Discrete transport problems and the concavity of entropy

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Motivating Problem I

- Suppose we have a pile of soil we need to move somewhere (say along $\mathbb{R}$, or along $\mathbb{Z}$).
- Each spadeful moved from point x to point y costs us something.
- Fix cost function e.g. $c(t) = |t|^p$ for $p \geq 1$.
- Moving one spadeful from x to y costs $c(y - x) = |y - x|^p$.
- Can we find a moving strategy that minimises the total cost $\ldots$?

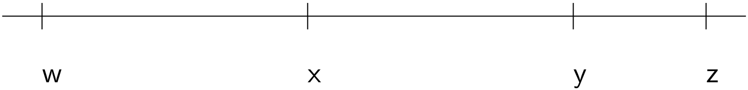
. . . Yes We Can!

- Source and destination piles need to have same size.
- Suppose piles have the same shape.
- Intuitive solution: just translate (move everything same distance).

More general case

- What if piles not the same shape?
- For many cost functions c, intuitive ‘non-crossing principle’.

Non-crossing principle



- Suppose spadefuls of soil at w and x to move to y and z.
- Take cost $c(t) = t^2$ for simplicity.
- Strategy 1: $w \longrightarrow z$, $x \longrightarrow y$. Cost $c_1 = (z-w)^2 + (y-x)^2$.
- Strategy 2: $w \longrightarrow y$, $x \longrightarrow z$. Cost $c_2 = (y-w)^2 + (z-x)^2$.
- $c_1 - c_2 = 2(x-w)(z-y) \geq 0$.
- Prefer Strategy 2: not to let soil cross over.
- Similar argument for any convex cost function.

Transport of probability measures

- Can rephrase problem more mathematically.
- Transport probability density function (or mass function) f_0 to f_1.
- Equivalently think in terms of distribution functions F_0 and F_1.
- Write $\Gamma(F_0, F_1)$ for the set of joint probability distributions with marginals F_0 and F_1 (couplings).
- Joint density $f(x, y)$ codes the amount of mass to be moved from x to y for particular strategy.

Transport of probability measures on $\{0, 1\}$

Example

- Consider marginals $f_0 = (3/4, 1/4)$ and $f_1 = (1/4, 3/4)$.
- Could define $f(x, y)$ as follows:

$f(x,y)$	$y = 0$	$y = 1$	
$x = 0$	$1/4$	$1/2$	$f_0(0) = 3/4$
$x = 1$	0	$1/4$	$f_0(1) = 1/4$
	$f_1(0) = 1/4$	$f_1(1) = 3/4$	

- Cost of strategy f is

$$\sum_{x,y} f(x,y)c(y-x) = \sum_{x,y} f(x,y)|y-x|^p.$$

Distance between probability measures

- This gives us a way to measure how similar F_0 and F_1 are ...
- ... measure cost to move one distribution to the other ...
- ... under optimal strategy.

Distance between probability measures

Definition

Given F_0 and F_1 and cost function $c(t) = |t|^p$, write

$$W_p(F_0, F_1) = \left(\inf_{F \in \Gamma(F_0, F_1)} \int |y - x|^p dF(x, y) \right)^{1/p}.$$

- Using non-crossing principle, optimal strategy gives

$$W_p(F_0, F_1) = \left(\int_0^1 |F_0^{-1}(t) - F_1^{-1}(t)|^p dt \right)^{1/p}.$$

- This is the Wasserstein distance ... (or Vasershtein) ... (or earth mover's) ... (or Mallows) ... (or Kantorovich) ... (or Kantorovich-Rubinstein) ... (or Monge-Kantorovich) ... (or Tanaka) ... (or transport) ... (or transportation) ... SEO hell!

Motivating problem II

- Suppose want to run from $x = 0$ to $x = D$ in T units of time.
- Suppose to maintain a speed of v costs us v^2 in energy.
- What is correct speed to run to minimise total energy use?
- Represent trajectory in terms of a function $x(t)$, with $x(0) = 0$ and $x(T) = D$.
- Wish to minimise $\int_0^T x'(t)^2 dt$.

Constant speed paths

- Obvious strategy: $x(t) = tD/T$.
- Gives $\int_0^T x'(t)^2 dt = T(D/T)^2 = D^2/T$.
- Now by Cauchy-Schwarz:

$$\left(\int_0^T 1 dt\right)\left(\int_0^T x'(t)^2 dt\right) \geq \left(\int_0^T x'(t) dt\right)^2 = D^2$$

- That is $T \int_0^T x'(t)^2 dt \geq D^2$.
- Obvious strategy (constant speed path) is optimal.

What does this tell us about the Wasserstein distance?

- We saw how to move probability density f_0 to f_1 on $\mathbb{R}$.
- Can think of this as taking 1 unit of time.
- Now suppose that we interrupt the process at time t.
- Where would we have got to?
- Can use ideas from fluid dynamics.
- Benamou–Brenier proved variational characterization of W_2.
- Works for $\mathbb{R}$, $\mathbb{R}^d$, Riemannian manifolds . . . but not e.g. $\mathbb{Z}$.

Benamou–Brenier formula

- Given distribution functions F_0 and F_1, write $\mathcal{P}_{\mathbb{R}}(F_0, F_1)$ for the set of densities $f_t(x)$ such that $F_0(x) = \int_{-\infty}^x f_0(y)dy$ and $F_1(x) = \int_{-\infty}^x f_1(y)dy$.
- Given a sequence of densities, define velocity field $v_t(x)$ by

$$\frac{\partial}{\partial t} f_t(x) = -\frac{\partial}{\partial x}\left(v_t(x) f_t(x)\right).$$

Theorem (Benamou–Brenier)

The quadratic Wasserstein distance on $\mathbb{R}$ is given by

$$W_2(F_0, F_1) = \left(\inf_{f_t \in \mathcal{P}_{\mathbb{R}}(F_0, F_1)} \int_0^1 \left(\int_{-\infty}^{\infty} f_t(y) v_t(y)^2 dy \right) dt \right)^{1/2}.$$

Benamou–Brenier geodesics

- If $f_t \in \mathcal{P}_{\mathbb{R}}(F_0, F_1)$ achieves infimum in Benamou–Brenier, call it a geodesic.
- Geodesics have nice properties.

Theorem

Geodesics satisfy fixed speed property:

$$W_2(F_s, F_t) = |t - s| W_2(F_0, F_1), \quad \textit{for all } s \textit{ and } t.$$

- Say that W_2 induces a length space.
- Fits with idea that geodesics are straight lines.

Entropy

Definition

Recall we measure ‘randomness’ of probability density f by entropy

$$H(f) = -\int_{\mathbb{R}} f(x) \log f(x) dx.$$

- Interested in how entropy varies along paths f_t.
- In particular, what is behaviour along geodesics?

Behaviour of entropy along paths

Definition

Given a path $f_t(x)$, introduce functions g_t and h_t such that

$$\frac{\partial f_t(x)}{\partial t} = -\frac{\partial g_t(x)}{\partial x}, \qquad \frac{\partial^2 f_t(x)}{\partial t^2} = \frac{\partial^2 h_t(x)}{\partial x^2}.$$

Theorem

Writing $H(t) = H(f_t)$ for the entropy along the path, under integrability conditions:

$$\begin{aligned} H''(t) &= -\int_{\mathbb{R}} \left(h_t(x) - \frac{g_t(x)^2}{f_t(x)} \right) \frac{\partial^2}{\partial x^2} (\log f_t(x))\, dx \\ &\quad -\int_{\mathbb{R}} f_t(x) \left(\frac{\partial}{\partial x} \left(\frac{g_t(x)}{f_t(x)} \right) \right)^2 dx. \end{aligned}$$

Behaviour of entropy along paths

Proof.

-
- $$H'(t) = -\int_{\mathbb{R}} \frac{\partial f_t(x)}{\partial t} \log f_t(x) dx$$

$$\begin{aligned} H''(t) &= -\int_{\mathbb{R}} \frac{\partial^2 f_t(x)}{\partial t^2} \log f_t(x) dx - \int_{\mathbb{R}} \frac{1}{f_t(x)} \left(\frac{\partial f_t(x)}{\partial t} \right)^2 dx \\ &= -\int_{\mathbb{R}} \frac{\partial^2 h_t(x)}{\partial x^2} \log f_t(x) dx - \int_{\mathbb{R}} \frac{1}{f_t(x)} \left(\frac{\partial g_t(x)}{\partial x} \right)^2 dx. \end{aligned}$$

- Integration by parts deals with these terms.
- Key is an explicit expression for $\frac{\partial^2}{\partial x^2} \log f_t(x)$.

□

Behaviour of entropy along geodesics

- Along BB geodesics turns out $g_t(x) = v_t(x) f_t(x)$ and $h_t(x) = v_t(x)^2 f_t(x)$.
- In above theorem

$$H''(t) = - \int_{\mathbb{R}} f_t(x) \left(\frac{\partial v_t(x)}{\partial x} \right)^2 dx \leq 0.$$

- This concavity used in information geometry.
- Properties of W_2 are key.
- Special case of Sturm–Lott–Villani theory. For example:

Theorem

For a Riemannian manifold (M, d) concavity of entropy along every geodesic is equivalent to positivity of the Ricci curvature tensor.

Discrete random variables

- Situation less clear for random variables supported on discrete sets.
- Will consider random variables supported on $\mathbb{Z}$ ...
- ...or in fact $\{0, 1, \ldots, n\}$.

For discrete problems, W_2 is not a length space

Example

- Consider marginals $f_0 = (3/4, 1/4)$ and $f_1 = (1/4, 3/4)$
- Obvious (and optimal) strategy $f_t = (3/4 - t/2, 1/4 + t/2)$.
- Could define $f_t(x, y)$ as follows:

$f_t(x,y)$	$y = 0$	$y = 1$	
$x = 0$	3/4 - t/2	t/2	$f_0(0) = 3/4$
$x = 1$	0	1/4	$f_0(1) = 1/4$
	$f_t(0) = 3/4 - t/2$	$f_t(1) = 1/4 + t/2$	

- Cost of f_t is $W_2^2(F_0, F_t) = \sum_{x,y} f_t(x,y)|y - x|^p = t/2$.
- Hence $W_2(F_0, F_t) = \sqrt{t} W_2(F_0, F_1)$ – not a length space.

Concavity of entropy: Shepp–Olkin conjecture

- Consider n independent Bernoulli random variables, with parameters $\mathbf{p} = (p_1, \ldots p_n)$.
- Their sum has mass function $f_{\mathbf{p}}(k)$ for $k = 0, 1, \ldots, n$.
- Consider the entropy of $f_{\mathbf{p}}$, defined by

$$H(\mathbf{p}) := -\sum_{k=0}^{n} f_{\mathbf{p}}(k) \log f_{\mathbf{p}}(k).$$

Conjecture (Shepp–Olkin (1981))

$H(\mathbf{p})$ is a concave function of $\mathbf{p}$.

- Sufficient to consider concavity for affine t, i.e. take

$$p_i(t) = p_i(0)(1-t) + p_i(1)t.$$

Known cases

- Folklore: $n = 1$.
- Shepp–Olkin (1981): $n = 2$, $n = 3$ (claim with no proof, in paper).
- Shepp–Olkin (1981): for all i, $p_i(t) = t$ (binomial case).
- Yu–Johnson (2009): for all i, either $p_i(0) = 0$ or $p_i(1) = 0$.
- Hillion (2012): for all i, either $p_i(t) = t$ or $p_i(t)$ constant (binomial translation case).

Motivating example: binomial case

Example

- Write spatial derivative $\nabla_1 f(k) = f(k) - f(k-1)$.
- For $0 \leq p < q \leq 1$, define $p(t) = p(1-t) + qt$.
- Write $\mathrm{Bin}_{n,p}(k) := \binom{n}{k} p^k (1-p)^{n-k}$.
- Write $f_t(k) = \mathrm{Bin}_{n,p(t)}(k)$.
- Simple calculation (e.g. Mateev, Shepp–Olkin) shows:

$$\frac{\partial f_t(k)}{\partial t} = -\nabla_1 \left(n(q-p) \mathrm{Bin}_{n-1,p(t)}(k) \right).$$

Motivating example: binomial case (cont.)

Example

- We rewrite this using an idea of Yu:

$$\mathrm{Bin}_{n-1,p}(k) = \frac{(k+1)}{n}\mathrm{Bin}_{n,p}(k+1) + \left(1 - \frac{k}{n}\right)\mathrm{Bin}_{n,p}(k).$$

- Suggests we introduce mixtures of mass functions:

$$\begin{aligned} \frac{\partial f_t(k)}{\partial t} &= -\nabla_1 \left(v g_t^{(\alpha)}(k) \right), \\ \text{for} \quad g_t^{(\alpha)}(k) &= \alpha_t(k+1) f_t(k+1) + (1 - \alpha_t(k)) f_t(k) \end{aligned}$$

- Here $\alpha_t(k) = k/n$ for all k and t and $v = n(q-p)$.
- Remember continuous equation $\frac{\partial}{\partial t} f_t(x) = -\frac{\partial}{\partial x} \left(v_t(x) f_t(x) \right)$.

Discrete Benamou–Brenier formula

Definition

- Write $\mathcal{P}_{\mathbb{Z}}(f_0, f_1)$ for the set of probability mass functions $f_t(k)$, given end constraints $f_t(k)|_{t=0} = f_0(k)$ and $f_t(k)|_{t=1} = f_1(k)$.
- Write $\mathcal{A}$ for the set of $\alpha(k)$ with $\alpha_t(0) \equiv 0$, $\alpha_t(n) \equiv 1$ and with $0 \leq \alpha_t(k) \leq 1$ for all k.

Discrete Benamou–Brenier formula

Definition

- For $f_t(k) \in \mathcal{P}_{\mathbb{Z}}(f_0, f_1)$ and $\boldsymbol{\alpha} \in \mathcal{A}$, define probability mass function $g_t^{(\boldsymbol{\alpha})}(k)$, velocity field $v_{\alpha,t}(k)$ and distance V_n by

$$g_t^{(\boldsymbol{\alpha})}(k) = \alpha_t(k+1) f_t(k+1) + (1 - \alpha_t(k)) f_t(k)$$

$$\frac{\partial f_t}{\partial t}(k) = -\nabla_1 \left(v_{\alpha,t}(k) g_t^{(\boldsymbol{\alpha})}(k) \right)$$

$$V_n(f_0, f_1) = \left(\inf_{\substack{f_t \in \mathcal{P}_{\mathbb{Z}}(f_0, f_1), \\ \alpha_t(k) \in \mathcal{A}}} \int_0^1 \left(\sum_{k=0}^{n-1} g_t^{(\boldsymbol{\alpha})}(k) v_{\alpha,t}(k)^2 \right) dt \right)^{1/2}.$$

- Refer to any path achieving the infimum as a geodesic.

Discrete Benamou–Brenier formula

Definition

- Example: binomial path is geodesic with $v_{\alpha,t}(k) \equiv n(q-p)$.
- Call path with $v_{\alpha,t}(k)$ fixed in k and t a constant speed path.

Proposition

- *V_n is a metric for probability measures on $\{0,\ldots n\}$.*
- *V_n defines a length space: for any geodesic f, distance $V_n(f_s, f_t) = |t-s| V_n(f_0, f_1)$.*
- *If there exists a constant speed path then*
  - *f_0 and f_1 are stochastically ordered.*
  - *Wasserstein distance W_1 and V_n coincide.*

Framework for concavity of entropy

- Want conditions under which entropy is concave.
- Give conditions in terms of $\alpha_t(k)$ to generalize binomial case.
- Recall that in that case, $\alpha_t(k) \equiv k/n$.

k-monotonicity condition

Condition (k-MON)

Given t, we say that the $\alpha_t(k)$ are k-monotone at t if

$$\alpha_t(k) \leq \alpha_t(k+1) \quad \textit{for all } k = 0, \ldots, n-1.$$

t-monotonicity condition

Condition (t-MON)

Given t, we say that the $\alpha_t(k)$ are t-monotone at t if

$$\frac{\partial \alpha_t(k)}{\partial t} \geq 0 \quad \textit{for all } k = 0, \ldots, n.$$

- Given a constant speed path

$$\frac{\partial f_t(k)}{\partial t} = -v \nabla_1 \left(g_t^{(\boldsymbol{\alpha})}(k) \right),$$

  introduce $h(k)$ such that

$$\frac{\partial^2 f_t(k)}{\partial t^2} = v^2 \nabla_1^2 \left(h(k) \right).$$

- t-MON condition provides an upper bound on $h(k)$.

GLC condition

Condition (GLC)

We say $f_t(k)$ is $\boldsymbol{\alpha}$-generalized log-concave at t, if for all $k = 0, \ldots, n-2$,

$$\begin{aligned} GLC(\boldsymbol{\alpha}_{\mathbf{t}})(k) &:= \alpha_t(k+1)(1-\alpha_t(k+1))f_t(k+1)^2 \\ &\quad -\alpha_t(k+2)(1-\alpha_t(k))f_t(k)f_t(k+2) \\ &\geq 0. \end{aligned}$$

Theorem (Hillion–Johnson 2014)

Consider constant speed path $f_t(k)$ and associated optimal $\alpha(t)$. If Conditions k-MON, t-MON and GLC hold at given $t = t^*$, the entropy $H(f_t)$ is concave in t at $t = t^*$.

Proof

- Dealing with logarithm remains key – but harder.
- k-MON and GLC together imply that

$$\frac{f_t(k)g_t(k+1)}{f_t(k+1)g_t(k)} \leq 1 \quad \text{and} \quad \frac{f_t(k+2)g_t(k)}{f_t(k+1)g_t(k+1)} \leq 1.$$

- Also $-\log v \leq \theta(v) = 1/(2v) - v/2$, for $v \leq 1$.
- Hence

$$\begin{aligned} & -\log\left(\frac{f_t(k)f_t(k+2)}{f_t(k+1)^2}\right) \\ = & \quad -\log\left(\frac{f_t(k)g_t(k+1)}{f_t(k+1)g_t(k)}\right) - \log\left(\frac{f_t(k+2)g_t(k)}{f_t(k+1)g_t(k+1)}\right) \\ \leq & \quad \theta\left(\frac{f_t(k)g_t(k+1)}{f_t(k+1)g_t(k)}\right) + \theta\left(\frac{f_t(k+2)g_t(k)}{f_t(k+1)g_t(k+1)}\right) \end{aligned}$$

Proof (cont.)

$$
\begin{aligned}
H''(t) &= \sum_{k=0}^{n} \frac{\partial^2 f_t(k)}{\partial t^2} \log f_t(k) - \sum_{k=0}^{n} \frac{1}{f_t(k)} \left(\frac{\partial f_t(k)}{\partial t} \right)^2 \\
&= -\sum_{k=0}^{n} v^2 \nabla_1^2 \left(h_t(k) \right) \log f_t(k) - \sum_{k=0}^{n} \frac{\left(\nabla_1 (v g_t(k)) \right)^2}{f_t(k)} \\
&= v^2 \sum_{k=0}^{n} h_t(k) \left(-\log \left(\frac{f_t(k) f_t(k+2)}{f_t(k+1)^2} \right) \right) - \sum_{k=0}^{n} \frac{\left(\nabla_1 (v g_t(k)) \right)^2}{f_t(k)} \\
&\leq v^2 \sum_{k=0}^{n} h_t(k) \left(\theta \left(\frac{f_t(k) g_t(k+1)}{f_t(k+1) g_t(k)} \right) + \theta \left(\frac{f_t(k+2) g_t(k)}{f_t(k+1) g_t(k+1)} \right) \right) \\
&\quad - \sum_{k=0}^{n} \frac{\left(\nabla_1 (v g_t(k)) \right)^2}{f_t(k)}
\end{aligned}
$$

Proof (cont.)

- ... and then, as if by magic, this becomes minus a perfect square!!
- Details best left to Mathematica ...
- $H''(t)$ becomes $\leq -v^2$ times ...

$$\sum_{k=0}^{n-2} \frac{f_t(k)f_t(k+1)f_t(k+2)}{2g_t(k)g_t(k+1)} \left(\frac{g_t(k)^2}{f_t(k)f_t(k+1)} - \frac{g_t(k+1)^2}{f_t(k+1)f_t(k+2)} \right)^2$$

- Would like to know how to interpret this cf (above)

$$H''(t) = -\int_{\mathbb{R}} f_t(x) \left(\frac{\partial v_t(x)}{\partial x} \right)^2 dx \leq 0.$$

Relating this to Shepp–Olkin

Proposition

For Shepp–Olkin interpolations, if all p_i' have the same sign ('monotone case'):

- *We have a constant speed path*
- *k-MON condition holds.*
- *GLC condition holds.*
- *However, t-MON condition fails for some Shepp–Olkin paths.*
- *Entropy remains concave if replace by t-MON by weaker 'Condition 4'.*
- *Condition 4 holds for Shepp–Olkin paths.*

Main result of our paper

Theorem (Hillion–Johnson 2014)

If all p_i' have the same sign, $H(\mathbf{p})$ is a concave function of $\mathbf{p}$.

- Call this monotone Shepp–Olkin theorem.
- General case remains open (not constant speed path).