Minimizing the Discrete Reflectivity of Perfectly Matched Layers

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Abstract

The perfectly matched layer (PML) method is widely used for truncating unbounded domains in simulations of optical wave-guiding structures. In this paper, we develop a practical procedure for selecting a PML profile for a given set of discretization parameters. Our approach is designed for frequency domain simulations and it is based on minimizing the average discrete reflectivity of the PML.

1 Introduction

The perfectly matched layer (PML) [1] is a widely used method for truncating unbounded domains in numerical simulations of wave propagation problems. The technique has been used in the beam propagation method [2, 3] and the mode matching method [4] for modeling optical waveguides. A PML can be regarded as a complex coordinate stretching [5] that turns outgoing waves to exponentially decaying solutions. If a PML is used to truncate the x-axis, then x is replaced by $\hat{x} = \int^x s(\tau)d\tau$, where $s(x) = 1 + i\sigma(x)$ and σ is a real function. The real part of s can also be replaced by a function to suppress waves evanescent in the x direction [6]. For actual numerical simulations, the PML has a finite thickness. This leads to a non-zero reflection for plane waves incident upon the PML.

The reflectivity of a PML in connection with a finite difference approximation has been studied by Yevick *et al.*[7] Such a discrete reflectivity depends on the actual profile of σ and it does not decrease indefinitely when σ is increased. In this paper, we present a simple method for selecting a profile for σ based on the average discrete reflectivity of the PML. For each profile of σ, an optimal scaling parameter is determined by minimizing the average discrete reflectivity.

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2 Reflectivity of a PML

Consider transverse electric waves in a two-dimensional wave-guiding structure. The y-component of the electric field satisfies a Helmholtz equation. If the structure is unbounded in the negative x direction and the medium is homogeneous (with a constant refractive index $n = n_0$) for $x < G$, we can truncate the negative x-axis by a PML. For D and H satisfying $D < H < G$, we define $\sigma(x)$ such that $\sigma(x) = 0$ for $x \geq H$ and $\sigma(x) > 0$ for $x < H$, then replace x by $\hat{x} = \int^x s(\tau)d\tau$, where $s = 1 + i\sigma$. This gives rise to

$$s^{-1}\partial_x(s^{-1}\partial_x u) + \partial_z^2 u + k_0^2 n^2(x, z)u = 0, \tag{1}$$

where k_0 is the free space wavenumber, n is the refractive index and the time dependence is $e^{-i\omega t}$. At $x = D$, we can use a simple zero boundary condition: $u = 0$. The actual PML is the layer $D < x < H$ where Eq. (1) is different from the original Helmholtz equation.

For $H < x < G$, Eq. (1) has a plane wave solution

$$u = e^{i(-\alpha x + \beta z)} + Re^{i(\alpha x + \beta z)},$$

where $\alpha > 0$ and $\alpha^2 + \beta^2 = k_0^2 n_0^2$. The first term is a plane wave propagating towards $x = -\infty$, the second term is the reflected wave due to the boundary $x = D$, R is the reflection coefficient and it satisfies[1, 7]

$$|R| = e^{-2\alpha \int_D^H \sigma(\tau)d\tau}.$$

Let θ be the angle between the z-axis and the wave vector $(-\alpha, \beta)$, then $\beta = k_0 n_0 \cos\theta$ and $\alpha = k_0 n_0 \sin\theta$. Clearly, R depends on the angle of incidence θ. In particular, $|R|$ can be close to 1, if the waves are nearly parallel to the z-axis (i.e. θ is small). For a fixed θ, $|R|$ depends only on $\int_D^H \sigma(\tau)d\tau$, not the actual profile of σ. Besides, $|R|$ can be arbitrarily small, if $\int_D^H \sigma(\tau)d\tau$ is sufficiently large.

When x is discretized, the reflection coefficient depends on the actual profile of σ and it cannot be reduced indefinitely by increasing σ [7]. Consider a second order finite difference approximation in the transverse direction x, Eq. (1) becomes

$$\frac{d^2 u_j}{dz^2} + \frac{a_j u_{j-1} + b_j u_j + c_j u_{j+1}}{h^2} + k_0^2 n^2(x_j, z)u_j = 0, \tag{2}$$

where $u_j \approx u(x_j, z)$, $x_j = x_0 + jh$, h is the grid size,

$$a_j = \frac{1}{s_j s_{j-1/2}}, \quad c_j = \frac{1}{s_j s_{j+1/2}}, \quad b_j = -a_j - c_j, \tag{3}$$

for $s_j = s(x_j)$ and $s_{j\pm 1/2} = s(x_j \pm h/2)$. An alternative discretization is based on $\hat{x}_j = \int^{x_j} s(\tau) d\tau$ and

$$\begin{aligned} \frac{1}{s}\frac{\partial}{\partial x}\left(\frac{1}{s}\frac{\partial u}{\partial x}\right)\Big|_{x=x_j} &= \frac{\partial^2 u}{\partial \hat{x}^2}\Big|_{x=x_j} \\ &\approx \frac{2}{\hat{x}_{j+1}-\hat{x}_{j-1}}\left(\frac{u_{j+1}-u_j}{\hat{x}_{j+1}-\hat{x}_j} - \frac{u_j - u_{j-1}}{\hat{x}_j - \hat{x}_{j-1}}\right). \end{aligned} \tag{4}$$

For $H < x_j < G$, the coefficients are simplified to $a_j = c_j = 1$ and $b_j = -2$. We also assume that $D = x_0$ and $x_m = H = D + mh$ for some integer m. For $H < x_j < G$, we have

$$u_j = u_j^{(1)} + u_j^{(2)} = e^{i(-\alpha x_j + \beta z)} + R e^{i(\alpha x_j + \beta z)},$$

where α is positive, α and β satisfy

$$\beta^2 + \frac{4}{h^2}\sin^2\frac{\alpha h}{2} = (k_0 n_0)^2. \tag{5}$$

In the above, $u_j^{(1)}$ represents a plane wave propagating towards $x = -\infty$. Due to the boundary condition at $x = D$ and the discretization of the PML, the plane wave gives rise to a reflected wave $u_j^{(2)}$ and R is the discrete reflection coefficient.

To find R, we write down Eq. (2) for $j = 1, 2, ..., m$. The zero boundary condition at $x = D$ gives $u_0 = 0$. After some simplifications, we obtain the following system:

$$\begin{bmatrix} \hat{b}_1 & c_1 & & \\ a_2 & \ddots & \ddots & \\ & \ddots & \hat{b}_{m-1} & c_{m-1} \\ & & a_m & d_m \end{bmatrix} \begin{bmatrix} v_1 \\ \vdots \\ v_{m-1} \\ \hat{R} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ -c_{m-1} \\ -e_m \end{bmatrix}, \tag{6}$$

where $\hat{R} = R e^{2i\alpha x_m}$,

$$\begin{aligned} d_m &= \hat{b}_m + c_m e^{i\alpha h}, \quad e_m = \hat{b}_m + c_m e^{-i\alpha h}, \\ \hat{b}_j &= b_j + 4\sin^2\tfrac{\alpha h}{2}, \quad v_j = u_j e^{-i(\alpha x_m + \beta z)}, \end{aligned}$$

for $j = 1, ..., m$. For the discretization scheme (4), an approximate formula for the discrete reflection coefficient R was developed in [7]. Since m is typically quite small, it is not expensive to find R exactly by solving (6). Notice that R depends on α. Alternatively, we consider R as a function of the angle θ between the wave vector $(-\alpha, \beta)$ and the z-axis. In the current discrete version, (5) is satisfied and θ is defined by

$$\beta = k_0 n_0 \cos\theta, \quad \frac{2}{h}\sin\frac{\alpha h}{2} = k_0 n_0 \sin\theta.$$

Our approach is to select a profile for σ and its scaling parameter so that the average of $|R|$, i.e.

$$\overline{|R|} = \frac{2}{\pi}\int_0^{\pi/2} |R(\theta)| d\theta \tag{7}$$

is minimized.

3 Numerical Results

In this section, we compare a few profiles of σ for practical discretization parameters. For $D < x < H$, we write $\sigma(x) = S\sigma_0(x)$, where S is a dimensionless scaling parameter and

$$\int_D^H \sigma_0(x)dx = H - D.$$

In the continuous case, $|R|$ depends only on $S|H - D|$. In the discrete case, the choice of σ_0 is important. We consider σ_0 given as simple powers:

$$\sigma_0(x) = (p+1)\left(\frac{x-H}{D-H}\right)^p, \quad p = 0, 1, 2, 3, ... \tag{8}$$

As an example, we consider a PML with a thickness of five grids (i.e. $m = 5$) where the grid size h is 1/20 of the wavelength in the medium. More precisely, we have $\lambda_0 = 1\,\mu m$, $k_0 = 2\pi/\lambda_0$, $n_0 = 1$ and $h = 0.05\,\mu m$. The average discrete reflectivity $\overline{|R|}$

p	0	1	2	3	4
$\overline{\lvert R\rvert}$	0.19	0.066	0.014	0.013	0.015
S	1.64	5.65	18.0	25.1	23.3

Table 1: Average reflectivity and optimal scaling parameter for PML profiles given in (8). The results correspond to a discretization using 20 points per wavelength and a PML with a thickness of five grids.

and the optimal values of S are listed in Table 1 for $p = 0, 1, 2, 3, 4$. For more details, we plot $|R|$ as functions of θ in Fig. 1 for $p = 2$, 3 and 4. From Table 1, it appears that the cubic profile is the best. In fact, the values of $\overline{|R|}$ for $p = 2$, 3 and 4 are quite close. It can be seen from Fig. 1 that the quadratic profile gives the lowest reflectivity for $\theta > 0.1\pi/2$, while the cubic profile has the lowest reflectivity for small angles. These results are obtained using the first discretization (3). The second discretization (4) is not recommended, since it gives a much larger reflectivity as shown in Fig. 2 for $p = 2$. To illustrate the dependence on the scaling parameter S, we plot the discrete reflectivity $|R(\theta)|$ of the quadratic profile for $S = 16$, $S = 18$ and $S = 20$ in Fig. 3. It can be observed that the smallest value of S (i.e. $S = 16$) gives the the lowest reflectivity for larger angles ($\theta > 0.5\pi/2$), while the largest value of S (i.e. $S = 20$) gives the lowest reflectivity for small angles ($\theta < 0.1\pi/2$). The optimal value of S (i.e. $S = 18$) gives a reasonable compromise, as it minimizes the average reflectivity.

Let S_* be the optimal value of the scaling parameter S for a given PML profile. It turns out that S_* depends only on m and $N = \lambda_0/(n_0 h)$, where N is the number of grid points per wavelength. We have calculated S_* for $5 \leq N \leq 25$, $m = 5, 6, ..., 15$ and $p = 2, ..., 5$. The results for $p = 3$ are shown in Fig. 4. We observe that S_* always

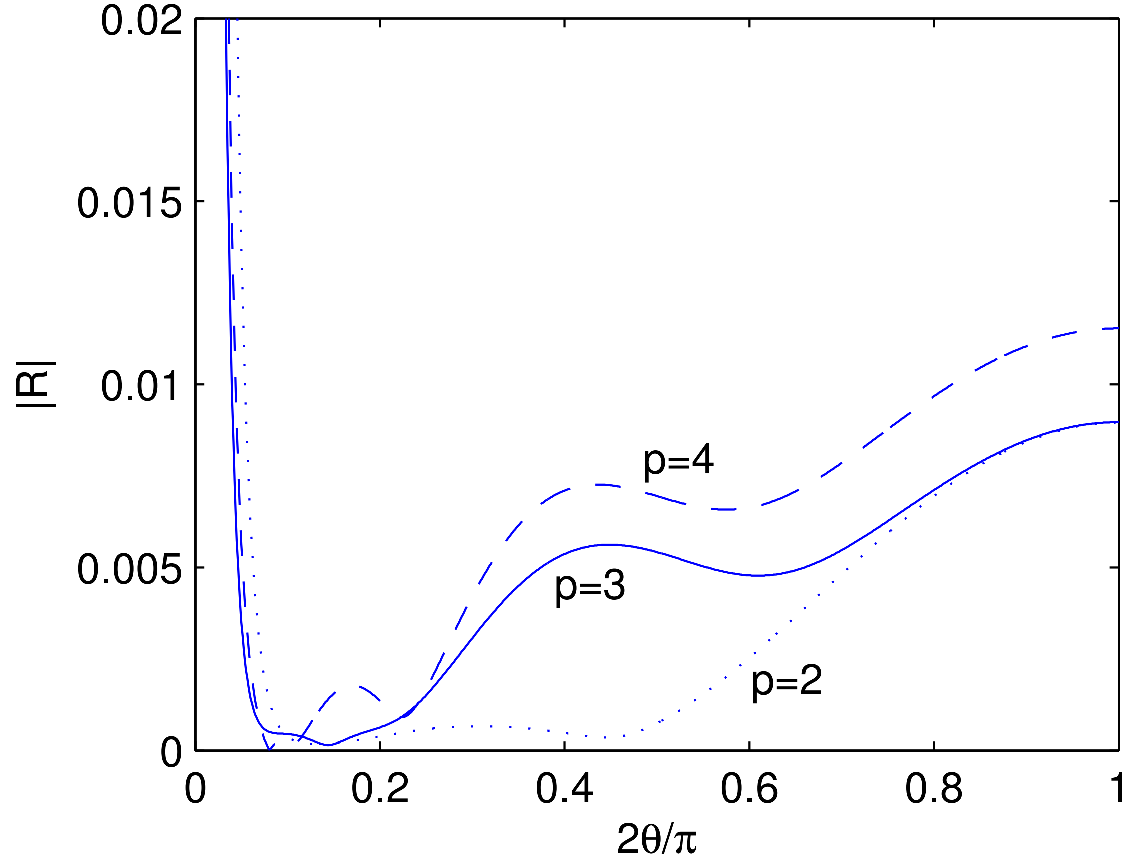

Figure 1: The discrete reflectivities of the quadratic (dotted line), cubic (solid line) and the 4th power PML profiles, using the optimal values of S given in Table 3.

increases with N, but it does not always increase with m. In Fig. 4, the curves for $m = 6$ and $m = 9$ have some unexpected behavior. When m and N are given, we choose the particular value of p which gives the smallest average reflectivity $\overline{|R|}$ when the corresponding S_* is used. For $5 \le m < 15$ and $5 \le N < 25$, the choice of p is summarized in Fig. 5.

4 Conclusion

In connection with a second order finite difference approximation, a practical procedure for calculating the optimal scaling parameter S of a PML profile is developed. Given the grid size, the free space wavelength, the refractive index and the thickness of the PML, we calculate the optimal value of S corresponding to the smallest average discrete reflectivity.

The method is presented for a PML with the simple zero boundary condition. The extension to other boundary conditions, such as $\partial_x u = \gamma u$ for some constant γ, is straight

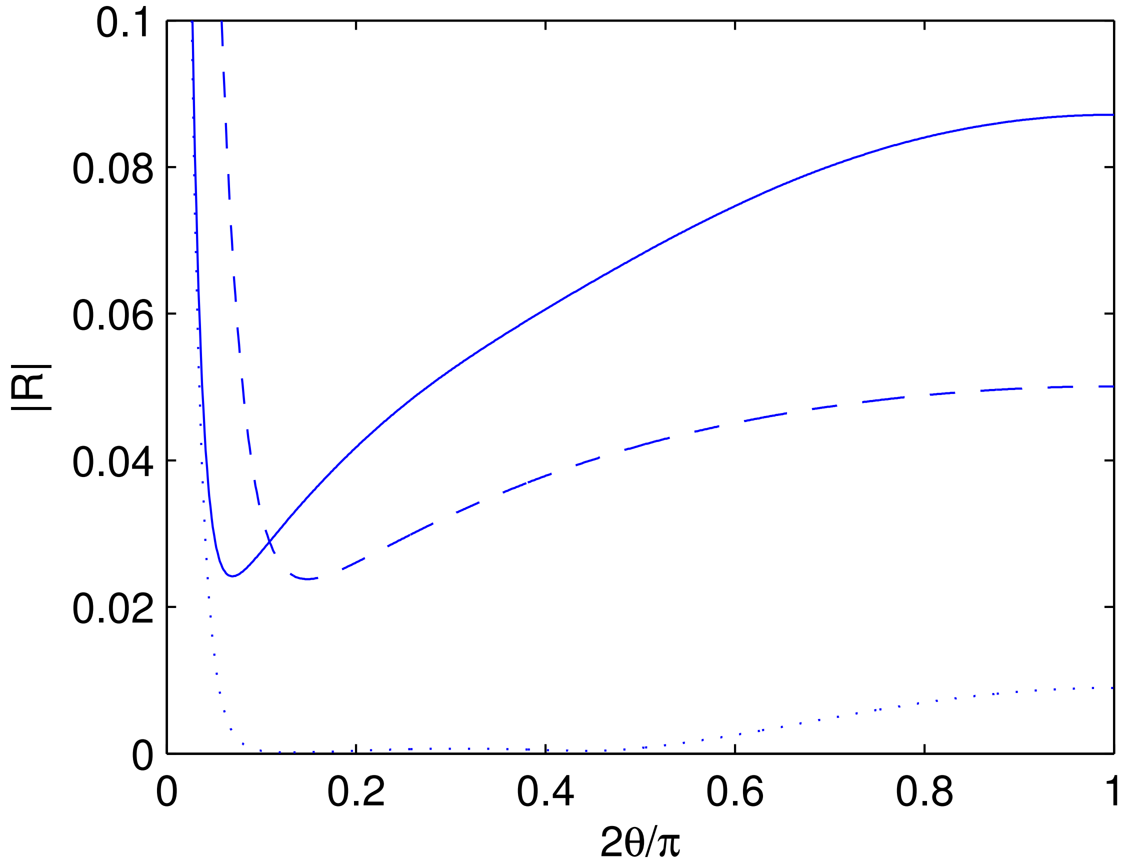

Figure 2: Comparison of reflectivity for discretization schemes (3) and (4) using the PML profile with $p = 2$. The dotted curve is for (3) with $S = 18$. The solid and the dashed curves are for (4) with $S = 18$ and $S = 8.4$, respectively. Here, $S = 8.4$ is the optimal value for discretization (4).

forward. We also considered other profiles besides those in (8). However, it appears that the four profiles corresponding to $p = 2, ..., 5$ of (8) are adequate for practical applications. A proper discretization in the PML is important. In particular, the widely used scheme (4) gives a poor performance. Although the method is presented for TE waves in 2-D structures, it actually applies to the TM case and to 3-D problems, as far as the PML is placed in a homogeneous medium.

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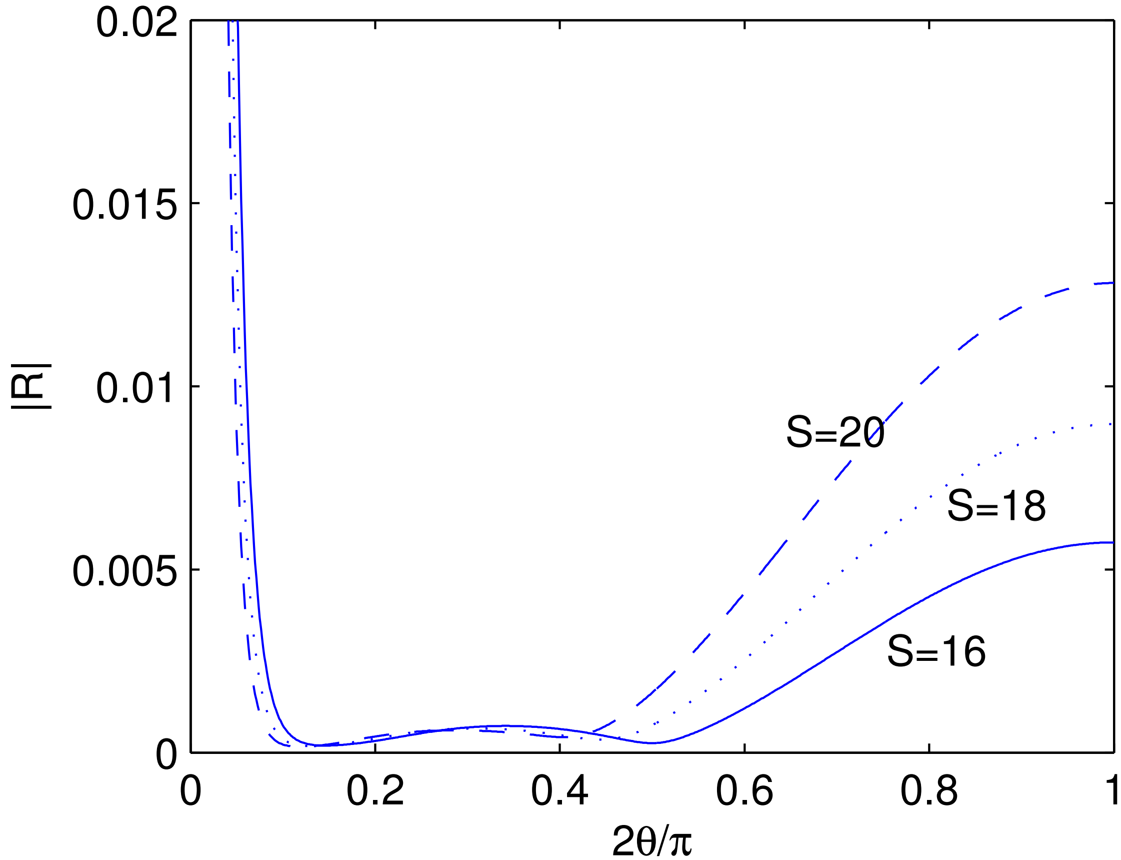

Figure 3: Discrete reflectivity for $p = 2$ and $S = 16$ (solid curve), $S = 18$ (dotted curve) and $S = 20$ (dashed line).

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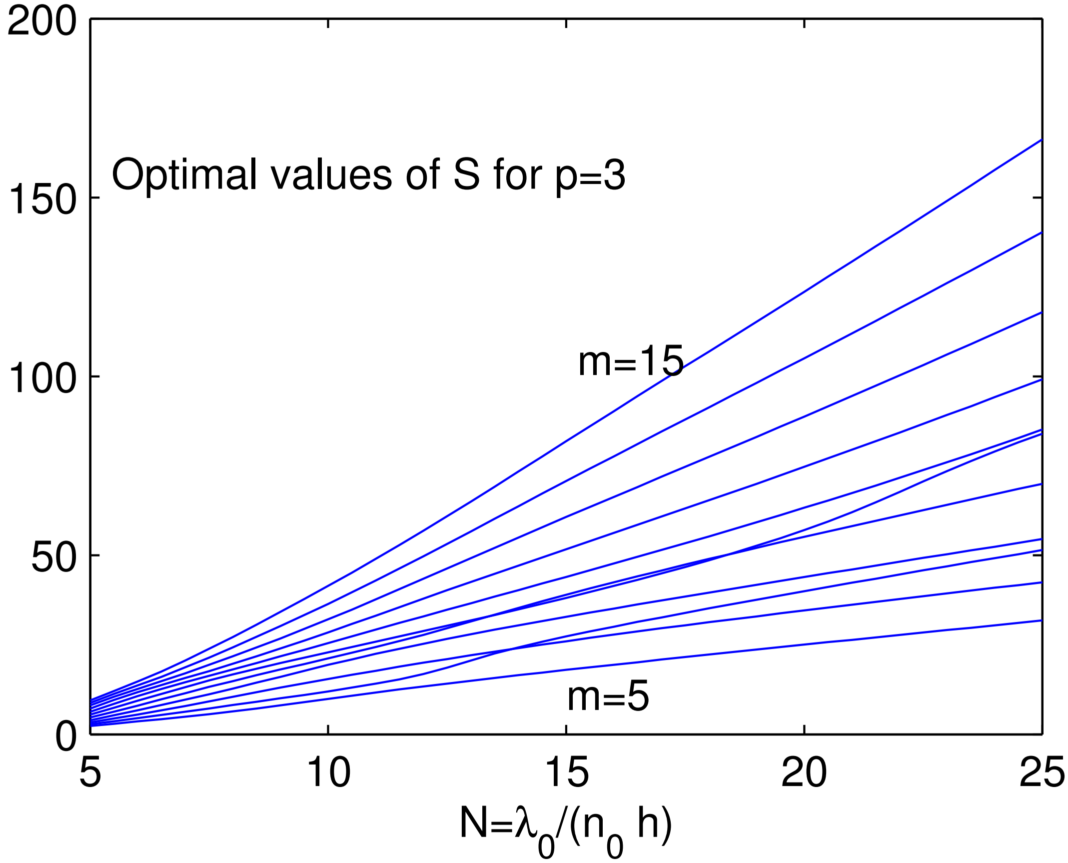

Figure 4: The dependence of the optimal scaling parameter S on N for the cubic profile and for different m.

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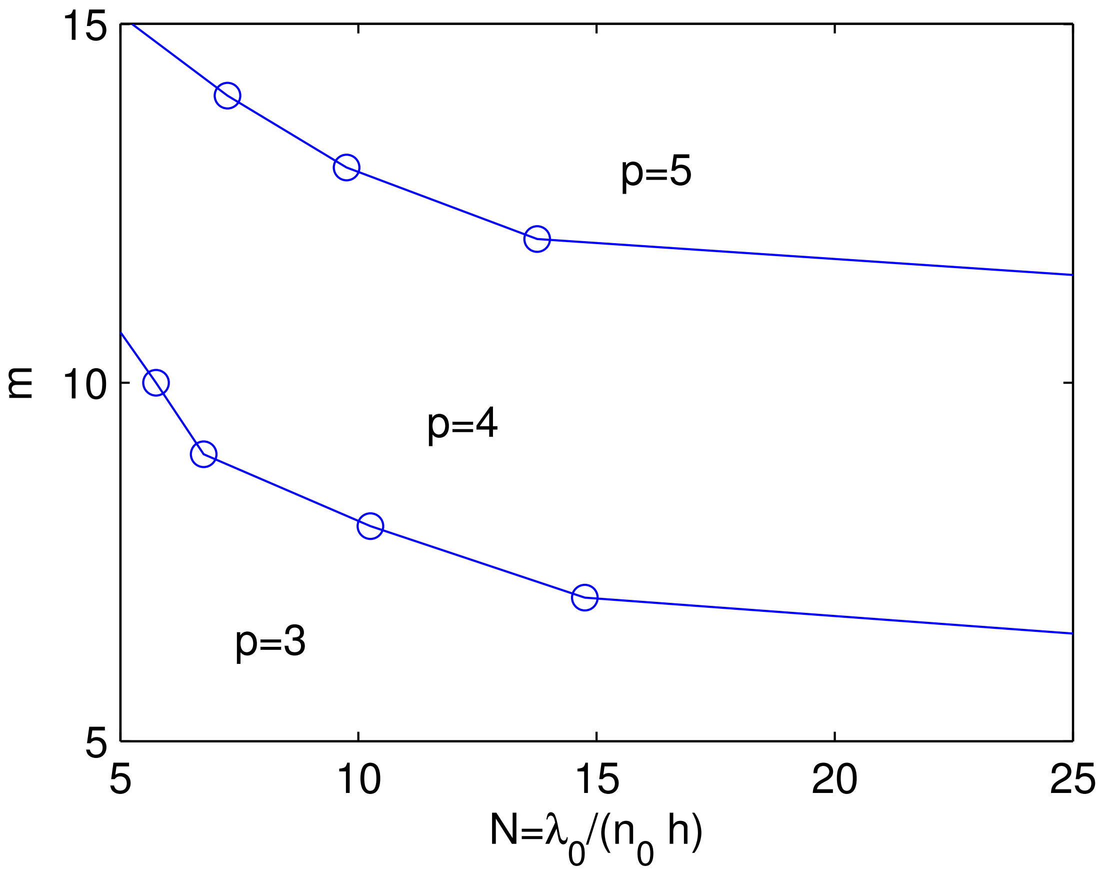

Figure 5: Selection of the PML profile (i.e., the integer p) based on the use of optimal scaling parameter S.