Reducing the two dimensional Green functions: Fourier mode decomposition

Reduciendo las funciones de Green bidimensionales: Descomposición en modos de Fourier

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Abstract

Often we encounter high dimensional differential equations. A clever representation of a generalized solution could be procured in certain cases using Green functions. We show how this representation could be achieved and via a clever Fourier mode decomposition for the particular disc case resulting in a highly correlated set of functions that transforming into a discrete representation – via a classical second order finite difference approximation – can be ultimately represented as a linear equation for matrices embedding all boundary conditions in the structure of such objects. The resulting problem could be solved using stochastic gradient descent with an additional on-the-fly optimization reducing required computation resources substantially.

Resumen

Comúnmente encontramos ecuaciones diferenciales en espacios de alta dimensionalidad. Una representación útil de la solución generalizada puede ser expresada en ciertos casos usando funciones de Green. Se muestra como esta representación se puede lograr por medio de una descomposición en modos de Fourier para el caso particular de un disco dando origen a un conjunto altamente correlacionado de funciones que transformando a una representación discreta – a través de una típica aproximación de segundo grado por métodos finitos – puede ser representado como una ecuación lineal para matrices que contienen las condiciones iniciales de tales objetos. El problema resultante se puede resolver por medio del método de *Gradient Descent* estocástico cuyos componentes se calculan sobre la marcha para optimizar el uso de recursos computacionales.

Introduction

We often encounter ourselves solving complex multidimensional second order differential equations. A clever artifact for this purpose is the known *Green function* construction that has been employed in a cornucopia of areas in Physics throughout history. This scenario is clearly seen in Quantum and Statistical Physics [1–8].

From a mathematical point of view, the Green function problem can be conveniently defined via a differential operator also known as the Liouville operator as follows

$$\hat{\mathcal{L}}_{\{\mathbf{r}\}} \boxdot = \left(\vec{\nabla}_{\{\mathbf{r}\}} + \vec{f}(\mathbf{r})\right) \cdot \left(\vec{\nabla}_{\{\mathbf{r}\}} \boxdot\right) + g(\mathbf{r}) \boxdot, \qquad (1)$$

acting on a scalar field $\boxdot$ in $\Re^d$, with d the dimension of the system – *i.e.* $\mathbf{r} \in \Re^d$.

In particular, our aim is to tackle the two dimensional case to allow a reduction in dimensionality using a Fourier expansion. Two dimensional systems are of great interest in material sciences, quantum computing, experimental and high energy physics, ionic fluids, theoretical mathematics, and many others. Numerical methods have been described to compute Green's functions, however, due to its increased complexity some remarkable efforts have been made for establishing a precise formulation of boundary conditions for their numerical calculation [9] and, more interestingly, for elaborating solutions in periodic systems in similar work by [10].

The key for introducing Green's function – or more accurately, distribution – formalism is writing the overall problem as the in-homogeneous equation

$$\hat{\mathcal{L}}\psi(\mathbf{r}) = \phi(\mathbf{r}), \qquad (2)$$

with $\psi(\mathbf{r})$ and $\phi(\mathbf{r})$ two scalar functions. It is proven that existence of Green's distribution relies on the likewise existence of a weight function introduced to guarantee symmetrical convolution in Hilbert's space $\mathcal{H}$ – also known as the space of functions.

The Green function formalism starts from the identity,

$$\hat{\mathcal{L}}_{\{\mathbf{r}\}} G(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'), \qquad (3)$$

with $\delta(\mathbf{r}-\mathbf{r}')$ the $\Re^d$ Dirac delta distribution, where the solution to the in--homogeneous equation (2) is postulated by the convolution identity from the distribution,

$$\psi(\mathbf{r}) = \int_{\mathbf{r}'} G\,(\mathbf{r},\mathbf{r}')\phi(\mathbf{r}')\,\mathrm{d}\mathbf{r}' + \text{b.c.}, \qquad (4)$$

with either Dirichlet or Neumann boundary conditions (b.c).

Fourier modes analysis and reduction

In polar coordinates eq. (3) is given by

$$\left[\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}+f_1(r,\theta)\frac{\partial}{\partial r}+f_2(r,\theta)\frac{1}{r}\frac{\partial}{\partial\theta}+g(r,\theta)\right]G(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'), \qquad (5)$$

where $f_1(r,\theta)$ and $f_2(r,\theta)$ are the components of $\vec{f}$ in the radial and angular directions respectively.

The presence of the delta function $\delta(\mathbf{r}-\mathbf{r}') = \frac{1}{r}\delta(r-r')\delta(\theta-\theta')$ suggests an expansion for the Green function of the form $\frac{1}{2\pi}\sum_l e^{il\theta}G_l(r-r')$ for the angular term where a separable solution can be procured by symmetry. However, in the most general case, an approximate method could be formulated to evaluate the *l*-modes G_l.

Completeness of the Fourier expansion and a divergence free system (f_1 and f_2 are well behaved within the domain), the effective one-dimensional system equation for *r* yields – multiplying eq. (5) by r^2 to avoid a pathological behavior at $r=0$ –,

$$\sum_l e^{il(\theta-\theta')}\left[r^2\frac{d^2}{dr^2}+A(r,\theta)\frac{d}{dr}+B_l(r,\theta)\right]G_l = \sum_l e^{il(\theta-\theta')}\,r\delta(r-r'). \qquad (6)$$

In terms of the functions introduced in eq. (5) we have the relations $A(r,\theta) = r(1+rf_1(r,\theta))$ and $B(r,\theta) = -l^2 + ilrf_2(r,\theta) + r^2 g(r,\theta)$. Following the same recipe for expansion in Fourier representation of both $A(r,\theta)$ and $B(r,\theta)$ yields in simplified form,

$$r^2 G_n'' + \sum_m A_m(r)e^{im\theta'}G'_{n-m} + \sum_m B_{n-m,m}(r)e^{im\theta'}G_{n-m} = r\delta(r-r'), \qquad (7)$$

after averaging over θ as $\int_0^{2\pi} d\theta\, e^{-in\theta}$ ...

In terms of the Fourier modes of the original functions $f_1(r,\theta)$, $f_2(r,\theta)$, and $g(r,\theta)$ (the modes of a function f (r,θ) are defined, as usually, as $f_m(r) = \frac{1}{2\pi}\int_0^{2\pi} f(r,\theta)e^{-im\theta}d\theta$ last equation takes the form

$$r^2 G_l'' + r(1 + r f_{1,0})G'_l - (l^2 - irlf_{2,0} - g_0)G_l + \sum_{m\neq 0}[\,ir(l-m)f_{2,m} + r^2 g_m]G_{l-m}$$
$$+ \sum_{m\neq 0} r^2 f_{1,m} G'_{l-m} = r\delta(r-r')e^{il\theta'}. \qquad (8)$$

This last equation represents an infinitely coupled system of differential equations. An exact solution for the effective one dimensional system can be found by adding the infinite modes of *m*. However, a numerical calculation of such problem is impractical. We are then forced to approximate the result by expanding over a finite number of modes. The rationale behind this cutoff is also justified by the limitations of numerical precision in floating point operations. Thus, the number of modes to be taken will depend entirely on how fast the functions $f_1(r,\theta)$, , and $g(r,\theta)$ decay on *m*. Textbook Fourier analysis shows that whenever a function $f(\theta)$ is at least twice differentiable, its Fourier series converges uniformly to the function and its coefficients decay as m^2 [11]. Additional convergence requirements in a numerical platform sets an upper bound to the utmost value of $|m|$ virtue of the first and second order derivatives approximation in Finite Elements.

Approximate solution using finite elements

A discretization of the radial variable, for both r and r' allows us to find an approximate solution to eq. (8) using the three-point-stencil. We now define a step size given by $h = R/N$, where *N* is the number of points along the grid. As the Green function for each mode has two degrees of freedom (r and r'), the Green function for each mode will be represented by an $N+1 \times N+1$ matrix, where we locate r and r' along the rows and columns of such matrix respectively.

Using a Taylor expansion [12–14] up to second order in h^2 to express the first and second derivatives of $G_l(r,r')$, eq. (8) can be written as

$$A_l^j G_l^{jj'} + B_l^j G_l^{j+1j'} + C_l^j G_l^{j-1j'} + \sum_{m\neq 0}^{M} D_{l\,m}^j G_{l-m}^{jj'} + \sum_{m\neq 0}^{M} E_{l\,m}^j \left(G_{l-m}^{j+1j'} - G_{l-m}^{j-1j'}\right) = F_l^j \delta^{jj'}, \qquad (9)$$

where A_l^j, B_l^j, C_l^j, $D_{l\,m}^j$, $E_{l\,m}^j$ and F^j are matrix elements, which can be written in terms of the discretized variable $r^j = hj$ and the Fourier modes of the functions: $f_{1\,m}^j$, $f_{2\,m}^j$, and g_m^j.

As the truncate the maximum number of Fourier *l*-modes by a value of *L*, we have a linear system (by blocks) of the form

$$\mathbf{P}_{(2L+1)(N+1)\times(2L+1)(N+1)} \cdot \mathbf{G}_{(2L+1)(N+1)\times 1} = \mathbf{V}_{(2L+1)(N+1)\times 1}\,.$$

More explicitly, the block linear system can be written as

$$\begin{pmatrix} \mathbf{P}_{-L\,-L} & \mathbf{P}_{-L\,-L+1} & \cdots & \mathbf{P}_{-L\,L-1} & \mathbf{P}_{-L\,L} \\ \mathbf{P}_{-L+1\,-L} & \mathbf{P}_{-L+1\,-L+1} & \cdots & \mathbf{P}_{-L+1\,L-1} & \mathbf{P}_{-L+1\,L} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \mathbf{P}_{L-1\,-L} & \mathbf{P}_{L-1\,-L+1} & \cdots & \mathbf{P}_{L-1\,L-1} & \mathbf{P}_{L-1\,L} \\ \mathbf{P}_{L\,-L} & \mathbf{P}_{L\,-L+1} & \cdots & \mathbf{P}_{L\,L-1} & \mathbf{P}_{L\,L} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{G}_{-L} \\ \mathbf{G}_{-L+1} \\ \vdots \\ \mathbf{G}_{L-1} \\ \mathbf{G}_{L} \end{pmatrix} = \begin{pmatrix} \mathbf{V}_{-L} \\ \mathbf{V}_{-L+1} \\ \vdots \\ \mathbf{V}_{L-1} \\ \mathbf{V}_{L} \end{pmatrix}, \qquad (10)$$

where the diagonal block matrices $\mathbf{P}_{ll}$ and the off-diagonal block matrices $\mathbf{P}_{lm}$ are $N+1 \times N+1$ matrices of the form

$$\mathbf{P}_{l\,l} = \begin{pmatrix} \mathrm{BC} & \mathrm{BC} & \cdots & 0 & 0 \\ C_l^1 & A_l^1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & A_l^{N-1} & B_l^{N-1} \\ 0 & 0 & \cdots & \mathrm{BC} & \mathrm{BC} \end{pmatrix}, \mathbf{P}_{l\,m} = \begin{pmatrix} 0 & 0 & \cdots & 0 & 0 \\ -E_{l\,m}^1 & D_{l\,m}^1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & D_{l\,m}^{N-1} & E_{l\,m}^{N-1} \\ 0 & 0 & \cdots & 0 & 0 \end{pmatrix}. \qquad (11)$$

In last expression, BC are elements associated with the boundary conditions chosen (either Dirichlet or Neumann). On the other hand, the same notation as in eq. (9) has been used. Similarly

$$\mathbf{G}_l = \begin{pmatrix} G_l^{00} & G_l^{01} & \cdots & G_l^{0N-1} & G_l^{0N} \\ G_l^{10} & G_l^{11} & \cdots & G_l^{1N-1} & G_l^{1N} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ G_l^{N-10} & G_l^{N-11} & \cdots & G_l^{N-1N-1} & G_l^{N-1N} \\ G_l^{N0} & G_l^{N1} & \cdots & G_l^{NN-1} & G_l^{NN} \end{pmatrix}, \mathbf{V}_l = \begin{pmatrix} \mathrm{BC} & 0 & \cdots & 0 & 0 \\ 0 & F^1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & F^{N-1} & 0 \\ 0 & 0 & \cdots & 0 & \mathrm{BC} \end{pmatrix}. \qquad (12)$$

Matrix inversion

A solution to the individual modes and hence, to the whole system (which can be found by adding the contribution of the different modes) can be found by obtaining the inverse of the full matrix P, or, likely, finding G *s.th* eq. (10). Although well-established numerical algorithms exist, such algorithms become unviable for *large* systems due to limitations on memory resources and time constraints. Particularly, these matrices are potentially highly sparse. In addition to, approximating via the 3 or 5 point stencil reflects an underlying structure of these matrices that suggests that an alternate solution method could be orchestrated.

An alternate method to find the required solution is an optimization scheme by means of the *gradient descent* method – and its faster sibling the *stochastic gradient descent* [15–17]. While this method does not directly find the inverse of the matrix P, it attempts to find the solution for the matrix G directly by the minimization of a cost function, usually the mean square error,

$$J = \frac{1}{N+1} \sum_{j,k=0}^{D} [\, V_{jk} - V_{jk}^{(i)}]^2 , \qquad (13)$$

where $V^{(i)}$ is an anzats satisfying the relation $P \cdot G^{(i)}=V^{(i)}$. Notice that by starting from an educated guess of $G^{(i)}$ we obtain a very crude estimate of $V^{(i)}$ distant from the expected V measured by the cost function *J*. Since the profile is quadratic, we can potentially improve $G^{(i)}$ iteratively by making multiple fractional updates in the opposite direction of the gradient to the hyper-surface profile for the cost function. The update is given by $\vec{G}_{(i)}^{a} = \vec{G}_{(i-1)}^{a} - \eta_{(i)} \vec{\nabla} J_{(i-1)}$. While this method

is guaranteed to converge – provided that the resulting matrix is invertible – it may require a significant number of updates, thus undermining its efficiency. For that matter, scientists often resource to Stochastic Gradient Descent to accelerate convergence. However, it is well known that high accuracy is not an outstanding trait of it. Lately, research on variations of the Stochastic Gradient Descent methods for higher accuracy have been developed which can be utilized in place such as variations of Kaczmarz's algorithm for solving systems of linear equations among others [17–19].

Results

In order to test the validity of the method, we will show a particular example in which the analytical solution to a second order differential equation is known. Let us suppose that we want to find the Green function associated with the Helmhotz equation

$$(\nabla^2 - m^2)G(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')\,. \qquad (14)$$

We will use units such that $m = 1$ and confine the system in a large disk of radius $R = 10$. Since the system can be solved by separation of variables and so the modes do not couple to each other $C_{l\,m} = D_{l\,m} = 0$. Additionally, $A_l^j = 2r_j^2 + h^2(l^2 + r_j^2)$, $B_l^j = r_j(r_j + \frac{h}{2})$, $C_l^j = r_j(r_j - \frac{h}{2})$,, and $F^j = -hr_j$. The analytical solution to eq. (14) with Dirichlet boundary conditions is

$$G(\mathbf{r},\mathbf{r}') = -\frac{1}{2\pi}\sum_l e^{il(\theta-\theta')}\left[I_l(r_<)K_l(r_>) - \frac{K_l(R)}{I_l(R)}I_l(r)I_l(r')\right], \qquad (15)$$

where $r_<$ and $r_>$ represent the smaller an the larger radii between r and r' respectively and $I_l(r)$ and $K_l(r)$ are the modified Bessel function of first and second kind. In the case in which $\theta = \theta'$ the numerical and analytical solutions are shown in figure 1. The average mean square error $\langle MSE\rangle$, representing the accuracy of the numerical solution is shown in table 1.

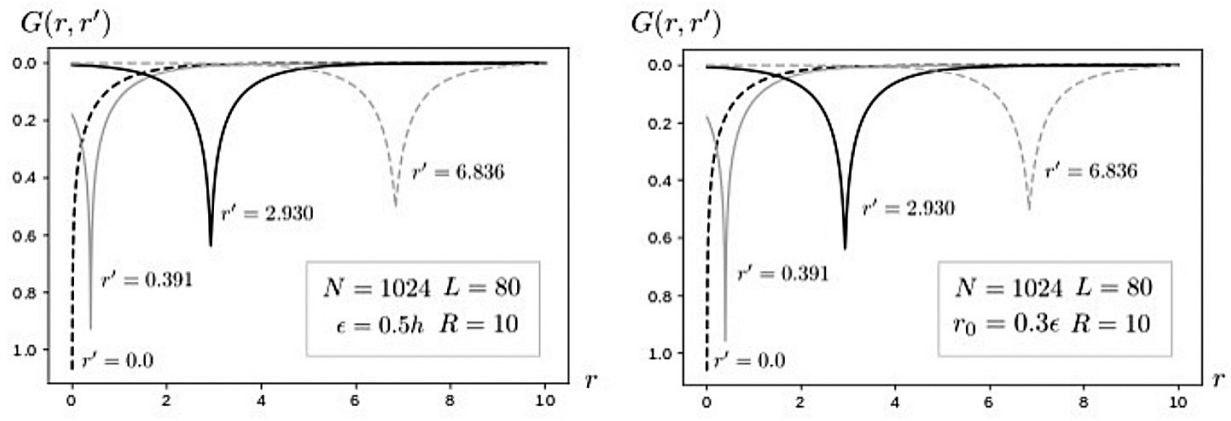

Figure 1: Left: numerical solution to eq. (14). Right: analytical solution provided by eq. (15). In each plot from left to right: $r' = 0$, $r' = 0.391$, $r' = 2.930$, and $r' = 6.836$. In both cases we took a maximum number of $L = 80$ modes; some other important parameters are shown in the plots. The parameters $\in$ and r_0 are necessary values introduced to avoid divergences, as the Green function diverges as a consequence of the Dirac Delta distribution.

Table 1. Mean square error associated with the numerical solution shown in figure 1. MSE_{max} represents the maximum error and r_{max} the value of r' at which it occurs. As expected, the maximum error takes place at the location of the peaks. While the height of the peaks is formally infinite, the cutoffs ∈ and r_0 are introduced to avoid such divergences.

r'	$\langle MSE \rangle$	MSE_{max}	r_{max}
0.000	1.44 x 10^{-7}	8.69 x 10^{-5}	0.000
0.391	9.26 x 10^{-7}	8.58 x 10^{-4}	0.391
2.930	2.21 x 10^{-10}	7.74 x 10^{-8}	2.930
6.836	6.11 x 10^{-9}	7.33 x 10^{-7}	6.836

Conclusions

We synthesized a prescription for finding solutions to the general Green functions formalism problem in two dimensions by using the well-known Fourier expansion arriving to a set of infinite countable coupled differential equations. In the process of describing solutions to G, we conceded in finding an alternate solution to an optimization problem where existence is guaranteed when we scale up to the structural properties of the Liouville operator. Ergo, a solution could always be found. Ultimately, this problem is paramount in an arena where the evolution of technology is highly dependent on the behavior and dynamics of two dimensional systems in material science.

References

[1] J. Schwinger, "Brownian motion of a quantum oscillator," *Journal of Mathematical Physics*, vol. 2, no. 3, pp. 407–432, 1961.

[2] J.-S. Wang, B. K. Agarwalla, H. Li, and J. Thingna, "Nonequilibrium green's function method for quantum thermal transport," *Frontiers of Physics*, vol. 9, no. 6, pp. 673–697, Dec. 2014.

[3] S. Foster and N. Neophytou, "Effectiveness of nanoinclusions for reducing bipolar effects in thermoelectric materials," *Computational Materials Science*, vol. 164, pp. 91–98, Jun. 2019.

[4] L. P. Kadanoff and G. Baym, "Quantum statistical mechanics. Green's function methods in equilibrium and nonequilibrium problems." New York: W. A. Benhamin, Inc. XI, 203 p. (1962)., 1962.

[5] V. Lucarini, "Revising and extending the linear response theory for statistical mechanical systems: Evaluating observables as predictors and predictands," *Journal of Statistical Physics*, vol. 173, no. 6, pp. 1698–1721, Dec. 2018.

[6] Z. Chen, J. de Gier, I. Hiki, and T. Sasamoto, "Exact confirmation of 1D nonlinear fluctuating hydrodynamics for a two-species exclusion process," *Phys. Rev. Lett.*, vol. 120, no. 24, p. 240601, Jun. 2018.

[7] I. Brevik, P. Parashar, and K. V. Shajesh, "Casimir force for magnetodielectric media," *Phys. Rev. A*, vol. 98, no. 3, p. 032509, Sep. 2018.

[8] F. Xu and J. Wang, "Statistical properties of electrochemical capacitance in disordered mesoscopic capacitors," *Phys. Rev. B*, vol. 89, no. 24, p. 245430, Jun. 2014.

[9] F. Tonon, E. Pan, and B. Amadei, "Green's functions and boundary element method formulation for 3D anisotropic media," *Computers & Structures*, vol. 79, no. 5, pp. 469–482, 2001.

[10] D. Duhamel, "Finite element computation of green's functions," *Engineering Analysis with Boundary Elements*, vol. 31, no. 11, pp. 919–930, 2007.

[11] M. Adams and V. Guillemin, "Fourier analysis," in *Measure theory and probability*, Boston, MA: Birkhäuser Boston, 1996, pp. 118–177.

[12] A. Tveito, H. P. Langtangen, B. F. Nielsen, and X. Cai, "Differential equations: The first steps," in *Elements of scientific computing*, Berlin, Heidelberg: Springer Berlin Heidelberg, 2010, pp. 31–73.

[13] J. Whiteley, *Finite element methods, a practical guide*. Springer, 2017.

[14] T. Grätsch and F. Hartmann, "Duality and finite elements," *Finite Elements in Analysis and Design*, vol. 40, no. 9, pp. 1005–1020, 2004.

[15] G. Montavon, G. Orr, and K.-R. Müller, *Neural networks: Tricks of the trade*, 2nd ed. Springer Publishing Company, Incorporated, 2012.

[16] S. Shalev-Shwartz and S. Ben-David, "Stochastic gradient descent," in *Understanding machine learning: From theory to algorithms*, Cambridge University Press, 2014, pp. 150–166.

[17] R. M. Gower, F. Hanzely, P. Richtárik, and S. U. Stich, "Accelerated stochastic matrix inversion: General theory and speeding up bfgs rules for faster second-order optimization," in *Proceedings of the 32Nd international conference on neural information processing systems*, 2018, pp. 1626–1636.

[18] D. Needell, R. Ward, and N. Srebro, "Stochastic gradient descent, weighted sampling, and the randomized kaczmarz algorithm," in *Advances in neural information processing systems 27*, Z. Ghahramani, M. Welling, C. Cortes, N. D. Lawrence, and K. Q. Weinberger, Eds. Curran Associates, Inc., 2014, pp. 1017–1025.

[19] N. Loizou, M. Rabbat, and P. Richtárik, "Provably accelerated randomized gossip algorithms," in *ICASSP 2019 - 2019 ieee international conference on acoustics, speech and signal processing (icassp)*, 2019, pp. 7505–7509.