

Fast computation of Toeplitz forms and some multidimensional integrals

E. E. Tyrtysnikov *

January 23, 2005

Abstract

A fast algorithm is proposed for computation of certain multilevel Toeplitz forms. It helps to implement some simple quadrature formulas in an efficient way, allowing for the use of more nodes. An application example is given with the volume integral equations in electromagnetics.

1 Introduction

Given a multilevel Toeplitz matrix [5] with entries $a_{i_1-j_1, \dots, i_p-j_p}$ and multilevel vectors with components $u_{i_1}^1 \dots u_{i_p}^p$ and $v_{j_1}^1 \dots v_{j_p}^p$ (p is the number of levels and $1 \leq i_k, j_k \leq n$, $k = 1, \dots, p$), consider a problem of computation of the following quantity:

$$f = \sum_{1 \leq i_1, \dots, i_p \leq n} \sum_{1 \leq j_1, \dots, j_p \leq n} u_{i_1}^1 \dots u_{i_p}^p a_{i_1-j_1, \dots, i_p-j_p} v_{j_1}^1 \dots v_{j_p}^p. \quad (1)$$

This is a p -level Toeplitz form. A direct computation of f , based on the Fast Fourier Transform (FFT), requires $O(N \log N)$ arithmetic operations, where $N = n^p$. In this paper, we present a faster algorithm that delivers f in $O(N)$ operations for any $p \geq 2$.

In the case $p = 1$ the direct FFT-based computation remains unbeaten. However, the new algorithm is faster for $p \geq 2$. Moreover, a special structure in the vectors $[u_{i_l}^l]$ and $[v_{j_l}^l]$ improves the performance to $O(N)$ operations even in the case $p = 1$.

The advantage is not only in removing the logarithmic factor. Since the FFT is not involved, the complexity is no longer dependent on the arithmetic properties of n . The new algorithm is noticeably faster in practice, for instance, in typical applications with n from units up to several tens (e.g. $n = 10$) and $p = 3$.

Fast computation of multilevel Toeplitz forms allows us to suggest a fast method of computation of some multidimensional integrals (arising in the method of moments when solving some integro-differential equations).

2 Fast computation of Toeplitz forms

Consider first the case $p = 1$. In order to compute

$$f = \sum_{1 \leq i \leq n} \sum_{1 \leq j \leq n} u_i a_{i-j} v_j, \quad (2)$$

*This work was supported by the Russian Fund for Basic Research (grants 02-1-00590; 04-07-90336).

let us set $k = i - j$ and restructure summation as follows:

$$f = \sum_{j=1}^n \sum_{k=1-j}^{n-j} a_k u_{k+j} v_j = \sum_{j=1}^n \sum_{k=-n+1}^{n-1} a_k u_{k+j} v_j s(k, j),$$

where

$$s(k, j) = \begin{cases} 1, & 1 - j \leq k \leq n - j, \\ 0, & \text{otherwise.} \end{cases} \quad (3)$$

Therefore,

$$v = \sum_{k=-n+1}^{n-1} a_k b_k, \quad (4)$$

where the quantities b_k are defined by

$$b_k = \sum_{j=1}^n u_{k+j} v_j s(k, j) \quad (5)$$

and can be computed in $O(n^2)$ operations.

At the first glance, this does not seem to give any gain. However, in some cases we need to compute f for the same u_i and v_j but various a_k . In all such cases, evaluation of b_k via (5) can be considered as precomputation and is the only step involving $O(n^2)$ operations, whereas the repeated computation by the formula (4) takes only $O(n)$ operations.

Moreover, in typical practical cases the values u_i and v_j depend polynomially on i and j , which makes it possible to compute b_k in $O(n)$ operations as well. For example, assume that

$$u_i = A + Bi, \quad v_j = C + Dj.$$

In this case the b_k can be computed analytically. Indeed,

$$\begin{aligned} b_k &= A_k + B_k k, & (6) \\ A_k &= AC b_k^0 + (BC + AD) b_k^1 + BD b_k^2, & B_k = BC b_k^0 + BD b_k^1, \\ b_k^0 &= \sum_{j=1}^m s(k, j), \\ b_k^1 &= \sum_{j=1}^m j s(k, j), \\ b_k^2 &= \sum_{j=1}^m j^2 s(k, j), \end{aligned}$$

and elementary calculations show that

$$\begin{aligned} b_k^0 &= m - |k|, \\ b_k^2 &= \frac{(m - |k|)(m - k + 1)}{2}, \\ b_k^3 &= \begin{cases} \sum_{j=1}^{m-k} j^2, & k \geq 0, \\ \sum_{j=|k|+1}^m j^2, & k < 0. \end{cases} \end{aligned}$$

The A_k and B_k in (6) can be evaluated altogether in $O(n)$ operations so long as the same holds true for the b_k^l . Consequently, we implement (4) capitalizing on (6) and find f eventually in just $O(n)$ operations. The same complexity stands when u_i and v_j are arbitrary polynomials of i and j , their orders being fixed and independent of n .

3 Multilevel case

Let f be defined by (1). Then, we may proceed by induction:

$$f = \sum_{1 \leq i_1, \dots, i_{p-1} \leq n} \sum_{1 \leq j_1, \dots, j_{p-1} \leq n} u_{i_1}^1 \dots u_{i_{p-1}}^{p-1} \tilde{a}_{i_1-j_1, \dots, i_{p-1}-j_{p-1}} v_{j_1}^1 \dots v_{j_{p-1}}^{p-1},$$

where

$$\tilde{a}_{i_1-j_1, \dots, i_{p-1}-j_{p-1}} = \sum_{k_p=-n+1}^{n-1} a_{i_1-j_1, \dots, i_{p-1}-j_{p-1}, k_p} \sum_{j_p=1}^n u_{k_p+j_p}^p v_{j_p}^p s(k_p, j_p).$$

Here, $s(k, j)$ is the function already defined by (3).

It is already obvious that f can be computed in $O(n^p)$ operations. The previous section's constructions now apply in succession on every level. Finally, we obtain

$$f = \sum_{k_1=-n+1}^{n-1} \dots \sum_{k_p=-n+1}^{n-1} a_{k_1, \dots, k_p} \beta_{k_1}^1 \dots \beta_{k_p}^p, \quad (7)$$

where

$$\beta_{k_l}^l = \sum_{j_l=1}^n u_{k_l+j_l}^l v_{j_l}^l s(k_l, j_l), \quad l = 1, \dots, p. \quad (8)$$

Evidently, only $O(n^2)$ operations appear through the implementation of (8) and $O(n^p)$ operations are required to compute (7).

Remark that there are special cases when the complexity can be further reduced. For instance, assume that

$$a_{i_1-j_1, \dots, i_p-j_p} = a_{i_1-j_1}^1 \dots a_{i_p-j_p}^p.$$

Then f can be found in just $O(n^2)$ operations. The same growth in n is kept when the above right-hand side is substituted with a sum of a few terms of similar structure.

4 Fast computation of integrals

Many integro-differential equations can be set in such a way that the kernel functions involved possess only weak singularity at $x = y$. Then simple quadrature rules can be used. The entries of the matrix of moments are typically assembled from those integrals precomputed over tensor products of some basic rectangular (cubic) cells.

Thus, a typical computation reads

$$(f, g) = \iiint_{\Pi_{i_1 i_2 i_3}} \iiint_{\Pi_{j_1 j_2 j_3}} G(x, y) f(x) g(y) dx dy,$$

where f, g are scalar functions (basis functions or their derivatives) and G is a scalar kernel with weak singularity at $x = y$. Choose a positive integer m , subdivide each cell into m^3

rectangular subcells and approximate the integral by multiple rule of rectangles, excluding the pairs with same subcells (where x may coincide with y). This suggests an approximate formula $(f, g) \approx I$ with the sextuple summation as follows:

$$I = \frac{(h_1 h_2 h_3)^2}{m^6} \sum_{\alpha_1} \sum_{\alpha_2} \sum_{\alpha_3} \sum_{\beta_1} \sum_{\beta_2} \sum_{\beta_3} G(X_{\alpha_1 \alpha_2 \alpha_3}, Y_{\beta_1 \beta_2 \beta_3}) f(X_{\alpha_1 \alpha_2 \alpha_3}) g(Y_{\beta_1 \beta_2 \beta_3}), \quad (9)$$

where $X_{\alpha_1 \alpha_2 \alpha_3}$ and $Y_{\beta_1 \beta_2 \beta_3}$ are the central points in the subcells. To exclude from summation the indices such that $(\alpha_1 \alpha_2 \alpha_3) = (\beta_1 \beta_2 \beta_3)$, we set $G(X, Y) = 0$ whenever $X = Y$.

Quite typically, $G(X_{\alpha_1 \alpha_2 \alpha_3}, Y_{\beta_1 \beta_2 \beta_3})$ is actually a function of $\alpha_1 - \beta_1$, $\alpha_2 - \beta_2$, $\alpha_3 - \beta_3$. It implies that

$$G(X_{\alpha_1 \alpha_2 \alpha_3}, Y_{\beta_1 \beta_2 \beta_3}) = a_{\alpha_1 - \beta_1, \alpha_2 - \beta_2, \alpha_3 - \beta_3}.$$

At the same time, in general $f(X_{\alpha_1 \alpha_2 \alpha_3})$ and $g(Y_{\beta_1 \beta_2 \beta_3})$ depend upon the indices in the following way:

$$\begin{aligned} f(X_{\alpha_1 \alpha_2 \alpha_3}) &= (a_1 + b_1 \alpha_1)(a_2 + b_2 \alpha_2)(a_3 + b_3 \alpha_3), \\ g(Y_{\beta_1 \beta_2 \beta_3}) &= (c_1 + d_1 \beta_1)(c_2 + d_2 \beta_2)(c_3 + d_3 \beta_3). \end{aligned}$$

The quadrature rule (9) provides a reasonable accuracy for moderate m . Using the algorithms proposed in this paper we also claim that the arithmetic complexity is $O(m^3)$.

5 Example from electromagnetics

Consider the Cartesian coordinate system (x_1, x_2, x_3) and a nonuniform inclusion \mathcal{V} with the (complex-valued) permittivity ε . The inclusion is in the shape of parallelepiped and located in the half-space $x_2 > 0$. The outer space \mathcal{W} (medium outside the inclusion) is uniform with the (complex-valued) permittivity ε_0 . The plane $x_2 = 0$ can be (optionally) the perfect conductor surface, in this case $\mathcal{W} = \{x_2 > 0\} \setminus \mathcal{V}$. The excitation is time-harmonic with the frequency ω (e.g. comes from a magnetic dipole located in the outer space under the bottom of the inclusion). The time-dependence factor is common for all quantities and cancelled in all formulas. As usual, all the quantities are considered without this factor.

It is well-known that the full electric field \mathbf{E} can be found from the following *volume integral equation* [1, 2, 3, 4, 6]:

$$\gamma^{-1} \mathbf{J}(x) - (k_0^2 + \text{grad div}) \int_{\mathcal{V}} G(x, y) \mathbf{J}(y) dy = \mathbf{E}^0, \quad x \in \mathcal{V}, \quad (10)$$

where \mathbf{E}^0 is the primary electric field, $\mathbf{J} = \gamma \mathbf{E}$, $k_0 = \sqrt{\varepsilon_0 \mu \omega^2}$, $\gamma \equiv \frac{\varepsilon}{\varepsilon_0} - 1$.

We solve the volume integral equation (10) by the Galerkin method with special locally-supported basis functions which are piecewise-linear (roof-like) in one direction and piecewise-constant (hat-like) in the other two directions [2, 4, 6].

Suppose that $\mathcal{V} = [a_1, b_1] \times [a_2, b_2] \times [a_3, b_3]$ and introduce regular one-dimensional grids with steps h_1, h_2, h_3 as follows:

$$\begin{aligned} x_1^{j_1} &= a_1 + (j_1 - 1)h_1, & h_1 &= (b_1 - a_1)/n_1, \\ x_2^{j_2} &= a_2 + (j_2 - 1)h_2, & h_2 &= (b_2 - a_2)/n_2, \\ x_3^{j_3} &= a_3 + (j_3 - 1)h_3, & h_3 &= (b_3 - a_3)/n_3. \end{aligned}$$

Thus, \mathcal{V} is a union of the basic 3D cells

$$\begin{aligned} \Pi_{j_1 j_2 j_3} &= [x_1^{j_1}, x_1^{j_1+1}] \times [x_2^{j_2}, x_2^{j_2+1}] \times [x_3^{j_3}, x_3^{j_3+1}], \\ 1 &\leq j_1 \leq n_1, \quad 1 \leq j_2 \leq n_2, \quad 1 \leq j_3 \leq n_3. \end{aligned}$$

The approximate unknown vector function \mathbf{J} is sought in the form

$$\begin{aligned} \mathbf{J}(x_1, x_2, x_3) &= \sum_{j_1=1}^{n_1-1} \sum_{j_2=1}^{n_2} \sum_{j_3=1}^{n_3} u_{j_1 j_2 j_3}^1 \mathbf{F}_{j_1 j_2 j_3}^1(x_1, x_2, x_3) + \\ &\quad \sum_{j_1=1}^{n_1} \sum_{j_2=1}^{n_2-1} \sum_{j_3=1}^{n_3} u_{j_1 j_2 j_3}^2 \mathbf{F}_{j_1 j_2 j_3}^2(x_1, x_2, x_3) + \\ &\quad \sum_{j_1=1}^{n_1} \sum_{j_2=1}^{n_2} \sum_{j_3=1}^{n_3-1} u_{j_1 j_2 j_3}^3 \mathbf{F}_{j_1 j_2 j_3}^3(x_1, x_2, x_3), \end{aligned} \quad (11)$$

where

$$\mathbf{F}_{j_1 j_2 j_3}^1 = \begin{bmatrix} \Phi_{j_1}^1 & \Psi_{j_2}^2 & \Psi_{j_3}^3 \\ 0 & & \\ 0 & & \end{bmatrix}, \quad \mathbf{F}_{j_1 j_2 j_3}^2 = \begin{bmatrix} 0 & & \\ \Psi_{j_1}^1 & \Phi_{j_2}^2 & \Psi_{j_3}^3 \\ 0 & & \end{bmatrix}, \quad \mathbf{F}_{j_1 j_2 j_3}^3 = \begin{bmatrix} 0 & & \\ 0 & & \\ \Psi_{j_1}^1 & \Psi_{j_2}^2 & \Phi_{j_3}^3 \end{bmatrix}, \quad (12)$$

$\Phi_{j_k}^k(x_k)$ are the roof-like functions:

$$\Phi_{j_k}^k(x_k) = \begin{cases} 1 - |x_k - x_k^{j_k+1}|/h_k, & |x_k - x_k^{j_k+1}| \leq h_k, \\ 0, & \text{otherwise,} \end{cases} \quad (13)$$

$\Psi_{j_k}^k(x_k)$ are the hat-like functions:

$$\Psi_{j_k}^k(x_k) = \begin{cases} 1, & x_k^{j_k} \leq x_k \leq x_k^{j_k+1}, \\ 0, & \text{otherwise.} \end{cases} \quad (k = 1, 2, 3) \quad (14)$$

The \mathbf{F}^k functions can be associated with the internal basic-cell faces orthogonal to the x_k axis. The boundary faces are ignored for all the functions to be zero outside \mathcal{V} .

In line with the Galerkin method, the unknown coefficients in the expansion (11) are found from the system of linear algebraic equations

$$(\gamma^{-1} \mathbf{J}, \mathbf{F}_{i_1 i_2 i_3}^k) - \left((k_0^2 + \text{grad div}) \int_{\mathcal{V}} \mathbf{G} \mathbf{J} dx, \mathbf{F}_{i_1 i_2 i_3}^k \right) = (\mathbf{E}^0, \mathbf{F}_{i_1 i_2 i_3}^k). \quad (15)$$

On suitable ordering of the unknowns and equations, it is of the form

$$\left(\begin{bmatrix} D_1 & & \\ & D_2 & \\ & & D_3 \end{bmatrix} + \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} \right) \begin{bmatrix} u^1 \\ u^2 \\ u^3 \end{bmatrix} = \begin{bmatrix} f^1 \\ f^2 \\ f^3 \end{bmatrix}, \quad (16)$$

where the block diagonal part of the matrix corresponds to the off-integral term of (15), and, specifically,

$$(D_k)_{i_1 i_2 i_3}^{j_1 j_2 j_3} = \int_{\mathcal{V}} \gamma^{-1} (\mathbf{F}_{i_1 i_2 i_3}^k(x), \mathbf{F}_{j_1 j_2 j_3}^k(x)) dx, \quad (17)$$

$$(A_{kl})_{i_1 i_2 i_3}^{j_1 j_2 j_3} = - \int_{\mathcal{V}} \left((k_0^2 + \text{grad div}) \int_{\mathcal{V}} (G(x, y) \mathbf{F}_{j_1 j_2 j_3}^l(y), \mathbf{F}_{i_1 i_2 i_3}^k(x)) dy \right) dx. \quad (18)$$

The right-hand side of (18) can be remarkably simplified. To this end, we need to observe that

$$\frac{\partial}{\partial x_l} G_l(x_1, x_2, x_3, y_1, y_2, y_3) = - \frac{\partial}{\partial y_l} G_1(x_1, x_2, x_3, y_1, y_2, y_3), \quad l = 1, 2, 3.$$

Then,

$$\text{div} \int_{\mathcal{V}} G(x, y) \mathbf{F}_{j_1 j_2 j_3}^l(y) dy = \iiint_{\Pi_{j_1 j_2 j_3}^l} \frac{\partial}{\partial x_l} G_l(x, y) \Phi_{j_l}^l(y_l) dy_1 dy_2 dy_3,$$

where

$$\begin{aligned} \Pi_{j_1 j_2 j_3}^1 &= [x_{j_1}^1, x_{j_1+2}^1] \times [x_{j_2}^2, x_{j_2+1}^2] \times [x_{j_3}^3, x_{j_3+1}^3], \\ \Pi_{j_1 j_2 j_3}^2 &= [x_{j_1}^1, x_{j_1+1}^1] \times [x_{j_2}^2, x_{j_2+2}^2] \times [x_{j_3}^3, x_{j_3+1}^3], \\ \Pi_{j_1 j_2 j_3}^3 &= [x_{j_1}^1, x_{j_1+1}^1] \times [x_{j_2}^2, x_{j_2+1}^2] \times [x_{j_3}^3, x_{j_3+2}^3]. \end{aligned}$$

Using integration by parts, we obtain

$$\int_{x^l}^{x_{j_l+2}^l} \frac{\partial}{\partial x_l} G_l(x, y) \Phi_{j_l}^l(y_l) dy_l = - \int_{x^l}^{x_{j_l+2}^l} \frac{\partial}{\partial y_l} G_1(x, y) \Phi_{j_l}^l(y_l) dy_l = \int_{x^l}^{x_{j_l+2}^l} G_1(x, y) \frac{\partial}{\partial y_l} \Phi_{j_l}^l(y_l) dy_l.$$

Hence,

$$\text{div} \int_{\mathcal{V}} G(x, y) \mathbf{F}_{j_1 j_2 j_3}^l(y) dy = \iiint_{\Pi_{j_1 j_2 j_3}^l} G_1(x, y) \frac{\partial}{\partial y_l} \Phi_{j_l}^l(y_l) dy_1 dy_2 dy_3.$$

One more integration by parts yields

$$\begin{aligned} & \int_{\mathcal{V}} \left(\text{grad div} \int_{\mathcal{V}} (G(x, y) \mathbf{F}_{j_1 j_2 j_3}^l(y), \mathbf{F}_{i_1 i_2 i_3}^k(x)) dy \right) dx = \\ & \iiint_{\Pi_{i_1 i_2 i_3}^k} \frac{\partial}{\partial x_k} \left(\iiint_{\Pi_{j_1 j_2 j_3}^l} G_1(x, y) \frac{\partial}{\partial y_l} \Phi_{j_l}^l(y_l) dy_1 dy_2 dy_3 \right) \Phi_{i_k}^k(x_k) dx_1 dx_2 dx_3 = \\ & \iiint_{\Pi_{i_1 i_2 i_3}^k} \iiint_{\Pi_{j_1 j_2 j_3}^l} G_1(x, y) \frac{\partial}{\partial x_k} \Phi^k(x_k) \frac{\partial}{\partial y_l} \Phi_{j_l}^l(y_l) dx_1 dx_2 dx_3 dy_1 dy_2 dy_3. \end{aligned}$$

Finally, (18) transforms into a simpler expression

$$(A_{kl})_{i_1 i_2 i_3}^{j_1 j_2 j_3} = -k_0^2 \delta_{kl} (P_k)_{i_1 i_2 i_3}^{j_1 j_2 j_3} + (Q_{kl})_{i_1 i_2 i_3}^{j_1 j_2 j_3} \quad (19)$$

with Kronecker's symbol δ_{kl} and

$$(P_k)_{i_1 i_2 i_3}^{j_1 j_2 j_3} = \iiint_{\Pi_{i_1 i_2 i_3}^k} \iiint_{\Pi_{j_1 j_2 j_3}^k} G_k(x, y) \Phi_{i_k}^k(x_k) \Phi_{j_k}^k(x_k) dx_1 dx_2 dx_3 dy_1 dy_2 dy_3, \quad (20)$$

$$(Q_{kl})_{i_1 i_2 i_3}^{j_1 j_2 j_3} = \iiint_{\Pi_{i_1 i_2 i_3}^k} \iiint_{\Pi_{j_1 j_2 j_3}^l} G_1(x, y) \frac{\partial}{\partial x_k} \Phi^k(x_k) \frac{\partial}{\partial y_l} \Phi^l(y_l) dx_1 dx_2 dx_3 dy_1 dy_2 dy_3. \quad (21)$$

Thus, our method for computation of multilevel Toeplitz forms can be applied to evaluate the integrals (20) and (21). If the perfect conductor plane is present, then G should be considered of the form

$$G(x_1, x_2, x_3, y_1, y_2, y_3) = \mathcal{T}(x_1 - y_1, x_2 - y_2, x_3 - y_3) + \mathcal{H}(x_1 - y_1, x_2 + y_2, x_3 - y_3), \quad (22)$$

for certain three-variate functions \mathcal{T} and \mathbf{H} . In this case $G(X_{\alpha_1 \alpha_2 \alpha_3}, Y_{\beta_1 \beta_2 \beta_3})$ is the sum of two functions, one being related to \mathcal{T} and depending on $\alpha_1 - \beta_1$, $\alpha_2 - \beta_2$, $\alpha_3 - \beta_3$, and the other being related to \mathbf{H} and depending on $\alpha_1 - \beta_1$, $\alpha_2 + \beta_2$, $\alpha_3 - \beta_3$. Using this observation, we can write

$$G(X_{\alpha_1 \alpha_2 \alpha_3}, Y_{\beta_1 \beta_2 \beta_3}) = a_{\alpha_1 - \beta_1, \alpha_2 - \beta_2, \alpha_3 - \beta_3} + b_{\alpha_1 - \beta_1, \alpha_2 + \beta_2, \alpha_3 - \beta_3}.$$

This allows us to split the sextuple summation in two parts, one with a and the other with b . The summation with b is easily reduced to the already considered case by substitution $\beta_2 \rightarrow m + 1 - \beta_2$.

References

- [1] V. I. Dmitriev, E. V. Zakharov, *Integral equations in boundary problems of electrodynamics*, Moscow State University, 1987 (in Russian).
- [2] V. I. Ivakhnenko, E. E. Tyrtshnikov, Block-Toeplitz-structure-based solution strategies for CEM problems, *11th Annual Review of Progress in Applied Comp. Electromagnetics, Conf. Proc.*, Monterey, CA, MArch 20–25, 1995, pp. 181–188.
- [3] A. B. Samohin, *Integral equations and iterative methods in electromagnetic scattering*, Radio i Sviaz, Moscow, 1998 (in Russian).
- [4] Yu. G. Smirnov, A. A. Tsupak, Volume singular integral equations for solving diffraction problem of electromagnetic waves in microwave oven, *Proc. of European Symp. on Numer. Meth. in Electromagnetics*, March 6–8, 2002, Toulouse, France, pp. 172–176.
- [5] V. V. Voevodin, E. E. Tyrtshnikov, *Computational processes with Toeplitz matrices*, Nauka, Moscow, 1987 (in Russian).
- [6] A. P. M. Zwamborn, Van der Berg, The three-dimensional weak form of the conjugate gradient FFT method for solving scattering problems, *IEEE Trans. Microwave Theory Tech.*, 1992, MTT-40, 9, pp. 1757–1765.