Inverse homogenization with diagonal Padé approximants

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The paper formulates inverse homogenization problem as a problem of recovery of Markov function using diagonal Padé approximants. Inverse homogenization or de-homogenization problem is a problem of deriving information about the micro-geometry of composite material from its effective properties. The approach is based on reconstruction of the spectral measure in the analytic Stieltjes representation of the effective tensor of two-component composite. This representation relates the n-point correlation functions of the microstructure to the moments of the spectral measure, which contains all information about the microgeometry. The problem of identification of the spectral function from effective measurements in an interval of frequency has a unique solution. The problem is formulated as an optimization problem which results in diagonal Padé approximation and exact formulas for the moments of the measure. The reconstructed spectral function can be used to evaluate geometric parameters of the structure and to compute other effective parameters of the same composite; this gives solution to the problem of coupling of different effective properties of a two-component composite material with random microstructure.

1 Uniqueness of reconstruction of Stieltjes representation of the effective property

The structural information is contained in the spectral measure μ in the Stieltjes representation of the effective complex permittivity ϵ^* developed in [1, 8, 6] in the course of computing bounds for the effective permittivity ϵ^* of an arbitrary two-component mixture. The spectral measure or its moments can be reconstructed from effective measurements and used to characterize parameters of the microstructure [7, 5, 10] or to estimate other effective properties of the same material [3, 4]. It is shown in [3] that the measure μ can be uniquely recovered from the effective complex permittivity given on an arc $\mathcal{C} \subset \mathbf{C}$ in the complex plane. The problem is reduced to inverse potential problem and solved using regularized method in [3, 4]. A concept of $S-equivalency$ of structures is introduced [3] for micro-geometries of composites which cannot be distinguished by effective measurements; it is shown that the $S-$equivalent structures correspond to the same spectral functions. Numerical algorithm based on $[p, q]$-Padé approximations is constructed in [10]. [2] develops application to viscoelastic torsion problem and evaluation of volume fractions of materials in the composite from torsion experiment.

We consider a stationary random fine-scale mixture of two materials with properties ϵ_1 and ϵ_2, and introduce a characteristic function χ of the region $\mathcal{O}_1$ occupied by the first material for a realization $\eta \in \Omega$, where Ω is the set of all realizations of the random medium, $\chi(x, \eta) = 1$ if $x \in \mathcal{O}_1$ and $\chi(x, \eta) = 0$ otherwise. The complex permittivity of the medium is modeled by a (spatially) stationary random field $\epsilon(x, \eta)$, $x \in \mathbf{R}^d$ and $\eta \in \Omega$, $\epsilon(x, \eta) = \epsilon_1 \chi(x, \eta) + \epsilon_2(1 - \chi(x, \eta))$. The stationary random fields $E(x, \eta)$ and $D(x, \eta)$, are related by $D(x, \eta) = \epsilon(x, \eta)E(x, \eta)$ and satisfy the equations $\nabla \cdot D = 0, \nabla \times E = 0, \langle E(x, \eta)\rangle = e_k$ with e_k being a unit vector in the k^{th} direction, for some $k = 1, \ldots, d$, where $\langle \cdot \rangle$ is ensemble average over Ω or spatial average over all of $\mathbf{R}^d$. The effective tensor ϵ^* is defined as coefficient of proportionality between the averaged fields: $\langle D\rangle = \epsilon^* \langle E\rangle$. The inverse homogenization problem [3] is a problem of characterization of function χ from the effective property ϵ^*:

$$\nabla \cdot (\epsilon_1 \chi(x, \eta) + \epsilon_2(1 - \chi(x, \eta)))\, E = 0, \qquad \epsilon^* = \langle \epsilon E\rangle \tag{1}$$

The approach is based on reconstruction of the spectral measure μ in the Stieltjes analytic representation, since the function μ contains all information about function χ.

The Stieltjes analytic representation of the effective complex permittivity ϵ^* was developed in [1, 8, 6] in the course of computing bounds for the effective permittivity ϵ^* of an arbitrary two-component mixture. Introducing $s = 1/(1 - \epsilon_1/\epsilon_2)$, (1) can be written as

$$\nabla \cdot \chi E = s \nabla \cdot\ E\ , \qquad s = \frac{1}{1 - \epsilon_1/\epsilon_2} \tag{2}$$

Let $\nabla\phi$ be a perturbation of the constant field e_k , so that $E = e_k + \nabla\phi$. Then, $\nabla \cdot\ \chi\,(\nabla\phi + e_k) = s\,\Delta\phi$. Introducing an operator $\Gamma = \nabla(-\Delta)^{-1}(\nabla\cdot)$, we can express E as a function of $\Gamma\chi$, $E = s(sI + \Gamma\chi)^{-1}e_k$. The spectral resolution of $\Gamma\chi$ with the measure Q results in the spectral representation for the field E, which is used to obtain the analytic representation for the function $F(s) = 1 - \epsilon^*(s)/\epsilon_2$. Indeed, the function $F(s) = F_{kk}(s) = \langle\, \chi\,(\, sI + \Gamma\,\chi\,)^{-1} e_k, e_k\rangle$ can be represented as

$$F(s) = \int_0^1 \frac{\langle\, \chi\, dQ(z)\, e_k,\, e_k\rangle}{s - z} = \int_0^1 \frac{d\mu(z)}{s - z} \qquad \text{with} \qquad d\mu(z) = \langle\, \chi\, dQ(z) e_k, e_k\rangle \tag{3}$$

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where μ is a positive function of bounded variation corresponding to the spectral measure Q. The spectral measure μ contains all information about the function χ and about the structure of the medium; having reconstructed it, we recover information about the structure χ.

Theorem 1.1 ([3]) *The measure μ can be uniquely reconstructed if the function $F(s)$ is known on an open set $\mathcal{C} \subset \mathbf{C}$ of the complex variable s with a limiting point.*

The proof is based on analytic continuation and reduction of the problem to Hausdorff moment problem. From theorem it follows immediately that the moments μ_n of the measure μ can be uniquely recovered under the same conditions.

2 Padé approximants

The integral representation (3) of $F(s)$ shows that function $F(s)$ is Markov function of the measure μ. Suggested approach to Padé approximations exploits this fact and is based on a number of special properties of Padé approximants to Markov functions ([9]). Diagonal Padé approximant of order n to the function $F(s)$ is a unique rational function π_n

$$\pi_n = \frac{P_n(s)}{Q_n(s)}, \qquad \text{s.t.} \qquad Q_n(s)F(s) - P_n(s) = O\left(\frac{1}{s^{n+1}}\right) \tag{4}$$

where polynomial $Q_n(s)$ has $\deg Q_n \le n$, and $P_n(s)$ is a polynomial part of the series $Q_n(s)F(s)$. It is known that the solution to this problem always exists with $\deg\ Q_n(s) = n, \deg\ P_n(s) \le n-1$.

It can be shown that $\{Q_n\}$ is a set of polynomials orthogonal with respect to the spectral measure μ, and zeros of orthogonal polynomials are all real, simple, and lie in the convex hull $\hat{S_\mu}$ of support of the measure μ. Then π_n has a partial fraction decomposition of the form:

$$\pi_n = \frac{P_n(s)}{Q_n(s)} = \sum_{j=1}^{n} \frac{r_{n,j}}{s - s_{n,j}} \qquad \text{with} \qquad r_{n,j} = res_{s=s_{n,j}} \pi_n(s) = \frac{P_n(s)}{Q\prime_n(s)}, \qquad j = 1, ..., n \tag{5}$$

where $s_{n,j}$ are zeros of polynomial Q_n, and $r_{n,j}$ are residues which are Christoffel coefficients.

Theorem 2.1 *Diagonal Padé approximant $\pi_n(s)$ to the Markov function $F(s)$ solves optimization problem: Find a rational function* $r(s) = \frac{P_n(s)}{Q_n(s)}, \deg\ r \le n$ *s. t.* $||F(s) - r(s)|| \to \inf$ *subject to the constraints:* $0 \le s_{n,j} \le 1, 0 \le r_{n,j} \le 1$

Proof is based on Gauss-Jacobi formula and the fact that support of the measure μ of the operator $\Gamma\chi$ belongs to the unit interval, $\hat{S_\mu} \in [0, 1]$. Theorem justifies numerical algorithm constructed in [10].

Convergence of the sequence of Padé approximants to the Markov function is given by Markov theorem.

Theorem 2.2 (Markov) *Diagonal Padé approximants π_n of the Markov function $\hat{\mu}$ converge to $\hat{\mu}$ uniformly on compact subsets of the domain $\hat{\mathbf{C}} \backslash \hat{S_\mu}$.*

Using Laurent expansion of the function $F(s)$ and expanding the integral Cauchy kernel, we obtain a series representation for $F(s)$ with the coefficients given by Stieltjes moments μ_n of the measure μ

$$F(s) = \sum_{n=0}^{\infty} \frac{1}{s^{n+1}} \int_0^1 z^n d\mu(z) = \sum_{n=0}^{\infty} \frac{\mu_n}{s^{n+1}}, \qquad \mu_n = \int_0^1 z^n d\mu(z)\,, \qquad n = 0, 1, 2, ... \tag{6}$$

Accuracy of diagonal Padé approximation is: $F(s) - \pi_n(s) = O\left(s^{-(2n+1)}\right)$. Expanding the partial fraction (5) into series, and comparing with power series expansion of $F(s)$, we obtain

Theorem 2.3 *The formulas for the moments μ_k of the spectral measure μ of operator $\Gamma\chi = \nabla(-\Delta)^{-1}(\nabla \cdot \chi)$ are given by* $\mu_k = \sum_{j=1}^{n} r_{n,j} s_{n,j}^k$. *The formulas are exact for $k = 0, 1, ..., 2n-1$.*

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