Efficient analytic computation of group delay dispersion from optical interference coatings

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Abstract: An inductive analytic method is presented for computing exact derivatives of phase with respect to frequency for arbitrary dielectric multilayer coatings. This algorithm is useful for the optimization of broadband dispersion compensating femtosecond laser optics.

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1. Introduction

The design and fabrication of dispersive optical thin-film filters and mirrors is very important for the generation of few-cycle laser pulses approaching the single-cycle regime [1]. For the design and optimization of these multilayer dielectric optical coatings efficient and accurate calculation of its dispersive properties is indispensable.

The standard method for computing the group delay dispersion is to compute complex reflection coefficients using the transfer matrix technique and then take successive finite differences over frequency. For mirror systems containing up to 160 layers this leads to a large numerical effort during optimization. In addition, accurately computing the mth order dispersion at a single wavelength requires computing at least $(m + 1)$ reflection coefficients and taking m finite differences. Unfortunately, numerical differentiation is inherently unstable [2] and achieving high accuracy requires careful optimization of sample spacing to balance the competing effects of round off error and truncation error. We demonstrate a method to analytically compute dispersion to any order and show how approximations in the derivative lead to highly efficient algorithms for dispersion calculations. In practice, the first m derivatives of phase at a given wavelength can be computed in less time than for m zeroth-order reflection coefficients, resulting in signicantly faster computation time than with numerical differentiation and yet without the associated issues of numerical stability.

2. General Method

Consider a dielectric stack whose total transfer matrix is given by

$$\mathbf{T}(k) = \begin{pmatrix} a(k) & b(k) \\ b^*(k) & a^*(k) \end{pmatrix} = \begin{pmatrix} |a(k)|e^{i\phi_a} & |b(k)|e^{i\phi_b} \\ |b(k)|e^{-i\phi_b} & |a(k)|e^{-i\phi_a} \end{pmatrix}. \tag{1}$$

The complex reflection coefficient is $r(k) = -b(k)/a(k)$. The phase of r is simply the difference between φ_b and φ_a. If we wish to find the mth derivative of the phase of r, we need to know the first m derivatives of the transfer matrix $\mathbf{T}$.

To avoid a combinatorial explosion of terms we must take derivatives inductively, stepping through the structure layer-by-layer and calculating each derivative of $\mathbf{T}$ from only the derivatives of the current single layer matrix and the derivatives of the total transfer matrix for the structure preceding the current layer. This can be done by recalling that matrix derivatives obey the same product rule as scalar functions: the mth derivative of a product of two matrices can be found as a function of the first m derivatives of each individual matrix. We can essentially follow the typical procedure for finding the zeroth-order reflectance of a structure, except now we must keep track of $m + 1$ matrices as we go along.

To calculate the recurrence relation for the mth derivative of the transfer matrix from the beginning of the structure up to the ℓth layer, we simply apply matrix product rules to the transfer matrices going from layer 0 to layer ℓ for the first m matrix derivatives:

$$\begin{aligned}
\frac{\partial \mathbf{T}_{(\ell,0)}}{\partial k} &= \frac{\partial\left(\mathbf{T}_\ell \mathbf{T}_{(\ell-1,0)}\right)}{\partial k} = \frac{\partial \mathbf{T}_\ell}{\partial k}\mathbf{T}_{(\ell-1,0)} + \mathbf{T}_\ell \frac{\partial \mathbf{T}_{(\ell-1,0)}}{\partial k}, \\
\frac{\partial^2 \mathbf{T}_{(\ell,0)}}{\partial k^2} &= \frac{\partial^2\left(\mathbf{T}_\ell \mathbf{T}_{(\ell-1,0)}\right)}{\partial k^2} = \frac{\partial^2 \mathbf{T}_\ell}{\partial k^2}\mathbf{T}_{(\ell-1,0)} + 2\frac{\partial \mathbf{T}_\ell}{\partial k}\frac{\partial \mathbf{T}_{(\ell-1,0)}}{\partial k} + \mathbf{T}_\ell \frac{\partial^2 \mathbf{T}_{(\ell-1,0)}}{\partial k^2}, \\
\frac{\partial^3 \mathbf{T}_{(\ell,0)}}{\partial k^3} &= \frac{\partial^3\left(\mathbf{T}_\ell \mathbf{T}_{(\ell-1,0)}\right)}{\partial k^3} = \frac{\partial^3 \mathbf{T}_\ell}{\partial k^3}\mathbf{T}_{(\ell-1,0)} + 3\frac{\partial \mathbf{T}_\ell}{\partial k}\frac{\partial^2 \mathbf{T}_{(\ell-1,0)}}{\partial^2 k} + 3\frac{\partial^2 \mathbf{T}_\ell}{\partial^2 k}\frac{\partial \mathbf{T}_{(\ell-1,0)}}{\partial k} + \mathbf{T}_\ell \frac{\partial^3 \mathbf{T}_{(\ell-1,0)}}{\partial k^3},
\end{aligned} \tag{2}$$

and so on, where $\mathbf{T}_{(\ell,0)}$ is the transfer matrix going from the zeroth layer to the ℓth layer and $\mathbf{T}_\ell$ is the transfer matrix for just the ℓth layer. Each term on the right hand side above is either known as an induction assumption (i.e. $\mathbf{T}_{(\ell,0)}$ terms) or can be calculated analytically (i.e. $\mathbf{T}_\ell$ terms). The only other pieces missing are the trivial statements of the starting matrices:

$$\mathbf{T}_{(0,0)} = \mathbf{I} \text{ and } \frac{\partial^n \mathbf{T}_{(0,0)}}{\partial k^n} = \mathbf{0}. \tag{3}$$

Since each successive derivative requires one more matrix multiplication than the last, the total number of matrix multiplications required to find the first m derivatives is $O[m^2]$. In general, each derivative of $\mathbf{T}_\ell$ will involve derivatives of material indices which break the symmetry inherent to a single layer transfer matrix. There is therefore no way to avoid doing each full matrix multiplication shown in (2). Thus, while this algorithm is still $O[n]$, where n is the number of layers, it becomes significantly slower than numerical differentiation for large m as numerical differentiation requires only $O[m]$ matrix multiplications per layer.

3. Fast Dispersion Computation

To see how the recursive scheme in (2) might be implemented quickly, consider the transfer function for a single layer and its derivative:

$$\begin{aligned}
\mathbf{T}_\ell(k) &= \begin{pmatrix} \left(1+p(k)\right)e^{-i\tilde{n}_\ell(k)d_\ell k} & \left(1-p(k)\right)e^{-i\tilde{n}_\ell(k)d_\ell k} \\ \left(1-p(k)\right)e^{i\tilde{n}_\ell(k)d_\ell k} & \left(1+p(k)\right)e^{i\tilde{n}_\ell(k)d_\ell k} \end{pmatrix} \\
\mathbf{T}'_\ell(k) &= \begin{pmatrix} \left[-id\left(1+p(k)\right)\left(\tilde{n}_\ell(k)+k\tilde{n}'_\ell(k)\right)+p'(k)\right]e^{-i\tilde{n}_\ell(k)d_\ell k} & \iddots \\ \left[id\left(1-p(k)\right)\left(\tilde{n}_\ell(k)+k\tilde{n}'_\ell(k)\right)-p'(k)\right]e^{i\tilde{n}_\ell(k)d_\ell k} & \ddots \end{pmatrix}
\end{aligned} \tag{4}$$

where $\tilde{n}(k)$ is the effective index of the layer and $p(k)$ is the ratio $\tilde{n}_{\ell\text{-}1}/\tilde{n}_\ell$ for TE waves and $n_\ell \tilde{n}_{\ell\text{-}1}/n_{\ell\text{-}1}\tilde{n}_\ell$ for TM.

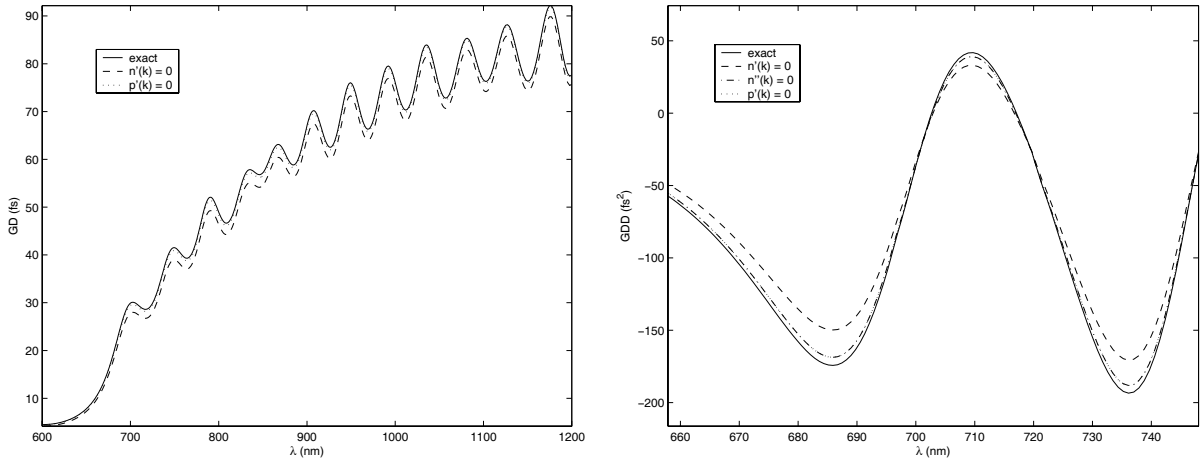

Fig. 1. Plots of GD and GDD for one 80 layer half of a DCM pair under various approximations.

Everything in the derivative is a simple multiplication with the exception of the $p'(k)$ terms, which break the symmetry. As it turns out, however, neglecting $p'(k)$ still leads to an excellent approximate calculation of the dispersion of an interference coating since dispersion is primarily due to the optical thickness of the layers and the associated phase shifts.

The result of neglecting the frequency variation of $p(k)$ is a dramatically simplified computation. Taking the mth derivative of a transfer matrix is then equivalent to multiplying by a complex scalar $D^{(m)}{}_{\ell}$, where ℓ is the layer to which it applies. In this context, the recursion relations in (2) can be rewritten as

$$\begin{aligned}
\frac{\partial \mathbf{T}_{(\ell,0)}}{\partial k} &= \frac{\partial\left(\mathbf{T}_{\ell}\mathbf{T}_{(\ell-1,0)}\right)}{\partial k} = D_{\ell}^{(1)}\mathbf{T}_{(\ell,0)} + \mathbf{T}_{\ell}\mathbf{T}'_{(\ell-1,0)}, \\
\frac{\partial^2 \mathbf{T}_{(\ell,0)}}{\partial k^2} &= \frac{\partial^2\left(\mathbf{T}_{\ell}\mathbf{T}_{(\ell-1,0)}\right)}{\partial k^2} = D_{\ell}^{(2)}\mathbf{T}_{(\ell,0)} + 2D_{\ell}^{(1)}\mathbf{T}_{\ell}\mathbf{T}'_{(\ell-1,0)} + \mathbf{T}_{\ell}\mathbf{T}''_{(\ell-1,0)}, \\
\frac{\partial^3 \mathbf{T}_{(\ell,0)}}{\partial k^3} &= \frac{\partial^3\left(\mathbf{T}_{\ell}\mathbf{T}_{(\ell-1,0)}\right)}{\partial k^3} = D_{\ell}^{(3)}\mathbf{T}_{(\ell,0)} + 3D_{\ell}^{(2)}\mathbf{T}_{\ell}\mathbf{T}'_{(\ell-1,0)} + 3D_{\ell}^{(1)}\mathbf{T}_{\ell}\mathbf{T}''_{(\ell-1,0)} + \mathbf{T}_{\ell}\mathbf{T}'''_{(\ell-1,0)}.
\end{aligned} \tag{5}$$

For a given derivative of $\mathbf{T}$, all terms on the right hand side are trivial scalar multiplications of previously computed matrices except for one; the sole new term which must be computed is always $\mathbf{T}_{\ell}\mathbf{T}^{(m)}_{(\ell-1,0)}$. As such, finding the first m derivatives can now be done with $O[m]$ matrix multiplications per layer, the same order of complexity of numerical differentiation methods. In practice, however, the analytic computation can be done significantly faster since all matrices involved are evaluated at a single wavelength and so only one new transfer matrix must be computed per layer.

4. Results

To gauge the efficacy of the approximation discussed above, we chose the rather extreme case of computing the dispersion of the off-axis reflection from one half of a double-chirped mirror pair having 80 layers with material indices of roughly 2.5 and 1.4, evaluated at an angle of incidence of 5 degrees. Such mirrors are used for the construction of octave spanning femtosecond laser systems emitting 5 fs pulses [1, 3]. Under MATLAB on a 2.4 GHz PC, the total computation time for the reflection, GD and GDD at 2024 wavelengths using the fully analytic method takes 1.53 s. The computation time when neglecting the $p'(k)$ terms becomes 0.6 s whereas the numerical calculation taking finite differences takes 1.1 s. Figure 1 shows the group delay (GD) and group delay dispersion (GDD) for several different levels of approximation, illustrating that the approximate calculation neglecting $p'(k)$ terms is a very accurate and efficient tool for the optimization of complex dielectric mirror structures with specified phase properties.

5. References

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