Software

We are pleased to make available two software repositories accompanying this analysis.

• Package compx for the R programming language implements computation of the information measures H(Y), I(X,Y), and J(X,Y), as well as a method for information-theoretic clustering. Access compx at

https://github.com/PhilChodrow/compx.

To install in R, install the package devtools at

https://cran.r-project.org/web/packages/devtools/index.html and run the command

devtools::install_github("PhilChodrow/compx")

in the R console.

• The analysis repository for this project, including data acquisition and processing; core computations; and figure generation. We hope that this repository will provide useful examples of how to use compx for others aiming to replicate and extend our results. Download the project files at

https://github.com/PhilChodrow/spatial_complexity.

Relation of mutual and Fisher informations

Let X be a continuous random variable taking values in \mathbb{R}^n , and let Y be a discrete random variable define on finite alphabet \mathcal{Y} . Suppose further that p(y|x) > 0 and that p(y|x) is differentiable as a function of x for all $x, y \in \mathbb{R}^n \times \mathcal{Y}$. Fix $x_0 \in \mathbb{R}^n$, and define $B_r \triangleq B_r(x_0) = \{x \in \mathbb{R}^n \mid ||x - x_0|| \le r\}$. Additionally, define the *local mutual information* in B_r as the mutual information between X and Y where X is restricted to B_r :

$$I_r(x_0) \triangleq \mathbb{E}_X[D[p(\cdot|X)||p(\cdot|X \in B_r)]|X \in B_r]$$
(1)

$$= \int_{B_r} p(x|X \in B_r) D[p(\cdot|x) || p(\cdot|X \in B_r)] d^n x.$$
 (2)

where $D[p||q] \triangleq \sum_{y} p(y) \log \frac{p(y)}{q(y)}$ is the Kullback-Leibler divergence of q from p.

Theorem 1. *Under the stated conditions,*

$$\lim_{r \to 0} \frac{I_r(x_0)}{r^2} = \frac{n}{2(n+2)} \text{trace } J_Y(x_0) . \tag{3}$$

where the Fisher information matrix J_Y is given by

$$J_Y(x) \triangleq \mathbb{E}_Y \left[\nabla_x S_Y(x) \nabla_x S_Y(x)^T \right]$$
 (4)

$$S_{y}(x) \triangleq \log p(y|x) . \tag{5}$$

The proof of Theorem 2 proceeds by the application of a number of Taylor approximations, in tandem with a fundamental relationship of information geometry. We first expand out $I_r(x_0)$ explicitly as

$$I_r(x_0) = \int_{B_r} p(x|X \in B_r) D[p(\cdot|x) || p(\cdot|X \in B_r)] d^n x.$$
 (6)

Lemma 1. The following approximation relationships hold for the components of (6):

- (a) $p(X \in B_r, Y) = p(x_0, Y)v(B_r) + O(r^{n+2})$
- (b) $p(Y|X \in B_r) = p(Y|x_0) + e_y$ where the error terms e_y satisfy $e_y \in O(r^2)$ and $\sum_{y \in \mathcal{V}} e_y = 0$.
- (c) $p(x|X \in B_r) = \frac{1+O(r)}{v(B_r)}$

Proof. For each approximation, we directly apply Taylor expansions about $X = x_0$.

(a) We have

$$p(X \in B_r, Y) = \int_{B_r} p(x, Y) d^n x \tag{7}$$

$$= \int_{B_r} p(x_0, Y) + \frac{\partial p(x_0, Y)}{\partial x} (x - x_0) + O(\|x - x_0\|^2) d^n x \qquad (8)$$

$$= p(x_0, Y)v(B_r) + \frac{\partial p(x_0, Y)}{\partial x} \int_{B_r} (x - x_0) d^n x$$
(9)

$$+O\left(\int_{B_r} \|x - x_0\|^2 \ d^n x\right) \tag{10}$$

$$= p(x_0, Y)v(B_r) + O(r^{n+2}), (11)$$

where the middle term vanishes due to spherical symmetry.

(b) The fact that the error terms e_y must satisfy $\sum_{y \in \mathcal{Y}} e_y = 0$ follows from the fact that $p(Y|X \in B_r)$ must be a valid probability distribution over \mathcal{Y} . We'll now show that $e_y \in O(r^2)$. First,

$$p(X \in B_r) = \sum_{y \in \mathcal{Y}} p(X \in B_r, y)$$
(12)

$$= \sum_{y \in \mathcal{V}} \left[p(x_0, y) v(B_r) + O(r^{n+2}) \right]$$
 (13)

$$= p(x_0)v(B_r) + O(r^2); (14)$$

from part (a). Next,

$$p(Y|X \in B_r) = \frac{p(X \in B_r, Y)}{p(X \in B_r)}$$
(15)

$$= \frac{p(x_0, Y)v(B_r) + O(r^{n+2})}{p(x_0)v(B_r) + O(r^{n+2})}$$
(16)

$$= p(Y|x_0) + O(r^2) , (17)$$

which completes this part of the argument.

(c) First,

$$p(X \in B_r) = \int_{B_r} p(x) \ d^n x \tag{18}$$

$$= \int_{B_r} \left[p(x_0) + \nabla p(x_0)(x - x_0) + O(r^2) \right] d^n x \tag{19}$$

$$= p(x_0)v(B_r) + O(r^{n+2}), (20)$$

where the middle term again vanishes through spherical symmetry. Thus, for $x \in B_r$, we have

$$p(x|X \in B_r) = \frac{p(x)}{p(X \in B_r)}$$
(21)

$$= \frac{p(x_0) + \nabla p(x_0)(x - x_0) + O(r^2)}{p(x_0)v(B_r) + O(r^{n+2})}$$
(22)

$$=\frac{1+O(r)}{v(B_r)}. (23)$$

Lemma 2. The following approximation holds for the divergence factor in the integral (6)

$$D[p(\cdot|x)||p(\cdot|X \in B_r)] = D[p(\cdot|x)||p(\cdot|x_0)] + O(r^3)$$
(24)

Proof. We compute directly:

$$D[p(\cdot|x)||p(\cdot|X \in B_r)] = \sum_{y \in \mathcal{Y}} p(y|x) \log \frac{p(y|x)}{p(y|X \in B_r)}$$

$$= -H[Y|X = x] - \sum_{y \in \mathcal{Y}} p(y|x) \log p(y|X \in B_r)$$

$$= -H[Y|X = x] - \sum_{y \in \mathcal{Y}} p(y|x) \log (p(y|x_0) + e_y))$$
(from Lemma 1)
$$= -H[Y|X = x] - \sum_{y \in \mathcal{Y}} p(y|x) \left[\log p(y|x_0) + \frac{e_y}{p(y|x_0)} + O(e_y^2) \right]$$

$$= D[p(\cdot|x)||p(\cdot|x_0)] + \sum_{y \in \mathcal{Y}} \frac{p(y|x)}{p(y|x_0)} e_y$$
(quadratic terms negligible)
$$= D[p(\cdot|x)||p(\cdot|x_0)]$$

$$+ \sum_{y \in \mathcal{Y}} \left(1 + \frac{1}{p(y|x_0)} \nabla p(y|x_0)(x - x_0) + O(r^2) \right) e_y$$
(29)
$$= D[p(\cdot|x)||p(\cdot|x_0)] + \sum_{y \in \mathcal{Y}} [e_y + O(r^3)]$$
($e_y \in O(r^2)$)
$$= D[p(\cdot|x)||p(\cdot|x_0)] + O(r^3)$$
($\sum_{y \in \mathcal{Y}} e_y = 0$)

Lemma 3. For any positive-semidefinite matrix $A \in \mathbb{R}^{n \times n}$,

$$\int_{B_r} \langle x - x_0, A(x - x_0) \rangle d^n x = \frac{n}{n+2} r^2 v(B_r) \operatorname{trace}(A)$$

Proof. Since A is positive-semidefinite, there exist an orthonormal matrix P and a diagonal matrix D such that $A = P^T D P$. Furthermore, the entries of D are the eigenvalues $\{\lambda_i\}$ of A. Then,

$$\int_{B_r} \langle x - x_0, A(x - x_0) \rangle d^n x = \int_{B_r} \langle x - x_0, P^T D P(x - x_0) \rangle d^n x \tag{30}$$

 $= \int_{B_n} \langle P(x - x_0), DP(x - x_0) \rangle d^n x . \tag{31}$

We can regard P as a reparameterization of B_r ; since det P = 1, we have

$$\int_{B_r} \langle P(x - x_0), DP(x - x_0) \rangle d^n x = \int_{B_r} \langle x - x_0, D(x - x_0) \rangle d^n x \tag{32}$$

$$= r^n \int_{B_n} \langle rx, rDx \rangle \, d^n x \tag{33}$$

$$=r^{n+2}\int_{B_n}\langle x,Dx\rangle\,d^nx\,, (34)$$

where B_n is the unit n-ball. We also let $S_n(r)$ be the n-sphere of radius r. Continuing,

$$r^{n+2} \int_{B_n} \langle x, Dx \rangle d^n x = r^{n+2} \int_{B_n} \sum_{i=1}^n x_i^2 \lambda_i d^n x$$
 (35)

$$= r^{n+2} \sum_{i=1}^{n} \lambda_i \int_{B_n} x_i^2 d^n x$$
 (36)

$$= \frac{r^{n+2}}{n} \sum_{i=1}^{n} \lambda_i \int_{B_n} \|x\|^2 d^n x$$
 (37)

(spherical symmetry)

$$= \frac{r^{n+2}}{n} \operatorname{trace}(A) \int_{B_n} ||x||^2 d^n x$$
 (38)

(spherical symmetry)

$$= \frac{r^{n+2}}{n} \operatorname{trace}(A) \int_{\rho \in [0,1]} \rho^2 S_{n-1}(\rho) d\rho$$
 (39)

$$= \frac{r^{n+2}}{n} \operatorname{trace}(A) \int_{\rho \in [0,1]} \rho^{n+1} S_{n-1}(1) d\rho \tag{40}$$

$$= \frac{r^{n+2}}{n} \operatorname{trace}(A) \frac{1}{n+2} S_{n-1}(1)$$
 (41)

$$= \frac{r^2}{n+2} \operatorname{trace}(A) n r^n v(B_n(1)) \tag{42}$$

$$= \frac{n}{n+2} r^2 v(B_r) \operatorname{trace}(A) , \qquad (43)$$

as was to be shown. \Box

Fact. The Kullback-Leibler divergence and the Fisher information J_Y are related according to the approximation

$$D[p(\cdot|x)||p(\cdot|x_0)] = \frac{1}{2} \langle x - x_0, J_Y(x_0)(x - x_0) \rangle + O(||x - x_0||^3)$$
(44)

We are finally ready to prove Theorem 2. Computing directly, we have

$$I_r(x_0) \triangleq \mathbb{E}_X[D[p(\cdot|X)||p(\cdot|X \in B_r)]|X \in B_r]. \tag{45}$$

$$= \int_{B_r} p(x|X \in B_r) D[p(\cdot|x) || p(\cdot|X \in B_r)] d^n x \tag{46}$$

$$= \int_{B_r} \left[\frac{1 + O(r)}{v(B_r)} \right] D[p(\cdot|x) || p(\cdot|X \in B_r)] d^n x$$
 (Lemma 1(c))

$$= \left[\frac{1 + O(r)}{v(B_r)} \right] \int_{B_r} \left(D[p(\cdot|x) || p(\cdot|x_0)] + O(r^3) \right) d^n x$$
 (Lemma 2)

$$= \left[\frac{1 + O(r)}{v(B_r)}\right] \int_{B_r} \left(\frac{1}{2} \langle x - x_0, J_Y(x_0)(x - x_0) \rangle + O(\|x - x_0\|^3) + O(r^3)\right) d^n x \tag{47}$$

$$= \frac{1}{2} \left[\frac{1 + O(r)}{v(B_r)} \right] \int_{B_r} \left(\langle x - x_0, J_Y(x_0)(x - x_0) \rangle + O(r^3) \right) d^n x \tag{48}$$

$$= \frac{1}{2} \left[\frac{1 + O(r)}{v(B_r)} \right] \left(\frac{n}{n+2} r^2 v(B_r) \operatorname{trace}(J_Y(x_0)) + v(B_r) O(r^3) \right)$$
(49)

$$= r^2 \frac{n}{2(n+2)} \left[1 + O(r) \right] \left(\operatorname{trace}(J_Y(x_0)) + O(r^3) \right) . \tag{50}$$

Dividing through by r^2 and computing the limit as $r \to 0$ proves the result.

Computational Methods and Assumptions

In this section, we provide a specification of the computational procedure used to estimate $I(X,Y) = \mathbb{E}_x[J_Y(X)]$ using blockgroup level data from the U.S. Census.

For fixed Census blockgroup i, let P_i be the population, let A_i be the area, let $\rho_i = P_i/A_i$ be the population density, and let $p_Y^i(y)$ be the observed proportion of racial group y. For hex k in our hexagonal grid, let N_k be the set of overlapping Census blockgroups. We also define $p_I^k(i) = \rho_i/\sum_{i \in N_k} \rho_i$ as the estimated proportion of population within hex k residing in blockgroup i. This definition embodies a computationally-simplifying assumption that each blockgroup in N_k overlaps hex k with equal area. Finally, $p_Y^k(y) = \sum_{i \in N_k} p_I^k(i) p_Y^i(y)$ is the estimated overall racial composition of hex k. Then, we estimate the mutual information in hex k as

$$I(k) = \sum_{i \in N_k} p_I^k(i) D[p_Y^i(\cdot) || p_Y^k(\cdot)].$$
 (51)

Using (??), the estimated Fisher information is

$$J(k) \approx \frac{4I(k)}{r^2} \tag{52}$$

where r is the grid radius. The estimated population in hex k is $P_k = A_k \sum_{i \in N_k} \rho_i$, where A_k is the cell area. We finally estimate $\mathbb{E}_X[J(X)]$ as

$$J(X,Y) = \mathbb{E}_X[J_Y(X)] \approx \frac{1}{\sum_k P_k} \sum_k P_k J(k)$$
 (53)

Mutual and Fisher Informations: Part 2

Let X be a continuous random variable taking values in \mathbb{R}^n , and let Y be a discrete random variable define on finite alphabet \mathcal{Y} . Suppose further that p(y|x) > 0 and that p(y|x) is differentiable as a function of x for all $x, y \in \mathbb{R}^n \times \mathcal{Y}$. Fix $x_0 \in \mathbb{R}^n$, and define $B_r \triangleq B_r(x_0) = \{x \in \mathbb{R}^n \mid ||x - x_0|| \le r\}$. Additionally, define the *local mutual information* in B_r as the mutual information between X and Y where X is restricted to B_r :

$$I_r(x_0) \triangleq \mathbb{E}_X[D[p(\cdot|X)||p(\cdot|X \in B_r)]|X \in B_r]$$
(54)

$$= \int_{B_r} p(x|X \in B_r) D[p(\cdot|x) || p(\cdot|X \in B_r)] d^n x.$$
 (55)

where $D[p||q] \triangleq \sum_{y} p(y) \log \frac{p(y)}{q(y)}$ is the Kullback-Leibler divergence of q from p.

Theorem 2. *Under the stated conditions,*

$$\lim_{r \to 0} \frac{I_r(x_0)}{r^2} = \frac{n}{2(n+2)} \text{trace } J_Y(x_0) . \tag{56}$$

where the Fisher information matrix J_Y is given by

$$J_Y(x) \triangleq \mathbb{E}_Y \left[\nabla_x S_Y(x) \nabla_x S_Y(x)^T \right]$$
 (57)

$$S_{y}(x) \triangleq \log p(y|x) . \tag{58}$$

We first define the following functions. For set *A*, let

$$f_A(x) \triangleq D[p(y|x)||p(y|x \in A)] . \tag{59}$$

Additionally, let

$$q_r(x) \triangleq p(x|X \in B_r) . \tag{60}$$

We can then write the local mutual information as

$$I_r(x_0) = \int_{B_r} q_r f_{B_r} d\lambda , \qquad (61)$$

where λ is the Lebesgue measure in \mathbb{R}^n . We also let $V_r \triangleq \int_{B_r} d\lambda$ be the volume of B_r , which we will explicitly compute later. Finally, define

$$a_r(y) \triangleq p(X \in B_r, Y).$$
 (62)

Lemma 4. For all $x \in B_r$,

$$q_r(x) = \frac{1 + O(r)}{V_r} \,. \tag{63}$$

Proof. First, Taylor's theorem implies that there exists a linear map *T* such that

$$p(x) = p(x_0) + T(x - x_0) + O(\|x - x_0\|^2)$$
(64)

$$= p(x_0) + T(x - x_0) + O(r^2). (65)$$

Then,

$$p(X \in B_r) = \int_{B_r} p \ d\lambda \tag{66}$$

$$= \int_{B_r} p(x_0) + T(x - x_0) + O(r^2) d^n x.$$
 (67)

The middle term vanishes by spherical symmetry, leaving

$$p(X \in B_r) = p(x_0)V_r + O(r^{n+2}). (68)$$

For $x \in B_r$, we therefore have

$$p(x|X \in B_r) = \frac{p(x, X \in B_r)}{p(X \in B_r)}$$
(69)

$$=\frac{p(x)}{p(X\in B_r)}\tag{70}$$

$$= \frac{p(x_0) + T(x - x_0) + O(r^2)}{p(x_0)V_r + O(r^{n+2})}$$
(71)

$$=\frac{p(x_0) + O(r) + O(r^2)}{p(x_0)V_r}$$
(72)

$$=\frac{1+O(r)}{V_r}\,,\tag{73}$$

as was to be shown. \Box

Lemma 5. For all $y \in Y$,

$$a_r(y) = p(x_0, y)V_r + O(r^{n+2})$$
 (74)

Proof. Taylor's Theorem again implies that, for any $(x,y) \in B_r \times \mathcal{Y}$, there is a linear map T such that

$$p(x,y) = p(x_0,y) + T(x - x_0) + O(\|x - x_0\|^2)$$
(75)

$$= p(x_0, y) + T(x - x_0) + O(r^2). (76)$$

We then have

$$p(X \in B_r, y) = \int_{B_r} p(x, y) d^n x \tag{77}$$

$$= \int_{B_r} p(x_0, y) + T(x - x_0) + O(r^2) d^n x$$
 (78)

$$= p(x_0, y)V_r + O(r^{n+2}) d^n x , (79)$$

where the middle term has again vanished due to spherical symmetry. \Box

Lemma 6. For any $y \in \mathcal{Y}$, we have $p(y|X \in B_r) = p(y|x_0) + e_y$, where the error terms e_y satisfy $e_y \in O(r^2)$ and $\sum_{y \in \mathcal{Y}} e_y = 0$.

Proof. That the errors must satisfy $\sum_{y \in \mathcal{Y}} e_y = 0$ follows from the fact that $p(\cdot | X \in B_r)$ must be a valid probability distribution on \mathcal{Y} . We'll now show that $e_y \in O(r^2)$. We then have

$$p(y|X \in B_r) = \frac{p(X \in B_r, Y)}{p(X \in B_r)}$$

$$= \frac{p(x_0, y)V_r + O(r^{n+2})}{p(x_0)V_r + O(r^{n+2})}$$
(81)

$$= \frac{p(x_0, y)V_r + O(r^{n+2})}{p(x_0)V_r + O(r^{n+2})}$$
(81)

$$= p(y|x_0)O(r^2) , (V_r \propto r^n)$$

as needed.

Specification of Spatially-Constrained Information-Theoretic Clustering 0.1