A Multiscale Measure for Mixing and its Applications

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Abstract

In spite of a large amount of recent research on the problem of fluid mixing and its control, there is no consensus on a proper measure for quantifying mixing. We present a measure of mixing that is based on the concept of weak convergence and is capable of probing the "mixedness" at various scales. The particular problem that this measure, called the Mix-Norm, resolves is the inability of the scalar variance (L^2 variance of the scalar concentration field) to resolve various stages of contour-level rearrangement by chaotic maps. The Mix-Norm is a pseudo-metric for the weak convergence topology on the space of scalar fields. We demonstrate the utility of the Mix-Norm by showing how it accurately measures the efficiency of mixing due to diffusion and discrete dynamical systems.

1 Introduction

Fluid mixing is a very important stage in many engineering applications. Aref [1] has stuied the use of chaotic advection to enhance mixing in laminar flows. Books by Ottino [2] and Wiggins [3] address the problem of mixing using concepts and methods of dynamical systems theory. In spite of this comprehensive study of mixing from the point of view of dynamical systems theory, there is no consensus on how to measure mixing and in particular how to compare the mixing rates of two different processes. Previous approaches to this fundamental problem of measurement of mixing include using the entropy of the underlying dynamical system as an objective for mixing and using the scalar variance of a concentration field which is being tranported by a dynamical system. Control of mixing using a maximum entropy approach for a prototypical mixing problem was studied in [5]. As the authors themselves point out in [5], the entropy of a dynamical system (given by a spatial intergral of the Lyapunov exponents) is independent of the initial fluid configuration. Therefore, if we are interested in mixing only certain portions of the phase space, the maximum entropy approach is no more applicable. In work by Ashwin et al. [4], interesting mixing protocols (combination of diffusion with permutation operations on phase space) are described. In [4] the L^2 and L^∞ norms are used to measure mixing. Any L^p norm fails to quantify mixing accurately because it is insensitive to the generation of small scale structures of the scalar concentration field which is being transported by a volume-preserving chaotic system. Mostly, this problem of the L^p norm has been ignored because typically there is diffusion associated with the mixing protocols as in [4]. In the absence of diffusion, the L^p norm of a scalar concentration being transported by a volume-preserving system will not decay. We develop a measure, called the Mix-Norm, which is based on the concept of weak convergence and demonstrate its relation to the definition of mixing as seen in dynamical systems literature [6]. The Mix-Norm was motivated by the *mixing variance coefficient* proposed in [7]. The formulation of the Mix-Norm overcomes the deficiences of the two approaches mentioned above. The Mix-Norm depends on the initial fluid configuration and also succeeds in capturing the mixing efficiency of measure preserving transformations (in the absence of diffusion) wherein the standard L^2 variance fails to do so. In this paper, we have restricted ourselves to periodic domains for ease of representation and clarity.

2 Structure of the Mix-Norm

A dynamical system can be considered to be mixing if every portion of the phase space gets spread uniformly throughout the phase space under the action of the dynamical system. If a scalar density field is being transported by a volume-preserving dynamical system, it can be said to be mixing if the mean of the scalar field in all subsets of the phase space become closer and closer to

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the mean of the scalar field over the whole phase space. These are the guiding lines behind the formulation of the Mix-Norm.

2.1 The Mix-Norm on the circle

First, we present the mix-norm on the circle and then generalize it to an n-dimensional torus. We parametrize the domain by a non-dimensional distance y ranging from 0 to 1. Let $c : S^1 \to \Re$ and $c \in L^2_{S^1}$. Let

$$d(c,p,s) = \frac{\int_{p-s/2}^{p+s/2} c(y)dy}{s}. \qquad (1)$$

for all $s \in (0,1)$ and $p \in [0,1]$. $d(c,p,s)$ is the mean value of the function c within the interval $[p-s/2, p+s/2]$. Define

$$\phi(c,s) = \left(\int_0^1 [d(c,p,s)]^2\, dp\right)^{\frac{1}{2}}. \qquad (2)$$

$\phi(c,s)$ is the root mean square(RMS) of the average values of c over all subsets $[p-s/2, p+s/2]$. Then the Mix-Norm of c is given by

$$\Phi(c) = \left(\int_0^1 \phi^2(c,s)ds\right)^{\frac{1}{2}}. \qquad (3)$$

The basic idea behind the Mix-Norm is to parametrize all sub-intervals of S^1 and to take the RMS of the average values of c over these sub-intervals.

2.2 The Mix-Norm on an n-dimensional torus

We consider scalar functions $c : T^n \to \Re$ and $c \in L^2_{T^n}$ where $T^n = [0,1]^n$ is an n-dimensional torus. For notational convenience, we make the following definitions.

For $x \in \Re^N$, $m(x) = x_1 x_2 ... x_N$
$S = (0,1)^n$
For a given $s \in S$ and $p \in T^n$,
$A_{[p,s]} = [p_1 - s_1/2, p_1 + s_1/2] \times [p_1 - s_2/2, p_2 + s_2/2] \times ....$
$... \times [p_N - s_n/2, p_N + s_N/2]$
$\chi_{A_{[p,s]}}$ is the characteristic function on the set $A_{[p,s]}$.
(4)

Also, in all the discussions, for any two functions $f, g \in L^2_U$, the inner product is assumed to be

$$\langle f,g\rangle = \int_U f(y)g(y)dy. \qquad (5)$$

To define the Mix-Norm let

$$d(c,p,s) = \frac{\int_{y\in A_{[p,s]}} c(y)dy}{m(s)} = \frac{\langle c, \chi_{A_{[p,s]}}\rangle}{m(s)}. \qquad (6)$$

for all $s \in S$ and $p \in A$. $d(c,p,s)$ is the mean value of the function c within the subset $A_{[p,s]}$. Now define

$$\begin{aligned}\phi(c,s) &= \left(\int_{A_{[p,s]}\subset T^n} [d(c,p,s)]^2\, dp\right)^{\frac{1}{2}} \\ &= \left(\langle d(c,\cdot,s), d(c,\cdot,s)\rangle\right)^{\frac{1}{2}}.\end{aligned} \qquad (7)$$

Just as in the case for the real line, $\phi(c,s)$ is the RMS of the average values of c over all subsets $A_{[p,s]}$. Then the Mix-Norm of c is given by

$$\Phi(c) = \left(\int_{s\in S} \phi^2(c,s)ds\right)^{\frac{1}{2}}. \qquad (8)$$

The following two limits can be easily verified.

$$\lim_{s\to 0} \phi(c,s) = \left(\int_A c^2(y)dy\right)^{\frac{1}{2}} \qquad (9)$$

$$\lim_{s\to(b-a)} \phi(c,s) = \int_A c(y)dy \qquad (10)$$

Expressions (9) and (10) are respectively the L^2 norm and mean of the scalar field c which are two fundamental measures associated with any scalar field. Therefore, $\phi(c,s)$ for different values of $s \in S$ can be seen as a smooth transition of measures associated with the scalar field c ranging from the L^2 norm to the mean and the Mix-Norm is the integral of these measures over all possible scales $s \in S$.

2.3 The Mix-Norm as an inner product

From the previous sections, one can observe that the Mix-Norm can be written as a triple integral on the real line and as a $3n$ integral on an n-dimensional torus. This sections shows that the Mix-Norm can be written in a much more compact form as an inner product. Let the linear operator $D_s : L^2_{T^n} \to L^2_{T^n}$ be defined as follows:

$$[D_s c](p) = \frac{\int_{y\in A_{[p,s]}} c(y)dy}{m(s)} = \frac{\langle c, \chi_{A_{[p,s]}}\rangle}{m(s)}. \qquad (11)$$

Now $\phi(c,s)$ can be written as:

$$\phi(c,s) = \left(\langle D_s c, D_s c\rangle\right)^{\frac{1}{2}} = \left(\langle c, D_s^* D_s c\rangle\right)^{\frac{1}{2}} \qquad (12)$$

where D_s^* is the adjoint operator of D_s. Then the Mix-Norm $\Phi(c)$ is given by

$$\begin{aligned}\Phi^2(c) &= \int_{s\in S} \phi(c,s)ds = \int_{s\in S} \langle c, D_s^* D_s c\rangle \, ds \\ &= \left\langle c, \left[\int_{s\in S} D_s^* D_s ds\right] c\right\rangle = \langle c, Mc\rangle\end{aligned} \tag{13}$$

where

$$M = \left[\int_{s\in S} D_s^* D_s ds\right] \tag{14}$$

and which we refer to as the Mix-Operator. Note that M is a symmetric definite operator by construction and that M depends only on the domain under consideration. Thus, the square of the Mix-Norm of any function c can be computed as the inner product of c and Mc. The formulation of the Mix-Norm as an inner product makes the computation and any kinds of analysis more efficient. Also, this quadratic form makes the problem of fluid mixing more tractable as an optimal control problem.

3 Properties of the Mix-Norm

The Mix-Norm is a pseudo-norm on the space of functions meaning that it satisfies the following properties. For any $c \in L^2_{T^n}$,

1. $\Phi(c) \geq 0$, and $c = 0 \Rightarrow \Phi(c) = 0$.
2. $\Phi(\lambda c) =\mid \lambda \mid \Phi(c)$, where λ is a scalar constant.
3. $\Phi(c_1 + c_2) \leq \Phi(c_1) + \Phi(c_2)$.

A pseudo-norm is different from a norm in that a pseudo-norm can be zero for nonzero functions. In particular, the mix-norm is zero for a special class of nonzero functions which have a mean of zero on all sets of nonzero measure, but have nonzero values on sets of zero measure. This is exactly the requirement for checking weak convergence and will be discussed in the next sub-section. The triangular inequality property of the mix-norm is not surprising because clearly each $\phi(c,s)$ is a pseudo-norm and $\Phi(c)$ is just a summation of these pseudo-norms. The proof for the triangular inequality property is included in the Appendix.

3.1 The Mix-Norm and weak convergence

This section describes how the mix-norm is useful as pseudo-metric for checking weak convergence.

Definition 3.1. *A sequence of functions $\{c_n\}$, $c_n \in L^2$ is weakly convergent to $c \in L^2$ if*

$$\lim_{n\to\infty} \langle c_n, g\rangle = \langle c, g\rangle \text{ for all } g \in L^2. \tag{15}$$

Theorem 3.1. *A sequence of functions $\{c_n\}$, $c_n \in L^2$ which is bounded in the L^2 norm is weakly convergent to $c \in L^2$ if and only if*

$$\lim_{n\to\infty} \Phi(c_n - c) = 0. \tag{16}$$

Proof. First, assume that $\{c_n\}$ weakly converges to c. Then $\lim_{n\to\infty}\langle c_n, g\rangle = \langle c, g\rangle$ for any $g \in L^2$. In particular, $\lim_{n\to\infty}\langle c_n, \chi_{A_{[p,s]}}\rangle = \langle c, \chi_{A_{[p,s]}}\rangle$ for all $s \in S$ and $p \in T^n$. Therefore

$$\begin{aligned}\lim_{n\to\infty} d(c_n - c, p, s) &= \lim_{n\to\infty} \frac{\langle c_n - c, \chi_{A_{[p,s]}}\rangle}{m(s)} \\ &= \lim_{n\to\infty} \frac{\langle c_n, \chi_{A_{[p,s]}}\rangle - \langle c, \chi_{A_{[p,s]}}\rangle}{m(s)} = 0\end{aligned} \tag{17}$$

for all $s \in S$ and $p \in T^n$. Therfore $\lim_{n\to\infty} \phi(c_n - c, s) = 0$ and $\lim_{n\to\infty} \Phi(c_n - c) = 0$.

Now, assume that $\lim_{n\to\infty} \Phi(c_n - c) = 0$. Then

$$\lim_{n\to\infty} \phi(c_n - c, s) = 0. \tag{18}$$

for all $s \in S$. This follows from the non-negativity and smoothness of $\phi(c_n - c, s)$ with respect to s. Therfore $\lim_{n\to\infty} d(c_n - c, p, s) = 0$ for all $p \in T^n$ because $d(c_n - c, p, s)$ is continuous with respect to p. ie,

$$\lim_{n\to\infty} \langle c_n, \chi_{A_{[p,s]}}\rangle = \langle c, \chi_{A_{[p,s]}}\rangle. \tag{19}$$

Since the set $K = \{\chi_{A_{[p,s]}} : s \in S \text{ and } p \in T^n\}$ is linearly dense in L^2 and $\{c_n\}$ is bounded, it follows that $\lim_{n\to\infty}\langle c_n, g\rangle = \langle c, g\rangle$ for any $g \in L^2$. Thus $\{c_n\}$ weakly converges to c. □

For example, the series $\{c_n\}$ where $c_n(x) = sin(n\pi x)$ weakly converges to zero. Therefore the function $c = \lim_{n\to\infty} c_n$ falls in the nullspace of the Mix-Operator M described in Section 2.3.

4 Applications of the Mix-Norm

In this section we demonstrate the effectiveness of the Mix-Norm in the context of mixing protocols generated by diffusion and discrete dynamical systems. An initial distribution $c(y, 0)$ of some passive tracer on a space U is assumed and the total quantity is normalized so that

$$\int_U c(y,0)dy = 1. \tag{20}$$

Let the distribution at time t be $c(y,t) \geq 0$. In work by P. Ashwin et al [4] the L^2 and L^∞ norms are used to measure mixing. Also, they define t_{95} is to be the smallest $t > 0$ such that

$$\|c(y,t) - 1\|_\alpha \leq 0.05 \tag{21}$$

where α refers to the norm used. Note that t_{95} is a function of the initial distribution, the norm chosen and the mixing protocol.

4.1 Mixing by diffusion

Here we consider diffusion occuring over a timestep of one unit with a normalized diffusivity rate $D > 0$. We assume the domain to be periodic during one time step, so that the total quantity of tracer is preserved. The diffusion equation over one unit time is given by

$$c_t = Dc_{yy}. \tag{22}$$

Assume that c(y,0) has a Fourier expansion

$$c(y,0) = \sum_{n=-\infty}^{n=\infty} a_n e^{2\pi i n y} \tag{23}$$

where $a_n = \int c(y,0)e^{-2\pi i n y}dy$. The distribution at time t is given by

$$c(y,t) = \sum_{n=-\infty}^{n=\infty} a_n e^{2\pi i n y} e^{-4\pi^2 n^2 Dt}. \tag{24}$$

Thus, one time step of diffusion can be explicitly written as the operator

$$(P_{diff}(c))(y) = \sum_n e^{2\pi i n y}\left(e^{-4\pi^2 n^2 D}\int_0^1 c(x)e^{2\pi i n x}dx\right). \tag{25}$$

A lower bound for t_{95} corresponding to the L^2 norm can be computed as in [4] to be

$$t_{95} = \frac{\log(20\|c(y,0) - 1\|_2)}{4\pi^2 D} \tag{26}$$

Doing the same computation corresponding to the Mix-Norm we obtain:

$$\begin{aligned}
&\Phi^2(c(y,t) - 1)\\
&= \left\langle \sum_{n\neq 0} a_n e^{2\pi i n y} e^{-4\pi^2 n^2 Dt}, M\left(\sum_{n\neq 0} a_n e^{2\pi i n y} e^{-4\pi^2 n^2 Dt}\right)\right\rangle\\
&\leq e^{-8\pi^2 Dt}\left\langle \sum_{n\neq 0} a_n e^{2\pi i n y}, M\left(\sum_{n\neq 0} a_n e^{2\pi i n y}\right)\right\rangle\\
&= e^{-8\pi^2 Dt}\Phi^2(c(y,0) - 1).
\end{aligned} \tag{27}$$

Thus a lower bound for t_{95} corresponding to the Mix-Norm can be found as

$$t_{95} = \frac{\log(20\Phi(c(y,0) - 1))}{4\pi^2 D}. \tag{28}$$

The changes in the estimates for t_{95} obtained using the Mix-Norm compared to that in (26) can be demonstrated as follows. Consider initial distributions of the form $c(y,0) = c_n = 1 + sin(2n\pi y)$. One can easily show that the series $\{c_n\}$ weakly converges to the uniform distribution of 1. In other words, $\lim_{n\to\infty}\Phi(c_n - 1) = 0$ whereas $\|c_n - 1\|_2 = 1$ for all n. According to Equation 28 diffusion will achieve almost perfect mixing in very less time for very large n whereas the estimate in (26) does not depend on how large n is. In general, if the initial distribution has strong high frequency Fourier modes, then the diffusion process will achieve mixing in very less time which is reflected by the estimate obtained using the Mix-Norm.

4.2 Mixing by discrete dynamical systems

We consider discrete dynamical systems and study their mixing properties using the Mix-Norm. First, we summarize some definitions concerning discrete dynamical systems and mixing. For a more detailed exposition, one can refer to [6].

Definition 4.1. *Let $(X, \mathbf{A}, \mu)$ be a measure space. If $T : X \to X$ is a nonsingular transformation the unique operator $P : L^2 \to L^2$ defined by (29) is called the* **Frobenius-Perron operator** *corresponding to T.*

$$\int_A Pc(x)\mu(dx) = \int_{T^{-1}(A)} c(x)\mu(dx), for\ A \in \mathbf{A} \tag{29}$$

The Frobenius-Perron operator P is a linear operator that expresses how a scalar density field on the domain evolves with time corresponding to a mapping T on the domain. For measure-preserving transformations the Frobenius-Perron operator reduces to (30).

$$Pc(x) = c(T^{-1}(x)). \tag{30}$$

Definition 4.2. *Let $(X, \mathbf{A}, \mu)$ be a normalized measure space and $T : X \to X$ be a measure-preserving transformation. T is called* **mixing** *if*

$$\lim_{n\to\infty} \mu(A \cap T^{-n}(B)) = \mu(A)\mu(B) \text{ for all } A, B \in \mathbf{A} \tag{31}$$

Theorem 4.1. *Let A be a normalized periodic domain and $T : A \to A$ a volume-preserving transformation. Then the following statements are equivalent*

1. *T is mixing.*
2. *The sequence of functions $\{P^n c\}$ is weakly convergent to $\langle c, \chi_A\rangle$ for all $c \in L^2_A$.*
3. $\lim_{n\to\infty} \Phi(P^n c - \langle c, \chi_A\rangle) = 0$ *for all $c \in L^2_A$.*

Proof. For the proof on the equivalence of statements 1 and 2, the reader can refer to [6]. The equivalence of 2 and 3 follows from Theorem 3.1. □

Statements 1 and 2 help us to classify transformations as mixing or non-mixing, but don't give a method for metrizing mixing or the mixing rate of a transformation. Statement 3 solves this problem and also makes it possible to compare the mixing performance of two different transformations.

4.2.1 Mixing properties of the Standard Map

We consider the standard map $T : [0,1] \times [0,1] \to [0,1] \times [0,1]$ in the following form.

$$\begin{aligned} x' &= x + y + \epsilon sin(2\pi x)[mod 1] \\ y' &= y + \epsilon sin(2\pi x)[mod 1] \end{aligned} \tag{32}$$

The above map is a diffeomorphism on the 2-torus and was first introduced by Chirikov [8]. Its behaviour changes with the value of ϵ and for values of ϵ close to one, it has been observed to have chaotic properties. Here we study its mixing properties. In this study, the computational domain is the square $[0,1] \times [0,1]$ whose sides are being identified(upper with lower, left with right).We discretize the computational domain and let the the grid points be (x_i, y_j) where $x_i = idx, y_j = jdy$ for $i = 0, 1, .., N_x$ and $j = 0, 1, .., N_y$ and where $dx = 1/(N_x - 1)$ and $dy = 1/(N_y - 1)$. To approximate the Frobenius-Perron operator corresponding to this map, for each grid point we compute $T^{-1}(x_i, y_j)$ by a Newton iteration. $T^{-1}(x_i, y_j)$ does not necessarily have to lie on a grid point. We employ a simple approach of assigning $T^{-1}(x_i, y_j)$ to the closest grid point around it. Interpolation schemes can be used to approximate $c(T^{-1}(x_i, y_j))$. But, this can introduce artificial diffusion effects which may not be desirable. Therefore, the discrete version of the Frobenius-Perron operator can be written as

$$\hat{P}c(x_i, y_j) = c(x_{i'}, y_{j'}) \tag{33}$$

where

$$\begin{aligned} i' &= round(x(T^{-1}(x_i, y_j))/dx) \\ j' &= round(y(T^{-1}(x_i, y_j))/dy). \end{aligned} \tag{34}$$

Figure 4.2.1 shows the mixing properties of the Standard Map when starting with an initial distribution

$$c_0(x, y) = \begin{cases} -1 \text{ if } y < 0.5 \\ 1 \text{ if } y > 0.5 \end{cases} \tag{35}$$

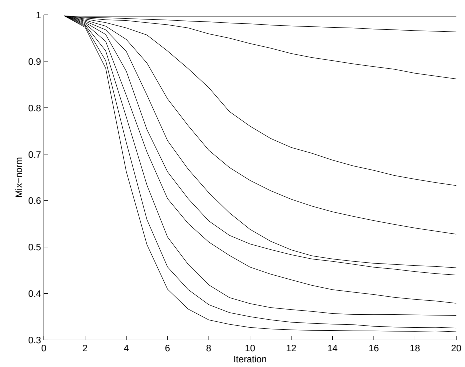

Figure 1: Plot showing the variation of the Mix-Norm with respect to number of iterations of the Standard Map for different epsilon values. For epsilon(ϵ) = 0, there is no mixing and as the value of epsilon(ϵ) increases, the mixing rate increases. These computations were done on a 500×500 grid. To compute the Mix-Norm we did not intergrate all they way up to the largest scale, but restricted ourselves to boxes of size up to 20 grid boxes

5 Conclusions

A multiscale measure for quantifying mixing has been presented. Its properties as a pseudo-norm induced by an inner product have been presented. We hope that the formulation of the Mix-Norm as an inner product makes the problem of fluid mixing more tractable as an optimal control problem. The effectiveness of the Mix-Norm in quantifying accurately the mixing rates due to diffusion and measure-preserving transformations have been discussed. Future applications include using it to optimize mixing in 3-D micromixer flows.

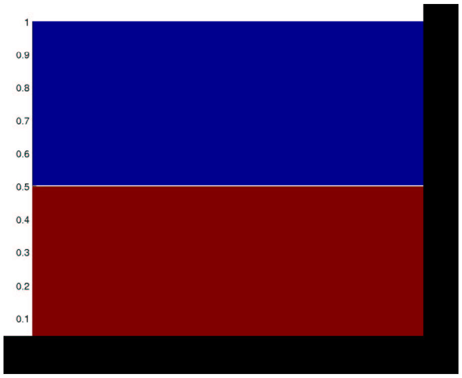

Figure 2: Contour plot of initial density distribution c_0

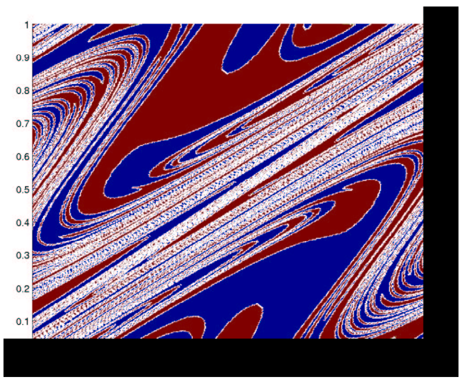

Figure 3: Contour plot of density distribution after 5 iterations for $\epsilon = 0.5$

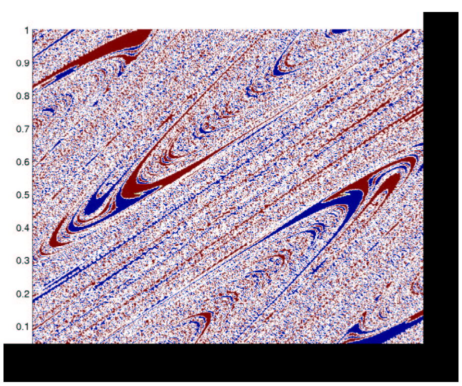

Figure 4: Contour plot of density distribution after 5 iterations for $\epsilon = 1$

6 Appendix

6.1 Proof for triangular inequality property of the Mix-Norm

Proof. Let $c_1, c_2 \in L^2_{T^n}$. We need to prove that $\Phi(c_1 + c_2) \le \Phi(c_1) + \Phi(c_2)$. Clearly,

$$d(c_1 + c_2, p, s) = d(c_1, p, s) + d(c_2, p, s) \tag{36}$$

Now,

$$\begin{aligned}
\phi^2(c_1 + c_1, s) &= \int\limits_{A_{[p,s]} \subset T^n} d(c_1 + c_2, p, s)^2 dp \\
&= \int\limits_{A_{[p,s]} \subset T^n} \left(d(c_1, p, s) + d(c_2, p, s)\right)^2 dp \\
&= \int\limits_{A_{[p,s]} \subset T^n} \left[\left(d(c_1, p, s)\right)^2 + \left(d(c_2, p, s)\right)^2 + 2\left(d(c_1, p, s)\right)\left(d(c_2, p, s)\right)\right] dp \\
&= \phi^2(c_1, s) + \phi^2(c_2, s) + 2 \int\limits_{A_{[p,s]} \subset T^n} \left[d(c_1, p, s) d(c_2, p, s)\right] dp
\end{aligned} \tag{37}$$

Applying the Cauchy-Schwartz inequality to above equation, we get

$$\begin{aligned}
\phi^2(c_1 + c_1, s) &\le \phi^2(c_1, s) + \phi^2(c_2, s) + 2\sqrt{\left(\int\limits_{A_{[p,s]} \subset T^n} [d(c_1, p, s)]^2 dp\right)\left(\int\limits_{A_{[p,s]} \subset T^n} [d(c_2, p, s)]^2 dp\right)} \\
&= \phi^2(c_1, s) + \phi^2(c_2, s) + 2\phi(c_1, s)\phi(c_2, s)
\end{aligned} \tag{38}$$

Then it follows that

$$\Phi^2(c_1 + c_2) \le \Phi^2(c_1) + \Phi^2(c_2) + \int\limits_{s \in S} 2\phi(c_1, s)\phi(c_2, s) ds \tag{39}$$

Applying the Cauchy-Schwartz inequality once again, we get

$$\begin{aligned}
\Phi^2(c_1 + c_2) &\le \Phi^2(c_1) + \Phi^2(c_2) + 2\sqrt{\left(\int\limits_{s \in S} \phi^2(c_1, s) ds\right)\left(\int\limits_{s \in S} \phi^2(c_2, s) ds\right)} \\
&= \Phi^2(c_1) + \Phi^2(c_2) + 2\Phi(c_1)\Phi(c_2) = \left(\Phi(c_1) + \Phi(c_2)\right)^2 \text{ (proved)}
\end{aligned} \tag{40}$$

□

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