The Optimal Transport Problem

Master Thesis

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Transport Problem

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by

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to obtain the degree of Master of Science in Mathematical Modelling and Engineering, to be defended publicly on September, 2018.

Project duration: September, 2016 - September, 2018

Thesis committee: Prof. Juan Enrique Martinez Legaz, UAB, supervisor



Preface

Preface...

Oscar Ramirez Barcelona, September 2018

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Notation Table.

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Ø
             Empty set
\mathbb{R}
             Real numbers field.
             \mathbb{R} \cup \{+\infty\}. That is [-\infty, \infty]
\mathbb{R}_{+}
            The set of nonnegative real numbers, that is the interval [0, \infty).
\bar{\mathbb{R}}_+
            The set of nonnegative extended real numbers, that is the interval [0, \infty]
\delta_x \\ \mathbb{R}^d
            The Dirac mass at point x.
            The d-dimensional Euclidean space.
            Identity map.
id
\mathcal{P}(X)
            Space of probabilities on X.
            The measure is absolutely continuous with respect to \nu.
\mu \ll \nu
            Indicator function of a set \Omega. If x \in \Omega then \mathbb{1}_{\Omega}(x) = 1. If x \in \Omega^c, we have \mathbb{1}_{\Omega}(x) = 0.
\mathbb{1}_{\Omega}
            A measure \mu restricted to a set A.
\mu \, \mathsf{L} \, A
            The Measure of the unite ball in \mathbb{R}^d.
\omega_d
            The min operator, that is a \wedge b := \min\{a, b\}.
Λ
            The max operator, that is a \lor b := \max\{a, b\}.
DT(x)
            Jacobian matrix of a map T(x).
            The image measure of \mu through the map T.
T_{\#}\mu
            The restriction of a function f to a set \Omega.
f_{|\Omega|}
\Pi(\mu,\nu)
            The set of transport plans from \mu to \nu.
\frac{\delta F}{\delta \rho}
            First variation of F: \mathcal{P}(X) \to \mathbb{R}, that is \frac{d}{d\epsilon} F(\rho + \epsilon \chi) \Big|_{\epsilon=0} = \int \frac{\delta F}{\delta \rho} d\chi
W_p
             Wasserstein distance of order p.
\dot{\mathbb{W}_p}
             Wasserstein space of order p.
            The transport plan in \Pi(\mu, \nu) induced by a map T. That is \gamma_T = (\mathrm{id}, T)_{\#}\mu and T_{\#}\mu = \nu.
\gamma_T M(T)
             Monge cost of a map T.
K(\gamma)
             Kantorovich cost of a plan \gamma.
            The product measure of \mu and \nu such that \mu \otimes \nu(A \times B) = \mu(A)\nu(B).
\mu \otimes \nu
M^{k \times h}
            The set of real matrices with k rows and h columns.
M^{\mathsf{T}}
            Transpose of a matrix M.
            Independent and identical probability distributions.
i.i.d.
1.s.c.
            Lower semicontinuous.
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Preliminaries.

Definitions and important theorems to remember.

We start this chapter reminding the basic definitions and theorems in topology and measure theory, since they are needed to have a suitable framework to discuss the optimal transport problem and its applications.

We start with the definition of topology that is needed to introduce a notion of continuity. We refer to [1] for more details.

Definition 1.1 (Topology). A topology on a set X is a collection \mathcal{T} of subsets of X having the following properties

- The space X itself and \emptyset are in \mathcal{T} .
- The union of the elements of any sub-collection of T is in T.
- The intersection of the elements of any finite sub-collection of T is in T.

A pair (X, \mathcal{T}) is called a topological space. The elements of \mathcal{T} are called open sets. The complements of the sets of \mathcal{T} are called closed sets. We call a neighborhood of x an element of \mathcal{T} containing x.

Definition 1.2 (Topological Basis.). Give a set X endowed with a topology T. We call a basis for T is a collection \mathcal{B} of subsets of X (called basis elements), such that,

- 1. For each $x \in X$, there is at least one basis element B containing x.
- 2. If x belongs to the intersection of two basis elements B_1 and B_2 , then there is a basis element B_3 containing x such that $B_3 \in B_1 \cap B_2$.

Definition 1.3 (Dense set). A subset D of a topological space X is dense in X if for any point x in X, any neighborhood of x contains at least one point from D.

Definition 1.4 (Separable space). A topological space is called separable if it contains a countable, dense subset.

Definition 1.5. Let X be a Hausdorff space. Let $\mathcal{V}(x_0)$ be a topological basis of X, such that all $V \in \mathcal{V}$ contains x_0 . Let $f: X \to \bar{\mathbb{R}}$ a functional valued in $\bar{\mathbb{R}}$. We define,

$$\liminf_{x \to x_0} f(x) = \sup_{V \in \mathcal{V}(x_0)} \inf_{s \in V} f(s)$$

$$\limsup_{x \to x_0} f(x) = \inf_{v \in \mathcal{V}(x_0)} \sup_{s \in V} f(s)$$

4 1. Preliminaries.

The above definitions can be expressed in terms of sequences of real numbers. Let $(x_n)_{n\in\mathbb{N}}$ be a sequence in X, the above formulation is equivalent to say.

$$\liminf_{n\in\mathbb{N}} x_n := \lim_{n\to\infty} \left(\inf_{m\geq n} x_m \right)$$

Equivalently for lim sup,

$$\liminf_{n\in\mathbb{N}} x_n := \lim_{n\to\infty} \left(\sup_{m\geq n} x_m \right)$$

Please note that the convergence to some point x_0 , $(x_n)_{n\in\mathbb{N}} \to x_0$ is not required in the last definitions.

Definition 1.6 (Lower Semicontinuity). On a complete metric space X, a function $f: X \to \mathbb{R}$ is said to be lower semi-continuous (l.s.c.) if for every sequence $(x_n)_{n\in\mathbb{N}}$ converging to $x\in X$, we have

$$f(x) \le \liminf_{n \in \mathbb{N}} f(x_n)$$

Definition 1.7 (Sequentially compact). A subset K of a metric space X is said to be compact if from any sequence x_n , we can extract a converging subsequence $x_{n_k} \to x \in K$.

We can see from the above definition that any continuous function is lower-semicontinuous.

Definition 1.8 (Compactness). A subset *K* of a metric space *X* is compact if every open cover of *K* has a finite subcover.

Theorem 1.1. A subset of a metric space is compact if and only if it is sequentially compact.

Theorem 1.2 (Maxima and Minima). Let X be a compact metric space and $f: X \to \mathbb{R}$ is continuous, real-valued function. Then f is bounded on X and attains its maximum and minimum. That is, there are x, y belonging to X such that,

$$f(x) = \inf_{z \in X} f(z)$$
 and $f(y) = \sup_{z \in X} f(z)$

Continuity is a strong requirement. Luckily we can assure the existence of a minimizer on lower-semicontinuous functions (or maximizer on upper-semicontinuous). The usual procedure to prove existence of a minimizer is making use of Weierstrass' criterion. We take a minimizing sequence and then we prove that the space in which we are trying to find a minimizer element is compact.

Theorem 1.3 (Weierstrass' criterion for existence of minimizers). If $f: X \to \mathbb{R}$ is lower semi-continuous and X is compact, then there exists $\hat{x} \in X$.

Proof. Define $l := \inf\{f(x) : x \in X\} \in \mathbb{R}$, notice that $l = +\infty$ only if f is identically $+\infty$, then this case is trivial since any point minimizes f. By compactness there exists a minimizing sequence x_n , that is $f(x_n) \to l$. By compactness we can extract a subsequence converging to some \hat{x} such that $\hat{x} \in X$. By lower-semicontinuity of f, we have that $f(\hat{x}) \liminf_n f(x_n) = l$. Since l is the infimum $l \le f(\hat{x})$. This proves that $l = f(\hat{x}) \in \mathbb{R}$.

We can apply the above analysis using a notion of upper-semicontinuity and compactness to find the maximum. Explanation about notions of convergence with bounded functionals and vanishing in infinity functions. If X is compact we have $C_0(X) = C_b(X) = C(X)$ if X and both notions of convergence coincide.

Definition 1.9 (Topological Dual). If X is a normed space, the dual space $X^* = \mathcal{B}(X, \mathbb{R})$. Consists of all linear and bounded functionals mapping from X to \mathbb{R} .

Definition 1.10 (Weak compactness in dual spaces). A sequence x_n in a Banach space X is said to be weakly converging to x, and we write $x_n \to x$, if for every $\xi \in X^*$. We have $\langle \xi, x_n \rangle \to \langle \xi, x \rangle$. A sequence $\xi_n \in X^*$ is said to be weakly-* converging to ξ , and we write $\xi_n \to \xi$, if for every $x \in X$ we have $\langle \xi_n, x \rangle \to \langle \xi, n \rangle$.

Theorem 1.4 (Banach-Alaouglu). If X is separable and ξ_n is a bounded sequence in X^* , then there exists a subsequence ξ_{n_k} weakly converging to some $\xi \in X^*$.

The Banach-Alaouglu's theorem is a well known result in functional analysis, an equivalent formulation is saying the closed unit ball in X^* is weak-* compact.

Definition 1.11. A sequence μ_n probability measures over X is said to be tight if for every $\epsilon > 0$, there exists a compact subset $K \subset XS$ such that $\mu_n(X \setminus K) < \epsilon$ for every n.

Definition 1.12 (Tightness). Let $(\mathcal{X},\mathcal{T})$ a topological space, and let \mathcal{A} a σ -algebra on \mathcal{X} that contains the topology \mathcal{T} . Let M be a collection of measures defined on \mathcal{A} . The collection M is called tight if for every $\epsilon > 0$ there is a compact subset K_{ϵ} of \mathcal{X} such that, for all measures $\mu \in M$ we have,

$$|\mu|(\mathcal{X}\backslash K_{\epsilon})<\epsilon$$

Theorem 1.5 (Prokhorov). Suppose that μ_n is a tight sequence of probability measures over a Polish space \mathcal{X} . Then there exists $\mu \in \mathcal{P}(X)$ and a subsequence μ_{n_k} such that $\mu_{n_k} \rightharpoonup \mu$, in duality with $\mathcal{C}_b(X)$. Conversely, every sequence $\mu_{n_k} \rightharpoonup \mu$ is tight.

Definition 1.13. Let $F: X \to \mathbb{R}$ be a given functional bounded from below on a metric space X. Let \mathcal{G} be the set of lower semicontinuous functions $G: X \to \mathbb{R}$, such that $G \leq F$. We call a relaxation the supremum of \mathcal{G} . This functional does exist since the supremum of an arbitrary family of lower semicontinuous functions is also lower semicontinuous. It is possible to have a representation formula as follows:

$$\bar{F}(x) = \inf \left\{ \liminf_{n \in \mathbb{N}} F(x_n) : x_n \to x \right\}. \tag{1.1}$$

As consequence of this definition we see that $F \geq \bar{F}$ implies $\inf F \geq \inf \bar{F}$. Let $l = \inf F$ then $F \geq l$. A constant function is lower semicontinuous. Therefore, $\bar{F} \geq l$ and $\inf \bar{F} \geq \inf F$. Implying that the infimum of both F and its regularization \bar{F} coincide, i.e. $\inf \bar{F} = \inf F$.

Definition 1.14. A measure over a set Ω is atomless if $\forall x \in \Omega$, we have $\mu(\{x\}) = 0$.

Definition 1.15 (Proper convex function). Let $f: X \to \mathbb{R}$, a function taking values in the extended real number line. We call it proper convex function if $\exists x \in X$ such that

$$f(x) < \infty$$

And $\forall x \in X$,

$$f(x) > -\infty \tag{1.2}$$

Basics in Convex Analysis.

Proposition 2.1. Let $f: X \to \mathbb{R}$ be a convex and lower-semicontinuous function. Assume that there exists $x_0 \in X$ such that $f(x_0) = -\infty$. Then f is nowhere finite on X.

Theorem 2.1. If f_{α} is an arbitrary family of lower semi-continuous functions on X, then $f = \sup_{\alpha} f_{\alpha}$ is also lower-semicontinuous.

Definition 2.1 (Convex conjugate function). Let X be a Banach space, let $f: X \to \overline{\mathbb{R}}$ be a functional over X. We call the convex conjugate to the function $f^*: X^* \to \overline{\mathbb{R}}$, defined as

$$f^*(x^*) = \sup_{x \in X} \{ \langle x^*, x \rangle - f(x) \}$$

Proposition 2.2. The convex conjugate $f^*: X^* \to \mathbb{R}$ of a function $f: X \to \mathbb{R}$ is convex.

Proof. Let x^*, y^* elements of the dual space X^* , and $t \in [0, 1]$,

$$f^{*}(tx^{*} + (1-t)y^{*}) = \sup_{x \in X} \{ \langle tx^{*} + (1-t)y^{*}, x \rangle - f(x) \}$$

$$= \sup_{x \in X} \{ \langle tx^{*} + (1-t)y^{*}, x \rangle - tf(x) - (1-t)f(x) \}$$

$$= \sup_{x \in X} \{ t \langle x^{*}, x \rangle + (1-t) \langle y^{*}, x \rangle - tf(x) - (1-t)f(x) \}$$

$$\leq \sup_{x, y \in X} \{ t \langle x^{*}, x \rangle + (1-t) \langle y^{*}, y \rangle - tf(x) - (1-t)f(y) \}$$

$$= t \sup_{x \in X} \{ \langle x^{*}, x \rangle - f(x) \} + (1-t)t \sup_{y \in X} \{ \langle y^{*}, y \rangle - f(y) \}$$

$$= tf^{*}(x^{*}) + (1-t)f^{*}(y^{*}).$$

Therefore f^* is convex regardless the convexity of f.

Theorem 2.2. A function $f: \mathbb{R}^d \to \bar{\mathbb{R}}$ is convex and lower-semicontinuous if and only if $f^{**} = f$.

Lemma 2.1 (Convex envelope theorem). Let X be a reflexive Banach Space. Then the convex conjugate function f^* is the maximum convex functional below f (also called convex envelope), i.e. if ϱ is convex functional and $\varrho(x) \leq f(x)$, $\forall x \in X$. Then, $f^{**}(x) \leq f(x)$, and $\varrho(x) \leq f^{**}(u)$, $\forall x \in U$. In particular $f^{**} = f$ if and only if J is convex.

Definition 2.2 (Legendre Transform). Let $f: \mathbb{R}^d \to \bar{\mathbb{R}}$ be a convex function, we call the Legendre transform f^*

$$f^*(y) = \sup_{x \in \mathbb{R}^d} \{x \cdot y - f(x)\}\$$

Corollary 2.1. A function $f: \mathbb{R}^d \to \overline{\mathbb{R}}$ is convex and l.s.c. if and only if $f^{**} = f$.

Definition 2.3 (Subdifferential). Given a proper convex function $f: X \to (-\infty, \infty]$, the subdifferential of such a function is the mapping $\partial f: X \to X^*$ defined by,

$$\partial f(x) = \{x^* \in X^*; f(x) - f(y) \le \langle x^*, x - y \rangle, \ \forall y \in X\}$$

Theorem 2.3 (Geometrical version of Hahn-Banach Theorem). Let M be a vector subspace of the topological vector space X. Suppose K is a non-empty convex open subset of X with $K \cap M = \emptyset$. Then there is a closed hyperplane $N \in X$ containing M with $K \cap N = \emptyset$.

Theorem 2.4. The epigraph of a convex and lower semicontinuous function is a closed convex set in $\mathbb{R}^d \times \mathbb{R}$, and can be written as the intersection of the half-spaces which contain it.

Linear Programming

Linear programming is a well studied branch of the mathematics that studies the optimization of linear functions under linear constrains. The study of linear programming started during the second part of the 1940s, as a technique military oriented problems.

We can formulate the problem in its general form as follows:

Problem 1. Given a cost vector $\mathbf{c} \in \mathbb{R}^n$, a linear operator $\mathbf{A} \in M^{m \times n}$

min
$$\mathbf{c}^{\mathsf{T}}\mathbf{x}$$
 (3.1)
subject to $\mathbf{A}\mathbf{x} = \mathbf{b}$ (3.2)
 $\mathbf{x} \ge 0$ (3.3)

Where . **A** is a $m \times n$ matrix, and **b** is an m-dimensional column vector. The vector inequality means $\mathbf{x} \geq 0$ means that each component is nonnegative. This problem has a solution if n > m.

Consider the system of equalities (3.2), the vector **b** belongs to \mathbb{R}^m .

Definition 3.1. Given the set of m simultaneous linear equations (3.2) with n unknowns, let \mathbf{B} be any nonsingular $m \times m$ submatrix made up of columns of \mathbb{A} . Then if all n-m

Definition 3.2. If one or more of the basic variables in a basic solution has value zero, that solution is said to be degenerate solution basic solution

Theorem 3.1 (Fundamental theorem of linear programming.). Given a linear program in

Simplex Method.

Optimal Transport Theory

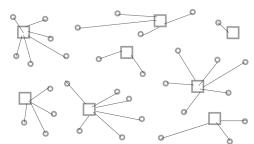
To introduce the optimal transport problem please imagine we are asked by a consortium of factories to design a plan for distributing their products among its many costumers in such a way that the transportation costs are minimal.

We can start the approach of this problem considering the costumers as members of the set X and the factories as members of a set Y. We want to know which factory $y \in Y$ is going to supply a costumer $x \in X$, i.e. $y = T(x) \in Y$. Therefore, we can estimate the transportation cost c(x,T(x)) of supplying a costumer x with a factory y = T(x). We see that our problem is reduced to find an assigning map from the set of costumers to the set of factories in such a way that the total cost $C(X,Y) = \sum_{x \in X} c(x,T(x))$ is minimal.

Figure 4.1: Illustration of the problem of Factories supplying Costumers.



(a) Factories represented by squares. Costumers represented by circles.



(b) Factories represented by squares. Costumers represented by circles. Assignation of a factory to a costumer represented by a line.

Gaspard Monge was a French mathematician who introduced for the first time the optimal transport problem as *déblais et remblais* in 1781. Monge was interested in finding a map that distributes an amount of sand or soil extracted from the earth or a mine distributed according to a density f, onto a new construction whose density of mass is characterized by a density g, in such a way the average displacement is minimal. In order to give a more precise idea of the problem, we make use of modern mathematical language and notation to state it as follows: Given two densities of mass f and g, Monge was interested in finding a map $T: \mathbb{R}^3 \to \mathbb{R}^3$ pushing the one onto the other,

$$\int_{A} g(y) dy = \int_{T^{-1}(A)} f(x) dx$$

For any Borel subset $A \subset \mathbb{R}^3$. And the transport also should minimize the quantity,

$$\int_{\mathbb{R}^3} \left| x - T(x) \right| f(x) \mathrm{d}x$$

We need to mention that given the context for which the problem was formulated, originally it was bind to \mathbb{R}^3 or \mathbb{R}^2 but we can consider the general case in \mathbb{R}^d . Notice that the problem requires a notion of measure. Then we find convenient to consider the measures μ on $X \subset \mathbb{R}^d$ and ν on $Y \subset \mathbb{R}^d$ induced by the densities f and g respectively. Therefore, we need to search for the optimum in the set of measurables maps $T: X \to Y$ such that the condition (4) is translated to,

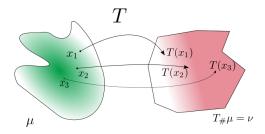
$$(T_{\#}\mu)(A) = \mu(T^{-1}(A)) \tag{4.1}$$

for every measurable set A. In other words, we need $T_{\#}\mu = \nu$. In the Euclidean frameworks if we assume f, g and T regular enough and T also injective, this equality implies,

$$g(T(x))\det(DT(x)) = f(x) \tag{4.2}$$

The equation (4.2) is nonlinear in T making difficult the analysis of the Monge Problem. Moreover, proving existence of a minimizer under this setting.

Figure 4.2: Monge problem. Finding a map.



Problem 2. Given two probability measures $\mu \in \mathcal{P}(X)$ and $\nu \in \mathcal{P}(Y)$ and a cost function $c: X \times Y \to \{0, +\infty\}$, the Monge's problem consists in finding a map $T: X \to Y$

$$\inf\left\{M\left(T\right) := \int_{X} c(x, T(x)) \mathrm{d}\mu(x) : \ T_{\#}\mu = \nu\right\} \tag{MP}$$

Definition 4.1. The space of Borel probability measures on \mathcal{X} is denoted by $\mathcal{P}(\mathcal{X})$. The weak topology on $\mathcal{P}(\mathcal{X})$ is induced by convergence against bounded continuous test functions on \mathcal{X} , that is $C_b(\mathcal{X})$.

Definition 4.2 (Coupling). Let (X, μ) and (Y, ν) be two probability spaces. Coupling μ and ν means constructing two random variables X and Y on some probability space (Ω, \mathcal{P}) such that $law(X) = \mu$, $law(Y) = \nu$. The couple (X, Y) is called a coupling of (μ, ν) .

Theorem 4.1. Let (X_i, μ_i) , i = 1, 2, 3, be Polish probability spaces. If (X_1, X_2) is a coupling of (μ_1, μ_2) and (Y_2, Y_3) is a coupling of (μ_2, μ_3) , then it is possible to construct a triple of random variables (Z_1, Z_2, Z_3) such that (Z_1, Z_2) has the same law as (X_1, X_2) and (Z_2, Z_3) has the same law as (Y_2, Y_3) .

Problem 3. Given $\mu \in \mathcal{P}(X)$, $\nu \in \mathcal{P}(Y)$, and $c: X \times Y \to [0, +\infty]$, we consider the problem

$$\inf\left\{K\left(\gamma\right):=\int_{X\times Y}c\mathrm{d}\gamma:\gamma\in\Pi\left(\mu,\nu\right)\right\} \tag{KP}$$

where $\Pi(\mu, \nu)$ is the set of transport plans.

Kantorovich formulation as relaxation

Theorem 4.2. Let X and Y be compact metric spaces, $\mu \in \mathcal{P}(X)$, $\nu \in \mathcal{P}$ and $c: X \times Y \to \mathbb{R}$ a continuous function. Then (KP) admits a solution.

Cyclical Monotonicity.

Definition 4.3 (c-transform). Let X and Y be sets, and $c: X \times Y \to (-\infty, \infty]$. A function $\psi: X \to \mathbb{R}$ is said to be c-convex if it is not identically to $+\infty$ and there exists $\psi^c: Y \to \mathbb{R}$

$$\psi^{c}(y) = \inf_{x \in X} c(x, y) - \psi(x). \tag{4.3}$$

Definition 4.4. Let X,Y be arbitrary sets, and $c: X \times Y \to (-\infty,\infty]$ be a cost function. A subset $\Gamma \subset X \times Y$ is said to be c-cyclically monotone if, for any $N \in \mathbb{N}$, and any family of points $(x_1,y_1), (x_2,y_2), ... (x_N,y_N)$ of Γ , the inequality

$$\sum_{i=1}^{N} c(x_i, y_i) \le \sum_{i=1}^{N} c(x_i, y_{i+1})$$

considering N + 1 = 1.

Since any permutation σ over the set $\{1, ..., N\}$ can be written as a product of disjoint cycles, we have that this property satisfies,

$$\sum_{i=1}^{N} c(x_i, y_i) \le \sum_{i=1}^{N} c(x_i, y_{\sigma(i)})$$
(4.4)

Definition 4.5 (Support of transport plan.). Given a separable metric space X, the support of a measure γ is defined as the smallest closed set on which γ is concentrated,

$$\operatorname{spt}(\gamma) := \bigcap_{\substack{\gamma(X \setminus A) = 0 \\ A = \bar{A}}} A \tag{4.5}$$

We can fix a point $(x_0, y_0) \in \operatorname{spt}(\gamma)$,

Theorem 4.3.

Wasserstein Spaces. \mathbb{W}_p

Computation of an Optimal Transport

The approximation of an optimal transport is a challenging problem, computationally speaking. We have found a rich literature on it, and many recent advances in this topic have arisen in the very last years.

Linear Programming Formulation.
Simplex Method Algorithm and Duality.
Sinkhorn-Knopp Algorithm.
Simulated Annealing.
Continuous Formulation.
Beckmann problem and

Applications

Nash Equilibrium.
Track of a Dynamic.
Domain Adaptation.
Isoperimetric Inequality.
Dynamical Optimal transport.
Barycenter of a Fourier Power Spectrum.****

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