Coordinate stretching for finite difference optical waveguide mode solvers

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Abstract

Numerical methods are necessary to calculate propagating modes in optical waveguides. The finite difference method is widely used because it is applicable to waveguides with arbitrary refractive index profiles and it is easy to implement. To improve the efficiency and to reduce the size of the resulting large sparse matrix, the finite difference method is often used with a variable grid size strategy. This is related to the technique of coordinate stretching. In this paper, we develop a technique for optimizing the coordinate stretching function based on discrete reflection coefficients. We demonstrate our method using a scalar model which is valid for weakly guided optical waveguides.

1 Introduction

In fiber and integrated optics, a fundamental problem is to compute the eigenmodes of optical waveguides. Unlike microwave waveguides, optical waveguides [1, 2, 3] are typically open structures for which the transverse domain is the entire plane perpendicular to the waveguide axis. A propagating mode of a waveguide is a special solution that depends on the variable z along the waveguide axis as $\exp(i\beta z)$ for a real β and decays to zero as the distance to the waveguide axis tends to infinity. Mathematically, it gives rise to an eigenvalue problem where β^2 is the eigenvalue and the mode profile is the eigenfunction defined on the transverse plane. Over the years, numerous numerical and semi-analytic methods have been developed for solving optical waveguide modes [4, 5, 6]. Some of the most effective methods rely on special geometric features of the waveguides and they may even turn the original linear eigenvalue problem to a nonlinear problem for

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the propagation constant β. Nevertheless, standard numerical methods such as the finite difference [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18] and finite element [19, 20, 21, 22] methods are still widely used, because they are very general, relatively easy to implement and compatible with other computation tasks.

For all numerical methods that approximate the differential operator by a matrix, so that the original linear eigenvalue problem is turned to a standard matrix eigenvalue problem, it is necessary to truncate the infinite transverse domain to a finite computation domain. Although the eigenfunctions decay to zero exponentially as the distance to the waveguide axis is increased, the decay rate is small if the eigenmode is near cut-off. In that case, a large truncation domain is necessary. For both finite difference and finite element methods, it is common to use large mesh size for grid points near the boundary of the truncated domain, since the eigenfunction does not change so much as it approaches zero. For the finite difference method, an alternative technique is to stretch the coordinate. Although variable grid size and coordinate stretching are closely related, they usually have different numerical properties when discretized. In all cases, these techniques are used with very little theoretical guidance. It is not clear how the grid size should be varied and how the coordinate should be stretched.

In this paper, we develop a technique for optimizing coordinate stretching parameters. We introduce a discrete reflection coefficient for any coordinate stretching profile in connection with a finite difference method. The concept of discrete reflectivity [23, 24] was originally developed to analyze and optimize perfectly matched layers (PMLs)[25, 26]. The parameters in the profile are determined by minimizing the reflection coefficient. The method is applied to the eigenvalue problem for a weakly-guided optical waveguide where the governing equation is the Helmholtz equation. Compared with the main task of solving the matrix eigenvalue problem, the work needed to find the best coordinate stretching parameters is negligible.

2 The eigenvalue problem

A straight optical waveguide can be described by its refractive index function $n = n(x, y)$, where x and y are the transverse variables and z is the variable along the waveguide axis. A propagating mode of the waveguide can be solved from eigenvalue problems involving two transverse components of the electric field, or two transverse components of the magnetic field, or the longitudinal components (i.e. z components) of both fields. If the two transverse components of the electric field are used, we have

$$\begin{bmatrix} E_x \\ E_y \end{bmatrix} = \begin{bmatrix} \Phi_x \\ \Phi_y \end{bmatrix} e^{i\beta z}$$

where E_x and E_y are the x and y components of the electric field, Φ_x and Φ_y are two functions of x and y only, and β is the unknown wavenumber in the z direction (i.e., the propagation constant). The mode is then solved from the following eigenvalue problem:

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} \Phi_x \\ \Phi_y \end{bmatrix} = \beta^2 \begin{bmatrix} \Phi_x \\ \Phi_y \end{bmatrix}, \tag{1}$$

where β^2 is the eigenvalue, Φ_x and Φ_y are the eigenfunctions, A_{11}, A_{12}, A_{21} and A_{22} are differential operators given as

$$\begin{aligned} A_{11} &= \frac{\partial}{\partial x}\left[\frac{1}{n^2}\frac{\partial(n^2 \cdot)}{\partial x}\right] + \frac{\partial^2}{\partial y^2} + k_0^2 n^2, \\ A_{12} &= \frac{\partial}{\partial x}\left[\frac{1}{n^2}\frac{\partial(n^2 \cdot)}{\partial y}\right] - \frac{\partial^2}{\partial x \partial y}, \\ A_{21} &= \frac{\partial}{\partial y}\left[\frac{1}{n^2}\frac{\partial(n^2 \cdot)}{\partial x}\right] - \frac{\partial^2}{\partial y \partial x}, \\ A_{22} &= \frac{\partial}{\partial y}\left[\frac{1}{n^2}\frac{\partial(n^2 \cdot)}{\partial y}\right] + \frac{\partial^2}{\partial x^2} + k_0^2 n^2. \end{aligned}$$

In the above, k_0 is the free space wavenumber related to the angular frequency and the speed of light in vacuum.

For conventional optical fibers, the refractive index of the fiber core is only slightly larger than that of the surrounding cladding, we can then replace the above full-vector eigenvalue problem by a much simpler scalar eigenvalue problem

$$\left(\partial_x^2 + \partial_y^2 + k_0^2 n^2\right) u = \beta^2 u, \tag{2}$$

where $ue^{i\beta z}$ represents a component of the electric or magnetic fields. The above eigenvalue problem is only valid for weakly-guided optical waveguides where the difference between the maximum and minimum of $n(x, y)$ is small. However, it also describes acoustic waveguides involving a medium with variable sound speed. For high index-contrast optical waveguides used in integrated optics, the full-vector eigenvalue problem (1) is more appropriate. In the following, we develop a coordinate stretching technique for the scalar eigenvalue problem (2). However, our method should be applicable to the full-vector problem (1) as well.

For simplicity, we also assume that the refractive index is a constant n_0 if the distance to the waveguide axis is sufficiently large. This is the case for conventional optical fibers, since the cladding is often assumed to extend to infinity in theoretical studies. For waveguides constructed in a layered background medium, this assumption is not valid, but our study concerning optimal coordinate stretching can still be applied to each region with a constant refractive index. Because of this assumption, we have a bounded domain Ω, such that $n = n_0$ if (x, y) is outside Ω. Let a be a characteristic length scale of Ω, we can non-dimensionalize the equation by introducing scaled variables $\hat{x}$ and $\hat{y}$ satisfying

$x = a\hat{x}$ and $y = a\hat{y}$. In terms of these new variables, the eigenvalue problem (2) can be written as

$$\left[\partial_{\hat{x}}^2 + \partial_{\hat{y}}^2 + \rho(\hat{x},\hat{y})\right] u = \lambda u, \tag{3}$$

where $\rho(\hat{x},\hat{y}) = (k_0 a)^2[n^2(x,y) - n_0^2]$ and $\lambda = a^2\beta^2 - k_0^2 a^2 n_0^2$. To simplify the notations, we also use x and y to denote $\hat{x}$ and $\hat{y}$ when the distinction is not important. In particular, we can see that for the eigenfunction to decay to zero exponentially as $\sqrt{x^2+y^2}$ tends to infinity, we must have $\lambda > 0$.

3 Coordinate stretching

The eigenvalue problem (3) is defined on the entire xy plane. For finite difference and finite element methods, it is necessary to truncate the xy plane to a finite computation domain. When the problem is discretized, the differential operator $\partial_x^2 + \partial_y^2 + \rho(x,y)$, where x and y now refer to $\hat{x}$ and $\hat{y}$ as in (3), is approximated by a matrix. In order to reduce the size of that matrix, we can use a larger grid size for grid points near the boundary of the truncated domain. Alternatively, we can use a uniform grid size in stretched coordinates. Let us consider a finite difference approximation to the second order derivative with respect to x. If we use the grid points $\{x_j\}$, then the second order derivative of a function $f(x)$ at x_j should be approximated as

$$f''(x_j) \approx \frac{2}{x_{j+1} - x_{j-1}} \left(\frac{f_{j+1} - f_j}{x_{j+1} - x_j} - \frac{f_j - f_{j-1}}{x_j - x_{j-1}} \right), \tag{4}$$

where f_j denotes $f(x_j)$, etc. If we use a coordinator stretching, the variable x is first changed to ξ by

$$x = \int_0^\xi s(\tau)d\tau.$$

The function s is chosen such that $s = 1$ in most part of the computation domain and $s > 1$ near the edges of this domain. The second order derivative f'' can be written as

$$\frac{d^2 f}{dx^2} = \frac{1}{s}\frac{d}{d\xi}\left(\frac{1}{s}\frac{df}{d\xi}\right).$$

Corresponding to a uniform discretization of ξ, satisfying $\xi_j = \xi_{j-1} + \Delta\xi$ for all j, we have

$$x_j = \int_0^{\xi_j} s(\tau)d\tau$$

and

$$f''(x_j) \approx \frac{1}{(\Delta\xi)^2}\left(\frac{f_{j+1} - f_j}{s_j s_{j+1/2}} - \frac{f_j - f_{j-1}}{s_j s_{j-1/2}} \right), \tag{5}$$

where $s_j = s(\xi_j)$, $s_{j\pm 1/2} = s(\xi_j \pm \Delta\xi/2)$. Clearly, the two approximations (4) and (5) can be related to each other by

$$\frac{x_{j+1} - x_j}{\Delta\xi} \approx s_{j+1/2}, \quad \frac{x_j - x_{j-1}}{\Delta\xi} \approx s_{j-1/2}, \quad \frac{x_{j+1} - x_{j-1}}{2\Delta\xi} \approx s_j.$$

However, they are not identical. If we insist that the first two conditions above are satisfied exactly, then we have $x_{j+1} - x_{j-1} = (s_{j+1/2} + s_{j-1/2})\Delta\xi$, but it is usually not the same as $2s_j\Delta\xi$. Since we can choose a smooth function s in the coordinate stretching approach, the approximation (5) usually gives better results.

For our waveguide eigenvalue problem (3), we need to use coordinate stretching for both x and y. Therefore, we also change y to η by

$$y = \int_0^\eta r(\tau)d\tau$$

for some real function r. The eigenvalue problem (3) now becomes

$$\frac{1}{s}\frac{\partial}{\partial\xi}\left(\frac{1}{s}\frac{\partial u}{\partial\xi}\right) + \frac{1}{r}\frac{\partial}{\partial\eta}\left(\frac{1}{r}\frac{\partial u}{\partial\eta}\right) + \rho u = \lambda u. \tag{6}$$

We can discretize the above as in Eq. (5) with a constant grid size for both ξ and η. More precisely, if we discretize η by $\{\eta_k\}$ satisfying $\eta_k - \eta_{k-1} = \Delta\eta$ for all k, and let

$$y_k = \int_0^{\eta_k} r(\tau)d\tau, \quad r_k = r(\eta_k), \quad r_{k\pm1/2} = r(\eta_k \pm \frac{\Delta\eta}{2}),$$

then (6) is discretized as

$$a_j u_{j-1,k} + b_j u_{j+1,k} + c_k u_{j,k-1} + d_k u_{j,k+1} + (\rho_{jk} - a_j - b_j - c_k - d_k)u_{jk} = \lambda\, u_{jk} \tag{7}$$

where

$$a_j = \frac{1}{(\Delta\xi)^2 s_j s_{j-1/2}}, \qquad b_j = \frac{1}{(\Delta\xi)^2 s_j s_{j+1/2}}, \tag{8}$$

$$c_k = \frac{1}{(\Delta\eta)^2 r_k r_{k-1/2}}, \qquad d_k = \frac{1}{(\Delta\eta)^2 r_k r_{k+1/2}}, \tag{9}$$

$$\rho_{jk} = \rho(x_j, y_k), \qquad u_{jk} \approx u(x_j, y_k). \tag{10}$$

In the following sections, we develop a strategy for choosing the functions s and r in connection with the discretized eigenvalue problem (7).

4 Discrete reflection coefficient

The optimal stretching functions s and r depend on many factors, including how the eigenfunction decays as $|x|$ or $|y|$ tend to infinity, how large the grid sizes $\Delta\xi$ and $\Delta\eta$ are and where the variables ξ and η are truncated, etc. To be more practical, we need to make a few assumptions. Concerning the discretization of ξ and η, we assume that ξ and η are truncated to a rectangular computation domain and discretized with grid sizes $\Delta\xi$ and $\Delta\eta$. We also assume that the region where s or r are greater than 1 is specified. Consider the positive ξ direction, we assume that $s = 1$ for $\xi \le H$ and $s > 1$ for $\xi > H$, and ξ is truncated at $\xi = D$ for $D = H + m\Delta\xi$ where m is a positive integer. Furthermore, we can specify the function s in a simple profile including one or two parameters, so that the difficult task of finding the function s is reduced to the simpler problem of finding the parameters in a given profile of s. Notice that the functions s and r are only numerical tools used to derive the discretization scheme (7). In the following, we consider a simple polynomial stretching function given by

$$s(\xi) = 1 + (p+1)S_0 \left(\frac{\xi - H}{D - H}\right)^p, \quad \xi > H, \tag{11}$$

where p is a positive integer and S_0 is a positive parameter of the profile. Since

$$\int_H^D s(\tau)d\tau = (D - H)(1 + S_0),$$

the length of the interval (H, D) for ξ is increased by a factor of $1 + S_0$, resulting the stretched interval $(H, D+S_0(D-H))$ for x. In other words, terminating the computation domain at $\xi = D$ corresponds to truncating x at $x = D + S_0(D - H)$.

A more difficult issue is that the optimal stretching functions also depend on the eigenfunction, at least the decay rate of the eigenfunction as $\sqrt{x^2 + y^2}$ tends to infinity. However, the decay rate depends on the eigenvalue and it is what we are trying to calculate. To resolve this difficulty, we propose to replace the exact eigenvalue by an approximation. If the eigenvalue problem (3) has a solution, then the eigenvalue λ must satisfy

$$0 < \lambda < \max_{x,y} \rho(x, y) = \rho_*.$$

To start, we may use $\rho_*/2$ as an approximation of λ to estimate the parameters in the stretching functions. Another approach is to perform a preliminary numerical calculation to find a first approximation of λ. Such a preliminary calculation can be done on a coarser grid without coordinate stretching. A rough estimate of λ should already allow us to find a good coordinate stretching function.

If we assume that the domain Ω in which ρ may be non-zero is given in the half plane $x < H$, then the differential equation (3) is reduced to

$$u_{xx} + u_{yy} = \lambda u,$$

for $x > H$. To find the optimal parameter for the stretching function s, we rely on the discrete reflection coefficient for y-independent solutions of the above equation. To avoid confusion with the original eigenfunction, we switch to the simple ordinary differential equation

$$\frac{d^2 f}{dx^2} = \lambda f. \tag{12}$$

For the ξ variable, we have

$$\frac{1}{s}\frac{d}{d\xi}\left(\frac{1}{s}\frac{df}{d\xi}\right) = \lambda f, \tag{13}$$

and it is discretized as

$$a_j f_{j-1} - (a_j + b_j) f_j + b_j f_{j+1} = \lambda f_j \tag{14}$$

where a_j and b_j are given in (8). Let us shift the index j, such that

$$\xi_0 = H, \quad \xi_m = D = H + m\Delta\xi,$$

then for $j \leq -1$, we have $a_j = b_j = 1/(\Delta\xi)^2$ and

$$\frac{f_{j-1} - 2f_j + f_{j+1}}{(\Delta x)^2} = \lambda u_j. \tag{15}$$

At the boundary of the truncated domain, we use a simple zero Dirichlet boundary condition. Therefore,

$$f_m = 0. \tag{16}$$

For $j \leq 0$, we can assume that the solution is a linear combination of two exponential functions

$$f_j = e^{-\gamma(\xi_j - H)} + Re^{\gamma(\xi_j - H)}, \tag{17}$$

where γ is a positive constant. The first term is an exponentially decaying solution that has been scaled to have amplitude 1 at $\xi = H$ and the second term is an exponentially growing solution that has amplitude R at $\xi = H$. From (15), we can find a simple equation for γ:

$$\frac{e^{-\gamma\Delta\xi} - 2 + e^{\gamma\Delta\xi}}{(\Delta\xi)^2} = \lambda. \tag{18}$$

The coefficient R is the discrete reflection coefficient and it is non-zero because ξ has to be truncated. To find R, we use Eq. (14) for $j = 0, 1, ..., m-1$, together with the extra condition (16) and the following two special cases of (17):

$$f_0 = 1 + R, \quad f_{-1} = e^{\gamma\Delta\xi} + Re^{-\gamma\Delta\xi}. \tag{19}$$

These conditions give rise to the following tridiagonal linear system:

$$\begin{bmatrix} \hat{c}_0 & b_0 & & & & \\ a_1 & c_1 & b_1 & & & \\ & a_2 & c_2 & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & c_{m-2} & b_{m-2} \\ & & & & a_{m-1} & c_{m-1} \end{bmatrix} \begin{bmatrix} R \\ f_1 \\ f_2 \\ \vdots \\ f_{m-2} \\ f_{m-1} \end{bmatrix} = \begin{bmatrix} d_0 \\ -a_1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}, \tag{20}$$

where

$$c_j = -a_j - b_j - \lambda, \quad \hat{c}_0 = c_0 + a_0 e^{-\gamma\Delta\xi}, \quad d_0 = -c_0 - a_0 e^{\gamma\Delta\xi}.$$

Notice that R is defined for a fixed λ, a given m, a given $\Delta\xi$ and a given function s. Meanwhile, s is related to the integer p and the coefficient S_0. In the following, we will solve only S_0 assuming that all other parameters are known. In particular, we assume that an approximate value of the exact eigenvalue λ is known. If we consider R as a function of S_0, then we find the optimal value of S_0 by minimizing the absolute value of R.

5 Numerical examples

In this section, we illustrate our method by a number of examples. First, we consider a rectangular waveguide with a $(3a) \times (2a)$ waveguide core, where $a = 2.4628\mu m$. In terms of the dimensionless variables defined by a scaling of a, the waveguide core is given by $|x| < 1.5$ and $|y| < 1$, where x and y correspond to $\hat{x}$ and $\hat{y}$ in Eq. (3). The refractive indices of the waveguide core and the cladding are $n_1 = 1.51$ and $n_0 = 1.50$, respectively. These two values are very close to each other, so that the weakly guidance approximation, leading to the simplified eigenvalue problem (2), is valid. For a free space wavelength of $1.55\mu m$, we have $k_0 = 2\pi/1.55(\mu m)^{-1}$ and $\rho = (k_0 a)^2(n_1^2 - n_0^2) = 3$ in the waveguide core. Due to the symmetry, we only need to solve the problem in the first quadrant. For the symmetric even mode, where the eigenfunction u is an even function of x and y, we have the boundary conditions $\partial_x u = 0$ at $y = 0$ and $\partial_y u = 0$ at $x = 0$.

The exact eigenvalue of this problem is unknown. When a finite difference method is used, the numerical approximation converges to the exact solution as the grid size tends to zero, but the convergence rate is quite slow for a second order finite difference scheme. This is not our main concern here, as we are considering techniques for effective truncation of the computation domain. Therefore, we will fix the grid size and compare various numerical solutions obtained with different ways of truncating the domain. For $h = \Delta x = \Delta y = 0.05$, we first calculate the numerical solution without using coordinate stretching. The domain is truncated to a square given by $0 < x < D$ and $0 < y < D$ and a simple zero Dirichlet boundary condition is used at $x = D$ and $y = D$. Due to the Neumann boundary conditions at $x = 0$ and $y = 0$, we have discretized x and y by $x_j = (j - 0.5)h$ and $y_k = (k - 0.5)h$ for $j \geq 1$ and $k \geq 1$. For $D - h/2 = 2$, 2.5, 3, 3.5, ..., 10, the approximate eigenvalues are shown in Fig. 1. As D is increased, the numerical eigenvalue converges to a constant $\lambda^{(0.05)} \approx 1.5226738587$.

To use the coordinate stretching technique, we need an approximation of the eigenvalue to find the best parameter S_0. Although an accurate solution is already found earlier, we choose to use the rough estimate $\lambda^{(appro)} = 1.5$ corresponding to 1/2 of the maximum of $\rho(x, y)$ (since $\rho = 3$ in the waveguide core). We also have to choose the integer m which is the number of points in the stretching layer. For $m = 7$ and a

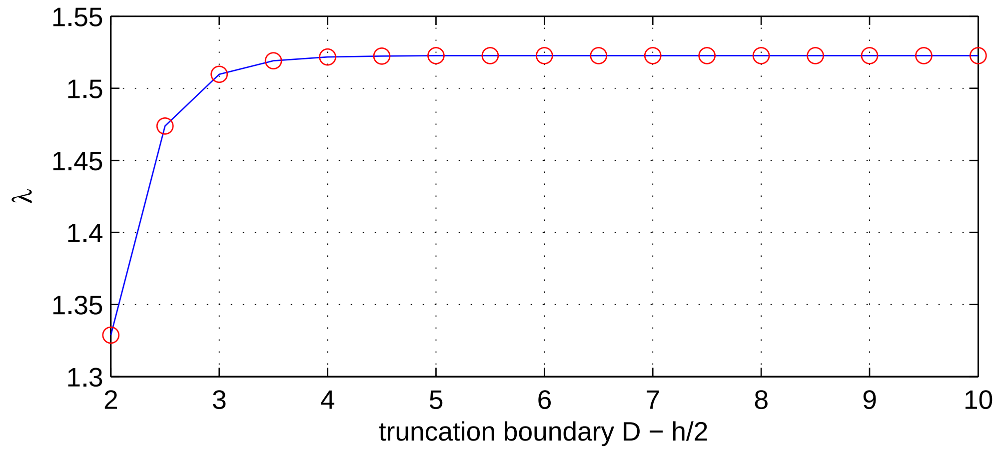

Figure 1: Numerical approximations of the eigenvalue calculated with the fixed grid size 0.05 in a truncated domain given by $0 < x, y < D$.

quadratic stretching function (i.e. $p = 2$), we find the optimal parameter $S_0 \approx 11.72$. In Fig. 2, we show the magnitude of the reflection coefficient R as a function of S_0. In

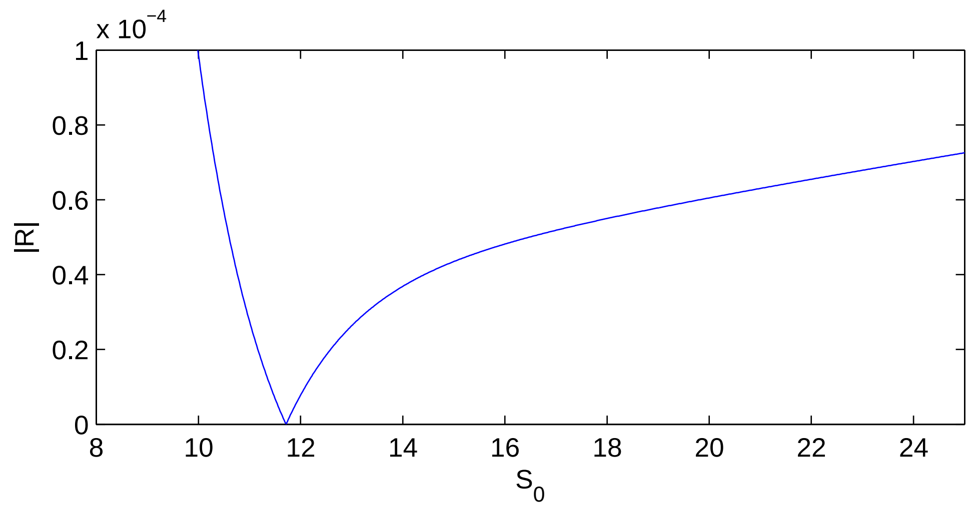

Figure 2: Magnitude of the reflection coefficient R as a function of S_0, for $m = 7$, $p = 2$, $\lambda \approx 1.5$ and $\Delta\xi = 0.05$.

fact, there is an S_0 such that R is exactly zero. However, this does not mean that we can use the m point stretching layer to exactly simulate the infinite domain, because the reflection coefficient is derived from a one-dimensional (1D) model. Since R can be easily found by solving the $m \times m$ tridiagonal linear system (20), it is straightforward to find the minimum of $|R|$. Besides, since the final numerical results are not sensitive to the stretching function, we do not need high accuracy for the optimal S_0, in fact, two or three digits are sufficient. For computations using the coordinate stretching technique, we switch to the transformed variables ξ and η. For these variables, the grid size is fixed at $h = \Delta\xi = \Delta\eta = 0.05$. In the ξ direction, the stretching layer where $s > 1$, is given by $H < \xi < D$ for $H = 2 - h/2 = 1.975$ and $D = H + mh = 2.325$. For $S_0 = 11.72$, the interval (D, H) is stretched by a factor of $S_0 + 1$. Therefore, $\xi = D = 2.325$ corresponds to $x = 6.427$. However, only seven points are used from $x = 1.975$ to $x = 6.427$. In the η direction, we use the same parameters, so that the stretching layer is $1.975 < \eta < 6.427$ and the stretching function r is identical to s (except ξ is replaced by η). For these selections, we found the approximate eigenvalue $\lambda_{cs}^{(0.05)} = 1.5226\underline{796}$. Using the accurate solution $\lambda^{(0.05)}$ given earlier as the reference solution, we found that the relative error of $\lambda_{cs}^{(0.05)}$ is 3.76×10^{-6}. Compared with earlier numerical results without coordinate stretching (as shown in Fig. 1), this result is more accurate than $1.5226\underline{682}$ obtained with $D = 6.025$ and less accurate than $1.52267\underline{23}$ obtained with $D = 6.525$. In the above calculation using coordinate stretching, the number of discrete points for both ξ and η is 46. Therefore, the discretized eigenvalue problem involves a 2116×2116 sparse matrix. In contrast, for $D = 6.025$ and if the coordinate stretching is not used, we have a 14400×14400 sparse matrix. Notice that the obtained numerical solution is also physically meaningful in the stretching region if we use the original variables x and y. For $\xi > H$ and the polynomial stretching function s given in (11), we have

$$x = \int_0^\xi s(\tau)d\tau = \xi + S_0 \frac{(\xi - H)^{p+1}}{(D - H)^p}.$$

In Fig. 3, we show the computed eigenfunction near the x and y axes. The seven points

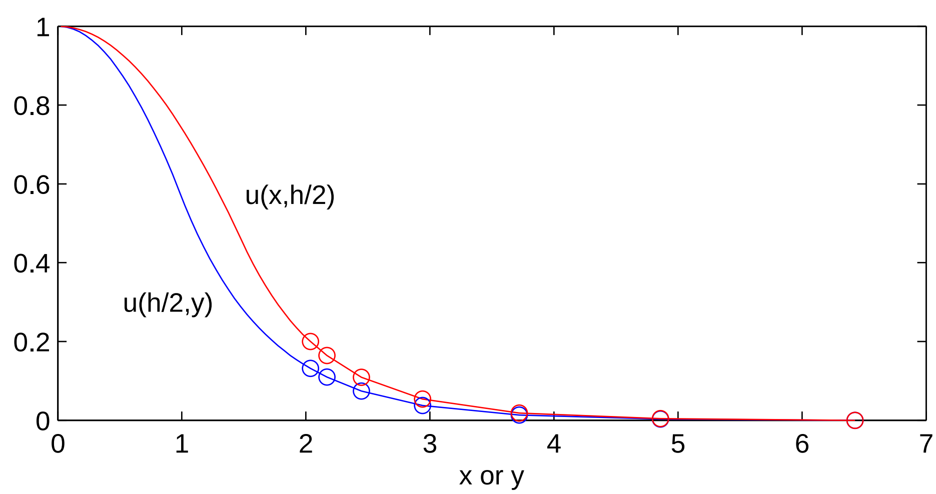

Figure 3: Eigenfunction near the x and y axes, computed using a coordinate stretching technique where the seven points in the stretched interval are shown as the small circles in the solution curves.

in the stretching intervals are marked by the little circles on the eigenfunction curves. We have compared this solution with the more accurate solutions obtained without coordinate stretching using $D \geq 6.525$, the difference can hardly be observed.

To analyze the sensitivity of the coordinate stretching technique with respect to the estimated eigenvalue, we carry out more calculations by varying $\lambda^{(appro)}$ from 1.0 to 2.0 with an increment of 0.1. The corresponding coefficient S_0 decreases monotonically from 14.92 to 9.84. The relative error of the computed eigenvalue decreases from 8.08×10^{-6} at $\lambda^{(appro)} = 1.0$ to 1.31×10^{-7} at $\lambda^{(appro)} = 1.7$, then increases to 6.49×10^{-6} at $\lambda^{(appro)} = 2.0$. We notice that the most accurate numerical solution is not obtained when $\lambda^{(appro)}$ is closest to the exact eigenvalue, this is possibly caused by the 1D model (12) which ignores the variation in y when a stretching in the x direction is concerned.

For the second example, we consider a square waveguide embedded in a slab. The waveguide core is a $(2a) \times (2a)$ square and it is embedded in a slab with a thickness of $2a$, where $a = 2.5\,\mu m$. The refractive indices of the core, the slab and the medium above and below the slab are $n_1 = 1.51$, $n_2 = 1.5$ and $n_0 = 1.4$, respectively. In terms of the variables scaled by a, the refractive index function satisfies

$$n(x,y) = \begin{cases} n_1, & |x| < 1 \text{ and } |y| < 1, \\ n_2, & |x| > 1 \text{ and } |y| < 1, \\ n_0, & |y| > 1. \end{cases}$$

We assume that the scalar model (2) is still applicable, although the index difference is small only in the x direction. The equation is again written in the dimensionless form (3), where $\hat{x}$ and $\hat{y}$ are denoted by x and y here. Notice that the function $\rho(x,y)$ in (3) satisfies $\rho = 0$ only for $|y| > 1$. For a free space wavelength of $1.55\,\mu m$, we have $\rho = \rho_1 \approx 32.8747$ and $\rho = \rho_2 \approx 29.7834$ in the core and the slab, respectively. As before, we consider the symmetric even mode and restrict the computation to the first quadrant using zero Neumann boundary conditions along the x and y axes.

To validate the coordinate stretching technique, we need an accurate numerical solution for a fixed grid size, on a very large computation domain, without using coordinate stretching. For $\Delta x = \Delta y = h = 0.05$, we have $\lambda^{(0.05)} \approx 30.140540418174$. This result is obtained in a sequence of calculations using $(2N) \times N$ discrete points, where $N = 25$, 30, 35, ..., 120. Since the discrete points are given by (x_j, y_k) for $1 \le j \le 2N$ and $1 \le k \le N$, the computation domain is given by $0 < x < D_x$ and $0 < y < D_y$, where $D_x = (2N+0.5)h$ and $D_y = (N+0.5)h$. For $N = 120$, we have $D_x = 12.025$ and $D_y = 6.025$. A convergence to all 14 digits of $\lambda^{(0.05)}$ given above is observed in this sequence of calculations. To use the coordinate stretching technique, we start with a 40×25 uniform mesh covering roughly a 2×1.25 rectangle, then add stretching layers of $m_x = 11$ and $m_y = 6$ grid points in the x and y directions, respectively. This leads to a total of $50 \times 30 = 1500$ discrete points. The decay rate of the eigenfunction is very different in the x and y directions. For the x direction, the 1D model (12) used to estimate the parameters of the stretching function should be replaced by $d^2 f/dx^2 = (\lambda - \rho_2) f$, since $\rho = \rho_2 \neq 0$ in the slab. For the y direction, (12) is still valid if x is replaced by y. For a quadratic stretching profile, i.e., $p = 2$ in (11), and using $(\rho_1 + \rho_2)/2 \approx 31.33$ as a rough estimate for λ, we obtain the optimal coefficients $S_0 = S_{0x} = 7.64$ and $S_0 = S_{0y} = 1.72$ for the x and y directions, respectively. Based on these parameters, we obtain the approximate eigenvalue $\lambda_{cs}^{(0.05)} = 30.140540\underline{11}$. Compared with $\lambda^{(0.05)}$ given earlier, the relative error of $\lambda_{cs}^{(0.05)}$ is 1.03×10^{-8}. If coordinate stretching is not used, the same level of accuracy can only be achieved with $N = 60$ which corresponds to a total of 7200 discrete points. In Fig. 4, we show the eigenfunction near the x and y axes. The small circles in Fig. 4

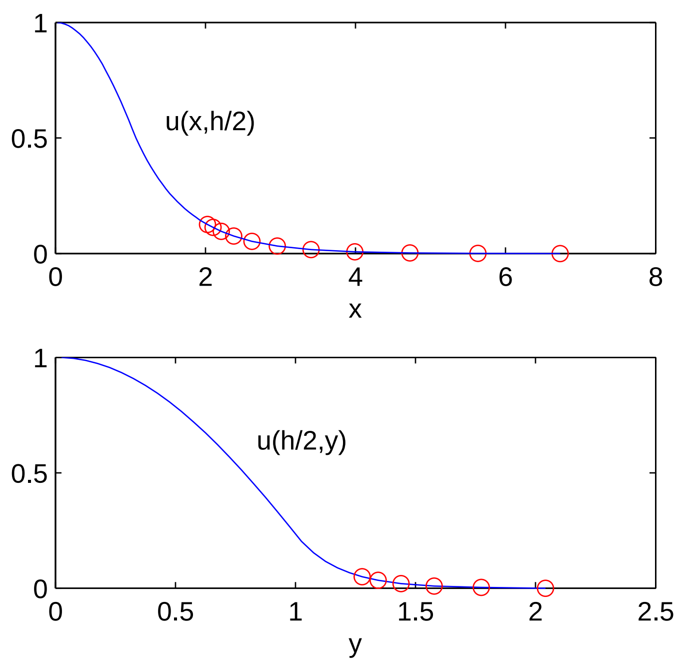

Figure 4: Eigenfunction near the x and y axes for a square waveguide embedded in a slab, computed with stretching coordinates.

denote the points in the stretched intervals. If $\lambda^{(appro)} = 31$ is used to estimate the optimal coefficients, we obtain $S_{0x} = 8.82$. In that case, the numerical solution is more accurate and the relative error of the computed eigenvalue is about 2.4×10^{-9}.

6 Discussions and conclusions

In this paper, we developed a simple technique for coordinate stretching in connection with a finite difference optical waveguide mode solver. The stretching function is given in the form of a simple polynomial with a scaling parameter S_0. The optimal scaling parameter is determined by minimizing the magnitude of the discrete reflection coefficient derived from a 1D model. The discrete reflection coefficient can be easily solved from a small tridiagonal linear system. Overall, the required computing effort to determine the scaling parameter is negligible compared with the main work for solving the matrix eigenvalue problem. Numerical examples indicate that the optimal coordinate stretching allows us to significantly reduce the size of the resulting matrix.

Our method is presented for the scalar eigenvalue problem (2), since it is much easier for us to find accurate numerical solutions to compare with the solution obtained using coordinate stretching. The method should be applicable to the more challenging full-vector eigenvalue problem (1). Consider a stretching layer for the x direction, we may assume that refractive index function in this layer depends only on y and is piecewise constant. In that case, ∂_x^2 appears in the two operators A_{11} and A_{22} defined in section 2 and it can be discretized as in (5). The other two operators A_{12} and A_{21} vanish where n is a constant, but they need to be properly discretized for grid points at and near the interfaces. The stretching profile can be selected based on the scalar model, since (2) is valid in each domain where n is a constant. Assuming that $n = n_\infty(y)$ as $|x| \to \infty$, the coefficients in the stretching profile can be estimated in the layer where n_∞ reaches its maximum. As in the scalar case, we need a rough estimate for the eigenvalue.

The technique developed in this paper is based on the assumption that the eigenfunction decays to zero exponentially as $|x|$ or $|y|$ tend to infinity. If the waveguide is composed of lossy material, the propagation constant becomes complex and the eigenfunction exhibit oscillations, but it still decays exponentially and our method should be useful. On the other hand, if the waveguide is leaky, the mode exhibit an outgoing wave behavior as $|x|$ or $|y|$ tends to infinity. In that case, it is necessary to use perfectly matched layers (PMLs) which correspond to complex coordinate stretchings [26]. For frequency domain propagation problems, we proposed to optimize a PML profile based on the average reflection coefficient for all plane waves incident upon the PML [24]. The 1D model used in this paper is simpler, as it corresponds to waves at normal incidence only. We are currently investigating the problem of optimizing the PMLs for leaky mode calculations.

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