Passive Scalar: Scaling Exponents and Realizability

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An isotropic passive scalar field $T$ advected by a rapidly-varying velocity field is studied. The tail of the probability distribution $P(\theta, r)$ for the difference $\theta$ in $T$ across an inertial-range distance $r$ is found to be Gaussian. Scaling exponents of moments of $\theta$ increase as $\sqrt{n}$ or faster at large order $n$, if a mean dissipation conditioned on $\theta$ is a nondecreasing function of $|\theta|$. The $P(\theta, r)$ computed numerically under the so-called linear ansatz is found to be realizable. Some classes of gentle modifications of the linear ansatz are not realizable.

In the past several years, a number of papers have dealt with the theory of a statistically isotropic passive scalar field advected by an incompressible velocity field that varies very rapidly in time (white velocity field) [1, 2]. Some exact statistical relations can be written for this problem, which leads to the hope that, for the first time, anomalous scaling exponents for the inertial range can be derived analytically in a turbulence problem.

Nevertheless, progress has been limited. Closed equations exist for each order of $n$-point moments of the scalar field [3], but above 2nd order the number of independent variables is daunting. Perturbation analysis has yielded predictions of finite-order scaling exponents at two remote borders of the problem: infinite space dimensionality and infinitely nonlocal interaction of spatial scales of the velocity and scalar fields, with diffusivity exponent $\xi \to 0$ in (10) below [4, 5]. Neither regime is accessible to test by direct numerical simulation (dns).

A physically-motivated “linear ansatz” for dissipation terms in the equation of motion [3, 6] predicts all exponents for the full domain of $d$ and $\xi$. It has quantitative support from dns [6, 7] and from some experiments [2]. The ansatz has not been derived analytically. The predictions in the limit $\xi \to 0$ are implausible and in conflict with the perturbation results. It is unclear whether the ansatz has any domain of exact validity.

In the present paper it is deduced that, contrary to common expectation, the tail of the probability distribution function (pdf) of spatial scalar-field differences is Gaussian in the inertial range, rather than exponential or stretched-exponential. This leads to a relation between the asymptotic behavior of scaling exponents and that of a conditional mean of dissipation. The linear ansatz is found to yield a realizable (everywhere positive) pdf, while some gentle deviations from it do not. A general apparatus is formulated for relating scaling exponents to the pdf shape in the inertial range. It is used to obtain the linear-ansatz pdf explicitly.

The passive scalar field $T(x, t)$ obeys
\[
\frac{\partial}{\partial t} + u(x, t) \cdot \nabla T(x, t) = \kappa \nabla^2 T(x, t). \tag{1}
\]

where $\kappa$ is molecular diffusivity. A statistically steady state may be maintained by adding an appropriate source term to (1).

The structure functions are defined by $S_q(r) = \langle |\theta(r)|^q \rangle$, where $\theta(r)$ denotes $T(x + r, t) - T(x, t)$ and $\langle \rangle$ denotes ensemble average over homogeneous, isotropic statistics. Suppose that there is power-law inertial-range scaling of the structure functions $S_q(r)$,
\[
S_q(r) \propto (r/L)^{\xi_q}, \tag{2}
\]
where $L \gg r \gg \ell_d$, $L$ is a large length scale, the order of initial or injection scales, and $\ell_d$ is a dissipation scale. A realizable (everywhere positive) pdf $P(\theta, r)$ for $\theta(r)$ requires that $d\xi_q/dq$ be a non-increasing function of $q$ (Hölder inequalities). This does not exhaust the realizability conditions on $\xi_q$. Necessary and sufficient conditions for an everywhere non-negative $P(\theta, r)$, nonzero at an infinite set of $\theta$ values, are [28]
\[
\det[S_{i+j}(r)]_{i,j=0,1,\ldots,n} > 0, \quad (n = 0, 1, 2, \ldots) \tag{3}
\]
where $S_{i+j}$ is set to zero for odd $i + j$. $P(\theta, r)$ is unique if, in addition, $\sum_q S_{2n}(r)^{-1/2n} = \infty$ (Carleman’s criterion [29]). This is satisfied if $P(\theta, r)$ falls off exponentially or faster as $|\theta| \to \infty$.

Direct calculation of the moments of $P(\theta, r)$ verifies that the $r$ dependence implied by (3) is
\[
P(\theta, r) = \int_0^\infty \rho(a, r/r') P\left(\frac{\theta}{a}, r'/a\right) \frac{da}{a}, \tag{4}
\]
where $r$ and $r'$ are both in the scaling range and $\rho(a, R)$ has moments $\int_0^\infty a^{2n} \rho(a, R) da = R^{\xi_2n}$. Explicitly,
\[
\rho(a, R) = \frac{2}{\pi} \int_0^\infty \cos(ka) \phi(k, R) dk, \tag{5}
\]
\[
\phi(k, R) = 1 + \sum_{n=1}^\infty R^{\xi_{2n}} (-k^2)^n/(2n!). \tag{6}
\]
Eqs. (3)–(5) are easily generalized to the case where the $S_{2n}(r)/S_{2n}(r')$ do not scale as powers of $r/r'$.

The Hölder relations are equalities for normal scaling $\zeta_{2n} = n\zeta_2$, which yields $\rho(a, R) = \delta(a - R^{\zeta_2/2})$. The smallest possible values of the higher $\zeta_n$ plausibly are $\zeta_2 = \zeta_2$, which yields $\rho(a, R) = (1 - R^{\zeta_2})\delta(a - (0 + 0)) + R^{\zeta_2}\delta(a - 1)$. This corresponds to regions of constant $T$ interspersed with regions where $\theta(r)$ is as large as the macroscale differences $\theta(L)$; (1) cannot magnify differences in the injected $T$, only change their spatial scale and relax them. Unless the scaling is normal, $\rho(a, R)$ increases in normalized width $a/R^{\zeta_2/2}$ as $R$ decreases, so that $P(\theta, r)$ cannot have a similarity form like $r^{-\beta}F(\theta/r^d)$.

In both cases $\zeta_{2n} = n\zeta_2$ and $\zeta_{2n} = \zeta_2$, the tail of $P(\theta, r)$ is Gaussian if $P(\theta, r)$ is Gaussian for $r \sim L$. In a Gaussian pdf $\rho(2n) \sim n \ln n$ for large $n$, to within terms of order $n$. If $\rho(2n) \sim n \ln n$ for $r \sim L$, it follows that, for all $n\zeta_2 \geq \zeta_2 \geq \zeta_2$, $\rho(2n) \sim n \ln n$ for large $n$ throughout the scaling range. This is asymptotically Gaussian behavior of the tail. An exponential or stretched exponential pdf with tail $P(\theta, r) \propto \theta^{-\beta}$, with $b < 2$, instead requires $\rho(2n) \sim (2/n) \ln n$ as $n \to \infty$. Thus the tail of $P(\theta, r)$ cannot fall off more slowly than Gaussian in the scaling range. This does not preclude exponential or slower fall-off in the dissipation range of $r$. The same result holds for the pdf of velocity differences in the inertial range of Navier-Stokes turbulence. Other arguments for faster-than-exponential tails in the inertial range have recently been given by Ching and Procaccia and by Noulez.

In interpreting this result, a distinction must be made between the presence of a central cusp in the pdf, expressing the existence of regions in which there is almost no excitation, and the shape of the far tail. Confusion between these two features can result in spurious fitting of a pdf to an exponential or stretched exponential. An example of a cusp pdf is that implied by the linear ansatz and shown in Fig. 2.

If there is a range of $r$ where the source term may be neglected, the steady-state balance equation for the even-integer structure functions $S_{2n}(r)$ is

$$-\frac{2}{r^{d-1}} \frac{\partial}{\partial r} \left( r^{d-1} \eta(r) \frac{\partial S_{2n}(r)}{\partial r} \right) = nJ_{2n}(r),$$

in the limit of rapidly-changing (white) velocity field. The left side of (7) is derived perturbatively from the $u \cdot \nabla$ term in (6) in the white limit. Here $d$ is space dimensionality, $\eta(r)$ is the two-particle eddy-diffusivity scalar exerted by the velocity field, and

$$J_{2n}(r) = 2n \left\langle \theta(r)^{2n-1} H[\theta(r)] \right\rangle,$$

$$H[\theta(r)] = \left\langle (\nabla_x^2 + \nabla^2_x) \theta(r) \right\rangle \theta(r),$$

where $\left\langle \cdot (\theta(r)) \right\rangle$ denotes ensemble average conditioned on a given value $\theta(r)$, and $x' = x + r$.

Power-law dependence of $S_{2n}(r)$ in the inertial range is assured from the exact, closed equation of motion for $S_{2n}(r)$, provided that $\eta(r)$ has the form

$$\eta(r) = \eta(L)(r/L)^\xi \quad (0 < \xi < 2),$$

for $L \gg r \gg \ell_d$. The steady-state scaling exponent for $S_{2n}(r)$ found from (8) is $\zeta_2 = 2 - \xi$.

There is no a priori assurance of power-law inertial-range scaling of $S_{2n}(r)$ for $n > 1$. If it exists, the balance of advection and $\kappa$ terms in (6) implies that the $J_{2n}(r)$ have the form

$$J_{2n}(r) = nC_{2n}J_2(r)S_{2n}(r)/S_2(r),$$

where the $C_{2n}$ are dimensionless constants and

$$C_{2n} = \frac{\zeta_{2n}(\zeta_{2n} + d - \zeta_2)}{nd\zeta_2}.$$

(12)

The Hölder inequalities $\zeta_{2n} \leq n\zeta_2$ give

$$C_{2n} \leq 1 + \frac{n - 1}{d - \zeta_2}.$$

Equality in (13) corresponds to normal scaling $\zeta_{2n} = n\zeta_2$.

The simplest candidate for an anomalous scaling solution to (6) is the “linear ansatz” (6):

$$H(\theta, r) = J_2(r)\theta/S_2(r).$$

It corresponds to $C_{2n} = 1$ for all $n$ and yields

$$\zeta_{2n} = \frac{1}{2} \sqrt{4nd\zeta_2 + (d - \zeta_2)^2} - \frac{1}{2}(d - \zeta_2).$$

Linear relations like (13) were earlier proposed by Ching and Pope.

Using Mathematica® 3.0, I have verified numerically, for a number of values of $d$ and $\zeta_2$, that (13) satisfies (6) up to $2n = 100$, even in the extreme case where $P(\theta, r')$ in (8) is taken as a $\delta$ function. The $\zeta_{2n}$ corresponding to $C_{2n} = 1 + \beta(n - 1)$ do not satisfy (6) for $0 < \beta < \zeta_2/d$. This case yields $\zeta_{2n} \propto n$ as $n \to \infty$; $\beta = \zeta_2/d$ is normal scaling. The perturbation analyses (8)–(12) give $n\zeta_2 - \zeta_{2n}$ that are quadratic in $n$ for moderate $n$. They also satisfy (13), and $P(\theta, r)$ are not predicted.

A conditional mean related to dissipation may be defined by

$$K(\theta, r) = \left\langle (\nabla_x \theta + \nabla_x' \theta') \theta \right\rangle .$$

(16)

If $r \gg \ell_d$, the $\nabla_x \nabla_x'$ crossterm in (14) is negligible, and $K(\theta, r) \approx \left\langle (\nabla_x \theta)^2 + (\nabla_x' \theta')^2 \right\rangle \theta$, the conditional mean of the average of the dissipation at the points $x$ and $x'$. $K(\theta, r)$, $K(\theta, r)$, and $P(\theta, r)$ are related by an identity that follows from homogeneity alone (21).
\[ H(\theta, r)P(\theta, r) \equiv \frac{\partial}{\partial \theta} [K(\theta, r)P(\theta, r)]. \] (17)

If the tail of \( P(\theta, r) \) is Gaussian, and \( K(\theta, r) \) is no stronger than a power of \( |\theta| \), the leading term on the right of (17) at large \( |\theta| \) is \( -\theta K(\theta, r)P(\theta, r) \), whence \( H(\theta, r)/\theta \propto -K(\theta, r) \).

Monotonic growth of \( K(\theta, r) \) with \( |\theta| \) at inertial-range \( r \) is a very weak, qualitative form of Kolmogorov refined similarity hypothesis [33,34]. If it holds, then the linear ansatz for \( H(\theta, r) \) and associated \( \zeta_{2n} \propto n^{1/2} \) behavior at large \( n \) represent a lower bound for the asymptotic growth of \( \zeta_{2n} \). This bound is achieved if \( K(\theta, r) \) tends to a constant as \( |\theta| \to \infty \). Sublinear growth of \( H(\theta, r) \) at large \( |\theta| \) would make \( K(\theta, r) \) a decreasing function of \( |\theta| \) and would yield slower growth of \( \zeta_{2n} \) than \( n^{1/2} \) at large \( n \). Yakhot [13] and Chertkov [17] predict \( \zeta_{2n} \to \text{constant} \) as \( n \to \infty \), which can be shown to imply \( K(\theta, r) \propto |\theta|^{-2} \) as \( |\theta| \to \infty \) [see (19) and (22)].

The analytical relations between \( H(\theta, r) \), \( P(\theta, r) \), and the \( \zeta_{2n} \) in the inertial range may be expressed in terms of a "co-pdf" \( P_H(\theta, r) \) with moments \( \int_{-\infty}^{\infty} \theta^{2n} P_H(\theta, r)d\theta = C_{2n}S_{2n}(r) \) (\( C_0 = 1 \)). Then by (3) and (4),

\[ \frac{H(\theta, r)}{\theta} = \frac{J_2(r)}{S_2(r)} P_H(\theta, r), \] \hspace{1cm} (18)

and \( \int_{-\infty}^{\infty} P_H(\theta, r)d\theta = 1 \). If (3) is satisfied with \( S_{2n}(r) \) replaced by \( S_{2n}^{(r)}(r) = C_{2n}S_{2n}(r) \), then \( P_H \) and \( H(\theta, r)/\theta \) are everywhere positive. By (17),

\[ P_H(\theta, r) \equiv \frac{1}{\theta} \frac{S_2(r)}{J_2(r)} \frac{\partial}{\partial \theta} [K(\theta, r)P(\theta, r)]. \] \hspace{1cm} (19)

\( P_H(\theta, r) \) is related to functions \( \rho_H(a, r) \) and \( \phi_H(k, r) \) by equations identical to (4)–(6) except that a factor \( C_{2n} \) appears in \( \phi_H(k, r) \):

\[ \phi_H(k, R) = 1 + \sum_{n=1}^{\infty} R^{2n} C_{2n} (-k^2)^n / (2n)! \] \hspace{1cm} (20)

\( P_H(\theta, r) = P(\theta, r) \) under the linear ansatz. \( P_H(\theta, r) \) can be found analytically in some other cases that are formal solutions of (12). One is \( C_{2n} = 1 + \beta(n-1) \). The associated \( P_H \) is

\[ P_H(\theta, r) = \left( 1 - \frac{3\beta}{2} \right) P(\theta, r) - \frac{\beta \theta P(\theta, r)}{2} . \] \hspace{1cm} (21)

Another case is \( \zeta_{2n} = \zeta_2 \) at all \( n \), for which (12) yields \( C_{2n} = 1/n \). These \( C_{2n} \) values are generated by

\[ P_H(\theta, r) = \frac{1}{|\theta|} \int_{|\theta|}^{\infty} P(\theta', r)d\theta'. \] \hspace{1cm} (22)

More generally, closed forms for \( P_H \) can be written if \( C_{2n} \) is a finite polynomial in \( n \).

Eqs. (3) and (4) converge rapidly because of the denominators \( 2n! \). They have infinite radii of convergence if the \( \zeta_{2n} \) satisfy the Hölder inequalities. In some cases it is feasible to sum (3) and (4) numerically, perform the transforms and explore the shapes of \( P \) and \( P_H \). Both \( \phi(k, R) \) and \( \phi_H(k, R) \) can be computed for large values of \( k \), far out in the tails, by the use of Mathematica® to sum hundreds of terms at precisions of the order of a hundred decimal digits.

**Fig. 1.** \( \phi(k, R) \) for \( d = 2, \zeta_2 = 1/2, R = 0.01 \) under the linear ansatz (solid line). The dashed line is \( \phi_H(k, R) \) if the linear-ansatz \( \zeta_{2n} \) are reduced by \( n^{1/10} \), and the dotted line is \( \phi_H(k, R) \) for that case.

**Fig. 2.** \( P(\theta, r) \) for the linear-ansatz case (solid line); \( \theta_{rms} = 10^{-1/2} \). The dashed curve is a normalized Gaussian. The inset is \( \rho(a, R) \) for the linear-ansatz case.

\[ \zeta_q = -(d - \zeta_2)/2, \quad q_c = -(d - \zeta_2)^2/(2d\zeta_2). \] \hspace{1cm} (23)
should mark the limit of applicability of \(C_2\), and \(q_c\) should represent the most-negative moment order that exists. The derivative \(P(\theta, r')\) is here taken as a \(\delta\) function so that its moments of all negative orders exist. I therefore conjecture that the ansatz gives \(\phi(k, R) \propto k^{-|\phi|} (k \to \infty)\) so that \(\rho(a, R) \propto q_2^{\phi-1}\) at the origin. The \(P(\theta, r')\) given by \(\delta\), then is a constant \(\propto |\phi|^{-1}\) at the origin if \(3 > \phi_c > 1\) and \(\propto |\phi|^{-|\phi|} (\text{infinite cusp})\) if \(|\phi_c| < 1\). The crossover is at \(C_2 = (2 - \sqrt{3})d\). The data shown in Fig. 2 appear to be consistent with exponent \(-1.25\) at \(k = \infty\), together with \(\int_0^\infty \phi(k, R)dk = 0\), in accord with this conjecture.

The primary fact here is that the linear ansatz appears to yield a \(\rho(a, R)\) that is positive everywhere, ensuring positive \(P(\theta, r')\) also. The positivity of \(\rho(a, R)\) is a stronger result than \(\delta\). It implies positive \(P(\theta, r')\) even in the unphysical case where \(P(\theta, r')\) is a \(\delta\) function. In Fig. 2 there is an absolute cutoff of \(\rho(a)\) at finite \(a\). This confirms that \(P(\theta, r')\) is Gaussian-like at large \(\theta\), despite its appearance, if \(P(\theta, L)\) is Gaussian.

Fig. 1, dashed curve is the \(\phi(k, R)\) that results from a gentle modification of these linear-ansatz exponents, \(\xi_2 = \xi_2^R n^{-1/10}\), where \(\xi_2^R\) satisfies \(\delta\). This leaves \(\xi_2\) unchanged and the \(\xi_2\) go as \(n^{-5/3}\) as \(n \to \infty\). The large-\(k\) \((k \approx 200)\) tail of \(\phi\) appears to go approximately as \(k^{-0.18}\), \(\delta\) is satisfied for \(2n \leq 100\). The implied behavior of \(P\) at small \(\theta\) is \(\theta^{-0.18}\). The result for \(\phi(k, r')\) is Fig. 1, dotted curve. Its large-\(k\) behavior is qualitatively different from that of \(\phi(k, R)\); \(\phi_H\) continues to grow more negative at \(k = 200\). Its tail is very different from that of \(\phi\), which suggests bizarre behavior of \(H(\theta, r')\) at small \(\theta\). The effective exponents \(c_H = C_2 n + C_2 n \ln R\) for this case differ little from the \(\xi_2\). If they are tried as exponents \(C_2 n\), they satisfy the Hölder inequalities, but they violate \(\delta\) at \(2n = 56\) if \(P(\theta, r')\) in \(\delta\) is taken as a \(\delta\) function. This illustrates that mild and innocent-looking deviations from the linear ansatz can destroy realizability.

Numerical investigation is feasible for other values of \(\xi_2\) and \(R\) and other deviations from the linear ansatz (e.g. \(\xi_2\) behaving as \(n^{1/2}\) at large \(n\), but with \(C_2 n\neq 1\)). The results appear to be consistent with the conjecture that \(\delta\) determines the behavior of \(P(\theta, r')\) at \(\theta = 0\) under \(\delta\). In particular, for \(d = 2, \xi_2 = 1, R = 0.01\), the large-\(k\) exponent of \(\phi(k, R)\) clearly lies between 0 and \(-1\) \((c_H = 0.356)\). Sensitivity to changes of the \(S_2\) away from unity seems to be widespread.

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