum in the buoyancy frequency where the mode is trapped; in this way the integration from both the centre and the surface is in the direction where the solution increases. Similarly, when integrating for a p mode of high degree, $r_f$ should be in the oscillatory region near the surface.

The solution of the full fourth-order problem proceeds in a very similar fashion. Here there are two linearly independent solutions that satisfy the boundary conditions at the centre, and two linearly independent solutions that satisfy the conditions at the surface. The condition that these two sets of solutions match continuously at a point $r_f$ leads to a set of equations whose solution requires the vanishing of a $4 \times 4$ determinant. It should be noted, however, that problems arise when the effect of the perturbation in the gravitational potential is small. In this case, although the two separate solutions from e.g. the centre are formally linearly independent, they are in practice very close to being linearly dependent, and the zeros of $\Delta_f$ are therefore ill-determined. This is no major concern in practice, since under these circumstances the Cowling approximation is in general adequate. However, as discussed below the problem may be avoided through the use of some variant of the relaxation technique.

6.3 Relaxation techniques

The relaxation technique considers the set of difference equations, such as equations (6.2), together with the homogeneous boundary conditions and a normalization condition, as a set of equations for the unknown quantities $\{y_i^{(n)}; i = 1, \ldots, I; n = 1, \ldots, N_{me}; \omega\}$. Due to the appearance of the eigenfrequency, the equations are non-linear in the unknowns. They are solved by linearizing around an assumed initial trial solution, and the solution is obtained by iteration. This technique is equivalent to what is commonly known as the Henyey technique in computations of stellar evolution (Henyey, Forbes & Gould 1964; see also Baker, Moore & Spiegel 1971; Kippenhahn & Weigert 1990).

A disadvantage of this technique is that it requires a reasonably accurate trial solution, both for the eigenfrequency and the eigenfunction, if the iteration is to converge to the desired mode. Also it is not immediately possible to search a given part of the spectrum. These problems may be avoided by dropping one of the boundary conditions, and regarding $\omega$ as given (e.g. Castor 1971; Osaki & Hansen 1973). The difference equations are then a linear set of equations for the $\{y_i^{(n)}\}$ which may be solved directly. Given the solution, the remaining boundary condition, now regarded as a function of $\omega$, is solved to obtain the
eigenfrequencies. Thus in this form the relaxation technique retains the advantages of the shooting method, in that a region of the spectrum can be scanned. Once a sufficiently close approximation to the solution has been found, the rate of convergence can be increased by switching to simultaneous iteration for the eigenfrequency and eigenfunction.

As for the shooting technique, the straight determination of the eigenfrequency through root-seeking on one of the boundary conditions is rather ill-behaved. This problem may be avoided by imposing all boundary conditions, but permitting for general \( \omega \) a discontinuity in one component of the eigenfunction at a suitable interior fitting point \( r_f \). The eigenfrequencies are then determined by requiring that the discontinuity vanish. I have found that this technique allows stable solution of the full set of equations for all relevant degrees and frequencies.

### 6.4 Formulation as a matrix eigenvalue problem

As discussed in Section 5.5 the equations of adiabatic oscillation, written as in equations (5.60) and (5.61), constitute a linear eigenvalue problem in function space. If the operator on the right hand side is discretized, the result is a linear discrete eigenvalue problem. By solving this, one obtains (approximations to) the eigenvalues and eigenfunctions of the continuous problem.

A method of this nature (but generalized to the non-adiabatic case) was used by Keeley (1977) for radial oscillations. Knölker & Stix (1983) used it for adiabatic non-radial oscillations in the Cowling approximation. In these cases, the operator describing the left hand side of the oscillation equations is a pure differential operator; hence its discrete representation only couples the solution at a few neighbouring meshpoints and results in an eigenvalue problem where the matrix is banded, with only a few off-diagonal elements. Consequently, efficient techniques exist for the determination of the eigenvalues. In contrast, in the full non-radial problem the terms in \( \Phi' \) couple all parts of the model [see also equation (5.11)]; then the corresponding matrix is full, although for large \( l \) it is diagonally dominated, due to the factors \((r'/r)^{l+1}\) and \((r/r')^l\) occurring respectively in the first and second term on the right hand side of equation (5.11). In this case it is not evident that sufficiently fast algorithms exist for the determination of the matrix eigenvalues to make the technique competitive with the shooting or relaxation techniques. No attempt has apparently been made to apply it to this problem.

The matrix eigenvalue problem can also be derived directly from the variational principle as expressed in equation (5.77), by means of the so-called Rayleigh-Ritz method (e.g. Strang & Fix 1973). To do so the eigenfunction is expanded on a set of suitable basis functions, and the expansion coefficients are determined by imposing the condition that the expression (5.77) be stationary. Although this method has proven useful in atomic physics (e.g. B. L. Christensen-Dalsgaard 1982), the effects of the gravitational potential once again lead to a full matrix in the resulting eigenvalue problem.

I finally note that Pesnell (1990) has developed an efficient algorithm, based on the method of Castor (1971), for computing nonradial oscillations both in the adiabatic and the nonadiabatic case. This involves formulating the oscillation equations as a generalized linear algebraic eigenvalue problem; in contrast to the techniques discussed above, Poisson's equation is left on differential form, and hence the resulting matrices are sparse. Cox et al. (1989) applied this method to the computation of solar oscillations.
6.5 Richardson extrapolation

The difference scheme (6.2), which is used by at least some versions of the shooting, relaxation and matrix eigenvalue techniques, is of second order. Consequently the truncation errors in the eigenfrequency and eigenfunction scale as $N^{-2}$. If $\omega(N_{\text{me}})$ and $\omega(N_{\text{me}}')$ are the eigenfrequencies obtained from solutions with $N_{\text{me}}$ and $N_{\text{me}}'$ meshpoints, the leading order error term therefore cancels in

$$\omega^{(\text{Ri})} = \frac{1}{3}[4\omega(N_{\text{me}}) - \omega(1/2N_{\text{me}}')] .$$

(6.7)

The evaluation of $\omega^{(\text{Ri})}$, known as Richardson extrapolation, was used by Shibahashi & Osaki (1981) to compute frequencies of solar oscillation. This provides an estimate of the eigenfrequency that is substantially more accurate than $\omega(N_{\text{me}})$, although of course at some added computational expense.

6.6 Variational frequencies

The variational property discussed in Section 5.5.2 can be used to obtain an estimate of the oscillation frequency which is at least formally more accurate than the frequency obtained as an eigenvalue of the solution of the oscillation equations (Christensen-Dalsgaard, Gough & Morgan 1979; J. Christensen-Dalsgaard 1982). It follows from equation (5.76) that if the computed eigenfunction is substituted into the functional $\Sigma(\xi)$, the result agrees with the squared eigenfrequency to within an error that is quadratic in the error in the eigenfunction. If the latter error goes as $N^{-2}_{\text{me}}$, the error in $\Sigma(\xi)$ would be expected to vary as $N^{-4}_{\text{me}}$; this assumes that the evaluation of $\Sigma(\xi)$, for given $\xi$, is sufficiently accurate.

For realistic solar models the complete expressions (5.77) or (5.79) must be used, including the surface terms. However, since these terms are in general relatively small, the variational property is still approximately satisfied. Hence the expressions may be used to provide estimates of the frequency which are less sensitive to numerical error than the eigenfrequency. On the other hand, it should be noted that the variational property, and the analysis leading to equations (5.77) and (5.79), assume that the solar model satisfies the equations of hydrostatic equilibrium and the mass equation exactly. When the model is itself the result of a numerical solution of the equations of stellar structure this is evidently not the case; then, even if they were to be evaluated with infinitely high precision for the given model, the variational frequency and the eigenfrequency would not agree. The discrepancy provides an estimate of the effect on the frequencies of the inconsistencies in the model. Examples of this were discussed by Christensen-Dalsgaard & Berthomieu (1991).

6.7 The determination of the mesh

Computational efficiency demands that the distribution of mesh points be chosen appropriately. It is immediately obvious from the eigenfunctions (cf. Figures 5.8 and 5.10 that a mesh uniform in $r$ is far from optimal; also the distribution of points should clearly be different for $p$ and for $g$ modes.

Procedures exist that determine the optimal mesh as part of the numerical solution of a set of differential equations (Gough, Spiegel & Toomre 1975). In the present case, however, the requirements on the mesh are essentially driven by the behaviour of the modes of high
radial order, whose eigenfunctions are given, with considerable precision, by the asymptotic expression (5.22). Thus to have a roughly constant number of meshpoints between the nodes in the eigenfunction, the mesh should be approximately uniformly spaced in terms of the integral in this equation.

To define a flexible method for setting up the mesh I have adopted a simplified version of the procedure developed by Gough et al. (1975). Thus I introduce a variable \( z \), with a range from 0 to 1, such that the mesh is uniform in \( z \), and determined by

\[
\frac{dz}{dr} = \lambda H(r) ;
\]

where \( \lambda \) is a normalization constant, relating the ranges of \( z \) and \( r \), and the function \( H \) determines the properties of the mesh. Given \( H \), \( z \) is obtained as

\[
z(r) = \lambda \int_0^r H(r')dr',
\]

with

\[
\lambda = \left( \int_0^R H(r)dr \right)^{-1}.
\]

The mesh \( \{r^{(n)}, n = 1, \ldots, N_{\text{me}}\} \) is finally determined by solving the equations

\[
z(r^{(n)}) = \frac{n - 1}{N_{\text{me}} - 1},
\]

by interpolating in the computed \( z(r) \).

The choice of the function \( H \) must be guided by the asymptotic behaviour of the modes, as described by the function \( K \) in equation (5.22). Specifically, I have used

\[
H(r)^2 = R^{-2} + c_1 \frac{\omega_g^2}{c^2} + c_2 \frac{|N|^2}{\omega_g^2 r^2} + c_3 \left( \frac{d \ln p}{dr} \right)^2,
\]

where \( \omega_g^2 \equiv GM/R^3 = t_{\text{dyn}}^{-2} \) is a characteristic squared frequency. Here the term in \( c_1 \) results from noting that in the limit of an extreme p mode \( K \propto c^{-2} \) [cf. equation (5.29)], whereas the term in \( c_2 \) similarly corresponds to the extreme g-mode case, where \( K \propto N^2/r^2 \) [cf. equation (5.33)]. The term in \( c_3 \) provides extra meshpoints near the surface, where the reflection of the p modes takes place. Finally the constant term ensures a reasonable resolution of regions where the other terms are small.

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<th>Table 6.1</th>
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<td>p-mode mesh</td>
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<td>g-mode mesh</td>
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Table 6.1: Parameters in equation (6.12) for determination of meshes suitable for computing p and g modes in a model of the present Sun.
The parameters in this expression can be determined by testing the numerical accuracy of the computed frequencies (e.g. Christensen-Dalsgaard & Berthomieu 1991). For normal solar models reasonable choices, based on a fairly extensive (but far from exhaustive) set of calculations, are given in Table 6.1. In the p-mode case the mesh is predominantly determined by the variation of sound speed, with the term in $N$ giving a significant contribution near the centre and the term in $d \ln p/dr$ contributing very near the surface. The g-mode mesh is dominated by the term in $N$ in most of the radiative interior, whereas in the convection zone, where $|N|$ is generally small, the constant term dominates; the term in $d \ln p/dr$ is again important in the surface layers.