The Monge–Ampère–Kantorovich approach to reconstruction in cosmology

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Motion of a continuous fluid can be decomposed into an “incompressible” rearrangement, which preserves the volume of each infinitesimal fluid element, and a gradient map that transfers fluid elements in a way unaffected by any pressure or elasticity (the polar decomposition of Y. Brenier). The Euler equation describes a system whose kinematics is dominated by incompressible rearrangement. The opposite limit, in which the incompressible component is negligible, corresponds to the Zeldovich approximation, a model of motion of self-gravitating fluid in cosmology.

We present a method of approximate reconstruction of the large-scale proper motions of matter in the Universe from the present-day mass density field. The method is based on recovering the corresponding gradient transfer map. We discuss its algorithmics, tests of the method against mock cosmological catalogues, and its application to observational data, which result in tight constraints on the mean mass density $\Omega_m$ and age of the Universe.

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I. INTRODUCTION

In the spectrum of possible models of fluid motion, the Euler equation of incompressible fluid constitutes an extreme. As was shown by Y. Brenier \cite{Brenier1, Brenier2}, any Lagrangian motion of fluid admits a polar factorization into a composition of an “incompressible” rearrangement, which preserves the volume of each infinitesimal fluid element, and an “absolutely compressible” transfer, which displaces fluid elements to their final locations prescribed by the gradient of a suitable convex potential, while expanding or contracting them in a way unaffected by any pressure or elasticity. Decomposing a fluid motion into a sequence of small time steps and factoring out the compressible transfer from the inertial fluid motion at each step yields a difference scheme for the incompressible Euler equation \cite{Brenier1}.

In this article we show how the opposite approach, in which only the compressible transfer is retained, can be applied to solving the problem of reconstructing peculiar motions and velocities of dark matter elements in cosmology. We also discuss algorithmics of this method, which gives an explicit discrete approximation to polar decomposition and can also be applied to model incompressible fluid as suggested in \cite{Brenier1}.

Recall that on scales from several to a few dozen of $h^{-1}$ Mpc the large-scale structure of the Universe is primarily determined by distribution of the dark matter. This distribution can be described by the mass density field and by the large-scale component of the peculiar velocity field \cite{Zeldovich}, controlled by dark matter itself via gravitational interaction. The dark matter distribution is traced by galaxies, whose positions and luminosities are presently summarized in extensive surveys \cite{SDSS, 2dF, WMAP}. On large scales luminosities of galaxies allow to determine their masses, from which the mass density of the dark matter environment can be estimated using well-established techniques \cite{Peebles1, Peebles2}.

It is appropriate to consider the reconstruction of the field of peculiar velocities as part of the more complex problem of reconstructing the full dynamical history of a particular patch of the Universe. Several approximate methods have been proposed to this end, of which we mention here two. The Numerical Action Method, based on looking for minimum or saddle-point solutions for a variational principle involving motion of discrete galaxies, was introduced by P. J. E. Peebles in the late 1980s \cite{Peebles1}; its modern state is addressed in the present volume by A. Nusser \cite{Nusser}. In this paper we concentrate on the Monge–Ampère–Kantorovich method introduced in \cite{MK} (hereafter the MAK method), specifically highlighting the structural relationship between the MAK method and the variational approach to the Euler equation of incompressible fluid \cite{Brenier2}.

In Section \textsuperscript{11} the mathematical setting of the MAK reconstruction is derived by application of the Zeldovich approximation to a suitable variational formulation of dark matter dynamics, which leads to the Monge–Kantorovich mass transfer problem and the Monge–Ampère equation. In Section \textsuperscript{11} we discuss algorithmics of solving the discretized Monge–Kantorovich problem, which gives as a byproduct an algorithm of polar decomposition for maps between discrete finite point sets. In Section \textsuperscript{11} we show that the MAK method performs very well when tested against direct numerical simulations of the cosmological evolution and review the recent applications of the MAK method to real observational data.
which yielded new tight constraints on the value of the mean mass density of the Universe. A detailed treatment of implementation and testing the MAK method against $N$-body simulations is presented in the companion paper by G. Lavaux in the present volume [20]. The paper is finished with a discussion and conclusions.

II. DYNAMICS OF COLD DARK MATTER AND THE ZEL'DOVICH APPROXIMATION

The most widely accepted explanation of the large-scale structure seen in galaxy surveys is that it results from small primordial fluctuations that grew under gravitational self-interaction of collisionless cold dark matter particles in an expanding universe (see, e.g., [12] and references therein). The relevant equations of motion are the Euler–Poisson equations written here for a flat, matter-dominated Einstein–de Sitter universe (for a more general case see, e.g., [13]):

$$\partial_\tau v + (v \cdot \nabla_x v) = -\frac{3}{2\tau} (v + \nabla_x \phi),$$  
$$\partial_\tau \rho + \nabla_x \cdot (\rho v) = 0,$$  
$$\nabla_x^2 \phi = \frac{1}{\tau} (\rho - 1).$$

Here $v(x, \tau)$ denotes the velocity, $\rho(x, \tau)$ denotes the density (normalized so that the background density is unity) and $\phi(x, \tau)$ is a gravitational potential. All quantities are expressed in comoving spatial coordinates $x$ and linear growth factor $\tau$, which is used as the time variable; in particular, $v$ is the Lagrangian $\tau$-time derivative of the comoving coordinate of a fluid element. A non-technical explanation of the meaning of these variables and a derivation of eqs. [13] in the Newtonian approximation can be found, e.g., in [14]; see also [15] in the present volume, where the growth factor is denoted by $a$.

The right-hand sides of the Euler and Poisson equations [13] contain denominators proportional to $\tau$. Hence, it suffices for the problem not to be singular as $\tau \to 0$ that

$$v(x, 0) + \nabla_x \phi(x, 0) = 0, \quad \rho(x, 0) = 1.$$  

Note that the density contrast $\rho - 1$ vanishes initially, but the gravitational potential and the velocity, as defined here, stay finite thanks to our choice of the linear growth factor as the time variable. Eq. [4] provides initial conditions at $\tau = 0$; at the present time $\tau = \tau_0$ the density is prescribed by a galaxy survey as explained above:

$$\rho(x, \tau_0) = \rho_0(x).$$

In parallel with the Euler equation of incompressible fluid, eq. [1] can be considered as the Euler–Lagrange equation for a suitable action $[14, 16]$:

$$\mathcal{I}_\alpha = \frac{1}{2} \int_0^{\tau_0} d\tau \int dx : \tau^\alpha (\rho |v|^2 + \alpha |\nabla_x \phi|^2),$$

where $\alpha = \frac{3}{2}$ for the flat Universe and minimization is performed under the constraints expressed by eqs. [2, 3]. Note that the term containing $|\nabla_x \phi|^2$ may be seen as a penalization for the nonuniformity of the mass distribution, which corresponds to the lack of incompressibility of the fluid; enhancing this penalization infinitely would suppress the “absolutely compressible” transfer of fluid elements, thus recovering the incompressible Euler equation.

However, according to eq. [4] the rotational component of the initial velocity field vanishes, which strongly suppresses the “incompressible” mode of the fluid motion at early times. Based on this observation, Ya. B. Zel'dovich proposed [17] an opposite approximation in which $\alpha \to 0$. In this approximation eq. [1] assumes the form

$$\partial_\tau v + (v \cdot \nabla_x v) v = 0.$$  

Much as the incompressible Euler system, the study of the Zel’dovich approximation benefits from the Lagrangian approach. Let $x(q, \tau)$ be the comoving coordinate at time $\tau$ of a fluid particle that was initially located at $q$: $x(q, 0) = q$. Then

$$\rho(x(q, \tau), \tau) = \left(\text{det}(\partial x/\partial q)\right)^{-1},$$

$$v(x(q, \tau), \tau) = \partial_\tau x(q, \tau),$$

where the $\tau$ derivative is taken as $q$ is fixed. As observed by Zel'dovich, in these new variables the nonlinear eq. [7] assumes a linear form

$$\nabla_x^2 x = 0.$$  

Moreover eq. [2] is satisfied automatically, and the action becomes

$$\mathcal{I}_0 = \frac{1}{2} \int_0^{\tau_0} d\tau \int dq |\partial_x x(q, \tau)|^2 = \frac{1}{2\tau_0} \int dq |x_0(q) - q|^2.$$  

Here we denote $x_0(q) = x(q, \tau_0)$ and use the fact that action minimizing trajectories of fluid elements, determined by eq. [10], are given by

$$x(q, \tau) = q + (\tau/\tau_0)(x_0(q) - q).$$

Note that according to the first condition [14], $v(q, 0) = (1/\tau_0)(x_0(q) - q) = \nabla_q \Phi(q)$ and the Lagrangian map [12] remains curl-free for all $\tau > 0$: $x(q, \tau) = q + \tau \nabla_q \Phi(q)$ and $\Phi(q, \tau) = |q|^2/2 + \tau \Phi(q)$; thus the “incompressible” rotational component of the fluid motion is indeed fully suppressed.

To find the motion of the fluid in the Zel’dovich approximation it is necessary to minimize the action [11] under the constraint provided by the representation of density [8] and the boundary conditions [4, 5],

$$\text{det}(\partial x_0(q)/\partial q) = 1/\rho(x_0(q)).$$

In optimization theory this problem is called the Monge–Kantorovich problem. Equivalently, one can solve the
In practice we choose all formulation, which is another linear program; such dual (Lagrange) ear program is treated simultaneously with a primal e.g., [18]. Often the original, of minimizing (17) under constraints (18) linearly. Problem where the maximum is attained at such that \( x = \nabla_q \Phi_0(q) \), gives (14) a simpler form
\[
\frac{1}{2} \sum_{i,j} \gamma_{ij} |x_j - q_i|^2,
\]
where \( \gamma_{ij} \geq 0 \) denotes the amount of mass transferred from \( q_i \) to \( x_j \) and mass conservation implies for all \( i, j \)
\[
\sum_k \gamma_{kj} = m_j, \quad \sum_i \gamma_{ij} = \mu. \quad (18)
\]
In practice we choose all \( m_j \) to be integer multiples of the elementary mass \( \mu \), which guarantees that all \( \gamma_{ij} \) assume only values 0 or \( \mu \).

Observe that the unknowns \( \gamma_{ij} \) enter into the problem of minimizing (17) under constraints (18) linearly. Problems of this form are called linear programs and can be efficiently solved by various optimization methods, see, e.g., [15]. Often the original, primal formulation of a linear program is treated simultaneously with a (Lagrange) dual formulation, which is another linear program; such algorithms are called primal-dual algorithms. For the linear program at hand the dual formulation is to maximize
\[
- \mu \sum_i \phi_i - \sum_j \psi_j m_j \quad (19)
\]
under the constraints
\[
\frac{1}{2} |x_j - q_i|^2 + \phi_i + \psi_j \geq 0 \quad \text{for all } i, j. \quad (20)
\]
Here \( \phi_i, \psi_j \) are Lagrange multipliers for constraints [18]; the duality comes from the following representation of the (coinciding) optimal values of the two problems:
\[
\min \max_{\gamma_{ij} \geq 0, \phi_i, \psi_j} \left( \frac{1}{2} \sum_{i,j} \gamma_{ij} |x_j - q_i|^2 + \sum_i \phi_i (\sum_j \gamma_{ij} - \mu) + \sum_j \psi_j (\sum_i \gamma_{ij} - m_j) \right),
\]
where taking max or min leads to the primal and dual problem respectively. The coincidence of the optimal values implies that \( \gamma_{ij}, \phi_i, \psi_j \) solve the respective problems if and only if
\[
\sum_{i,j} \gamma_{ij} \left( \frac{1}{2} |x_j - q_i|^2 + \phi_i + \psi_j \right) = 0. \quad (21)
\]
In view of the nonnegativity conditions this means that for each pair \((i, j)\) either \( \gamma_{ij} = 0 \) or constraint (20) is satisfied with equality (and then \( \gamma_{ij} = \mu \)). For all other values of \( \gamma_{ij} \geq 0 \) and \( \phi_i, \psi_j \) that satisfy constraints (18, 20), the left-hand side of (21) is strictly positive and thus the value of (17) is strictly greater than that of (19); such \( \gamma_{ij}, \phi_i, \psi_j \) cannot be solutions to the respective optimization problems.

A typical primal-dual algorithm starts with a set of values of \( \phi_i, \psi_j \) for which all inequalities (20) hold and proceeds in a series of steps. At each step a constraint of the form (20) is found that is, in a certain sense, the easiest to be turned into equality, values of the corresponding \( \phi_i, \psi_j \) are updated accordingly, and the \( \gamma_{ij} \) is set to \( \mu \). An algorithm stops when the number of equalities in (20) equals the number of masses \((\mu, q_i)\), so that (21) is satisfied.

We found the auction algorithm of D. Bertsekas [19] (see also [20]) to be a particularly efficient primal-dual algorithm for the huge data sets arising from the cosmological application. The search for the constraint (20) that is to be satisfied with equality at each step may be performed very efficiently using a specially developed geometrical search routine, which is based on suitably modified routines of the ANN library [21]. Further details of this numerical implementation of the MAK method are given in [14] and in our forthcoming publication with M. Hénon. A new implementation in a parallel computing environment is reported in the companion paper of G. Lavaux [20].

We finally show why the solution of the Monge–Kantorovich problem in the discrete case gives a discrete analogue of polar decomposition. Let a discrete “map” \( \gamma \) between two sets of points \((\mu, q_i)\) and \((m_j, x_j)\) be given such that \( m_j = \sum_i \gamma_{ij} \) and \( \gamma_{ij} \) take only values 0 and \( \mu \). Solving the corresponding Monge–Kantorovich problem will give a discrete analogue \( \gamma_{ij} \) of the gradient...
transfers. To see this observe that for \( \Phi_i = \frac{1}{2}|q_i|^2 + \phi_i \), \( \Psi_j = \frac{1}{2}|x_j|^2 + \psi_j \) equality in (20) means that
\[
\Psi_j = \max_k (q_k \cdot x_j - \Phi_k)
\]
(c.f. (15)), i.e., the map sending \( q_i \) to \( x_j \) is a discrete analogue of the gradient map \( x(q) = \nabla_q \Psi(q) \) of the previous section. The corresponding discrete analogue of “incompressible” rearrangement is a permutation of \( (\mu, q_i) \) that for any \( j \) sends the set of points \( i \) such that \( \gamma_{ij} > 0 \) to the set of points \( i' \) such that \( \gamma_{ij'} > 0 \); if furthermore \( n_j = \mu \) for all \( j \), both sets are singletons and the permutation is recovered uniquely.

In the MAK method we are interested in the “gradient” part of the Lagrangian map sending elements of dark matter to their present positions, whereas in the difference scheme for the Euler equation proposed by Y. Brenier in [3] it is the permutation part that is retained.

Finally note that an alternative approaches to solve the Monge–Kantorovich problem, based on direct numerical resolution of eqs. (7, 2), was proposed in [22].

IV. TESTING AND APPLICATION OF THE MAK METHOD TO COSMOLOGICAL RECONSTRUCTION

The validity of the MAK method depends on the quality of the Zel’dovich approximation, which is hard to establish rigorously. To be able to apply the method to real-world data we have instead to rely on extensive numerical tests.

We report here a test of the MAK method against an \( N \)-body simulation with over \( 2 \times 10^6 \) particles [29]. The \( N \)-body simulation had the following characteristics: \( 128^3 \) particles were assembled in a cubic box of \( 200 \, h^{-1} \) Mpc, giving the mean inter-particle separation of \( 1.5 \, h^{-1} \) Mpc; the initial conditions for the velocity field \( v(q, 0) \) were taken Gaussian; the density parameter was chosen to be \( \Omega_m = 0.3 \), the Hubble parameter to be \( h = 0.65 \), the normalization of the initial power-spectrum \( \sigma_8 = 0.99 \), and the mass of a single particle in this simulation was \( M = 3.2 \times 10^{11} \, h^{-1} M_{\odot} \) where \( M_{\odot} \) is the solar mass.

The scatter plot in Fig. 1 demonstrates the performance of the MAK method in finding Lagrangian positions of the particles. At the scales that were probed, positions of about 20\% of particles are reconstructed exactly (for detailed data see Table I). This low rate is due to large multi-streaming at such small scales; at larger scales

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|}
\hline
Scale & \( \leq 1 \) & \( \leq 2 \) & \( \leq 3 \) & \( \leq 4 \) & \( \leq 5 \) \\
\hline
\% & 18\% & 41\% & 54\% & 66\% & 74\% \\
\hline
\end{tabular}
\caption{MAK reconstruction: percentage of successfully reconstructed initial positions at different scales (measured in units of mesh size in a box of \( 128^3 \) grid points).}
\end{table}

\*Exact reconstruction.
This procedure is illustrated in Fig. 2, taken from [24]. The catalog of galaxies \((m_j, x_j)\) that is used here is a 40% augmentation of the Nearby Galaxies Catalog, now including 3300 galaxies within 3000 km s\(^{-1}\) [4]. This depth is more than twice the distance of the dominant component, the Virgo cluster, and the completion to this depth in the current catalog compares favourably with other all-sky surveys. The second observational component is an extended catalog of galaxy distances (or radial component of peculiar velocities). In this catalog, there are over 1400 galaxies with distance measures within the 3000 km s\(^{-1}\) volume; over 400 of these are derived by high quality observational techniques that give accurate estimates of the radial components of peculiar velocities. The important feature of Fig. 2 is that the MAK contours are transversal to contours provided by other methods, which largely reduces the degeneracy of constraints in the parameter space.

V. CONCLUSION

According to the polar decomposition theorem of Y. Brenier [1, 2], kinematics of continuous fluid motion can be decomposed into “incompressible” rearrangement and “infinitely compressible” gradient transfer. The Euler equation of describes a system whose kinematics is dominated by incompressible motion. In this paper we show that the opposite limit, in which the incompressible component is negligible, corresponds to the Zel’dovich approximation, a physically meaningful model of motion of self-gravitating fluid arising in cosmology.

This result enables us to approximately reconstruct peculiar motion of matter elements in the Universe from information on their present-day distribution, without any knowledge of the velocity field; indeed, the latter itself can be recovered from the reconstructed Lagrangian map. The viability of this method is established by testing it against a large-scale direct N-body simulation of cosmological evolution; when applied to real observational data, the method allows to get very tight constraints on the value of the mean mass density and the age of the Universe.

Another contribution is an efficient numerical method decomposing a given displacement field into “incompressible” and “infinitely compressible” parts. This method is not limited to cosmological reconstruction but can also be used for modeling the dynamics of incompressible fluid as suggested by Y. Brenier in [3].

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