The UMAP algorithm, reimagined

Rick Jardine

April 7, 2021

Rick Jardine The UMAP algorithm, reimagined

UMAP: "Uniform Manifold Approximation and Projection for Dimension Reduction"

Healy-McInnes, 2018 [4], Healy-McInnes-Melville, 2020 [5]

Outline

- \bullet Fuzzy sets, Fuzzy sets in $[0,\infty]$
- \bullet ep-metric spaces, coefficients in $[0,\infty]$
- \bullet TDA in $[0,\infty]$
- UMAP complex, excision
- Dimension reduction
- Optimisation: cross entropy

[0,1] is a locale.

A **locale** *L* is a poset (\leq) with infinite joins (least upper bounds) and finite meets (greatest lower bounds), in which finite meets distribute over all joins.

Facts: *L* has a terminal object (empty meet), an initial object (empty join), and infinite meets $(\bigvee_{x \leq all \ a_i} x)$.

Examples: 1) [a, b] and $[a, b]^{op}$ are locales, so $[0, 1]^{op}$ is a locale.

- 2) $[0,\infty]$ and $[0,\infty]^{\it op}$ are locales.
- 3) op_X (open subsets of a space X) is a locale.

Locales are topos-theoretic abstractions of topological spaces.

4) $[0, a) \hookrightarrow a$ defines an isomorphism of poset of half-open intervals in [0, 1] with elements of [0, 1].

Classical definition: A **fuzzy set** is a function $p: X \rightarrow [0, 1]$,

aka. a "fuzzy subset" of a universal set X.

Barr, 1974 [1]: A **fuzzy set** with coefficients in a locale *L* is a function $\phi : X \to L$.

A **morphism** $\phi \rightarrow \psi$ of fuzzy sets is a function $f : X \rightarrow Y$ such that in the picture



 $\phi(x) \leq \psi(f(x))$ for all $x \in X$. i.e. the diagram homotopy commutes.

There is a category Fuzz(L) of fuzzy sets with coefficients in L. Cases to care about: $L = [0, \infty], [0, \infty]^{op}, [0, 1], [0, 1]^{op}$.

Fuzzy sets and sheaves (Barr)

Every fuzzy set $\phi: X \to [0, \infty]$ defines a system of subsets $\phi^{-1}[0, a]$ for $a \in [0, \infty]$.

NB: If $a \leq b$ then $\phi^{-1}[0, a] \rightarrow \phi^{-1}[a, b]$ is an inclusion.

The assignment

$$\mathcal{T}(\phi)(a) = egin{cases} \phi^{-1}[0,a] & a\in[0,\infty] \ st & a=+ \ \end{cases}$$

defines a **sheaf** $T(\phi)$ on $[0, \infty]^{op}_+$, where $[0, \infty]^{op}_+ = [0, \infty]^{op} \sqcup \{+\}$ and + is new initial object (or new point at infinity for $[0, \infty]$).

Theorem 1 (Barr).

The functor $\phi \mapsto T(\phi)$ determines an equivalence of categories

$$\mathsf{Fuzz}([0,\infty]^{op})\simeq\mathsf{Mon}([0,\infty]^{op}_+)$$

with sheaves of monomorphisms on the locale $[0,\infty]^{op}_+$.

Classical fuzzy sets

Barr's theorem: there is an equivalence of categories

$$Fuzz([0,1]^{op}) \simeq Mon([0,1]^{op}_+).$$

Start with a sheaf F of monomorphisms on $[0,1]^{op}_+$, $F(s) \subset F(1)$ ("generic fibre"):

Given $x \in F(1)$ there is a minimum s_x such that $x \in F(s_x)$.

The assignment $x \mapsto s_x =: \phi_F(x)$ defines a function (fuzzy set) $\phi_F : F(1) \to [0, 1]$.

Meets, joins: $A, B \subset F$ in the sheaf category. Then $A \cup B$ and $A \cap B$ (sheaf theoretic) are subobjects of F, and

$$\phi_{A\cup B}(x) = \max\{\phi_A(x), \phi_B(x)\} \quad \text{``t-conorm''} \\ \phi_{A\cap B}(x) = \min\{\phi_A(x), \phi_B(x)\} \quad \text{``t-norm''} \\ \end{cases}$$

We have

$$\phi_A(x) \cdot \phi_B(x) \le \phi_{A \cap B}(x),$$

 $\phi_{A \cup B}(x) \le \phi_A(x) + \phi_B(x) - \phi_A(x) \cdot \phi_B(x).$

For $s, t \in [0, 1]$,

$$1-(1-s)(1-t)=s+t-s\cdot t$$

whereas $(A^c \cap B^c)^c = A \cup B$ for subobjects $A, B \subset X$.

The function $s \mapsto 1 - s =: e(s)$ defines a poset isomorphism (idempotent) $e : [0,1] \to [0,1]^{op}$ that I call the **dual**.

Classical: If $p: X \to [0, 1]$ is a fuzzy subset of X, its **complement** p^c is defined by $p^c(x) = 1 - p(x)$.

Alternatively, $p^c = e \cdot p$.

Definition: p^c is the **dual** of p.

Duality in the large

We have poset isomorphisms

$$\phi: [0,1] \stackrel{\cong}{\leftrightarrows} [0,\infty]^{op}: \psi$$

with $\phi(s) = -\log(s)$ and $\psi(t) = e^{-t}$ (order reversing).

 ϕ is Shannon's information function [6].

The commutative diagram of poset isomorphisms

$$\begin{array}{c} [0,\infty] \xrightarrow{\psi} [0,1]^{op} \\ \stackrel{e_{\psi}}{\longrightarrow} & \psi^{e} \\ [0,\infty]^{op} \xrightarrow{\psi} [0,1] \end{array}$$

$$(1)$$

defines a duality isomorphism (idempotent) $e: [0,\infty] \rightarrow [0,\infty]^{op}$.

$$x^* := e(x) = -\log(1 - e^{-x}) = x - \log(e^x - 1), \ x \in [0, \infty].$$

Facts: $x \mapsto x^*$ is continuous. x and x^* are close if x is near log(2).

Duals II

X is a set: there is a poset map $s : \mathcal{P}(X) \to \mathsf{Fuzz}([0,1])$, with

$$s(A)(x) = \begin{cases} 1 & \text{if } x \in A, \\ 0 & \text{if } x \notin A. \end{cases}$$

The fuzzy subset $s(A): X \to [0,1]$ of X is "crisp".

Any morphism $f : L \to L'$ of locales induces a functor $Fuzz(L) \to Fuzz(L')$, by composition with f.

There is a commutative diagram of poset morphisms

$$\begin{array}{c|c} \mathcal{P}(X) \xrightarrow{s} \mathsf{Fuzz}([0,1]) \xrightarrow{\phi} \mathsf{Fuzz}([0,\infty]^{op}) \\ c & \downarrow^{e} & \downarrow^{e} \\ \mathcal{P}(X)^{op} \xrightarrow{s^{op}} \mathsf{Fuzz}([0,1]^{op}) \xrightarrow{\phi} \mathsf{Fuzz}([0,\infty]) \end{array}$$

where c(A) = X - A is the complement of A in X.

Suppose that $u, v : X \to [0, 1]$ are fuzzy sets. The **cross entropy** from v to u is defined by

$$C(u,v) = \sum_{x \in X} (u(x)\log(\frac{u(x)}{v(x)}) + (1-u(x))\log(\frac{1-u(x)}{1-v(x)}))$$

(Bhandari 1993 [2]).

C(u, v) is a sum of elements of the form

$$F(s,t) = s \cdot \log(\frac{s}{t}) + (1-s) \cdot \log(\frac{1-s}{1-t}) \ge 0.$$

with $s, t \in [0, 1]$ (Kullback-Liebler divergence, 1951).

u (hence s) is fixed. C(u, v) is a (non-symmetric) measure of the distance of v from u.

Cross entropy II

Suppose
$$s = e^{-y}$$
 and $t = e^{-x}$. Then
 $F(s,t) = F(e^{-y}, e^{-x}) = e^{-y}(x-y) + e^{-y^*}(x^* - y^*).$
 $|F(e^{-y}, e^{-x})|$ depends on $|x - y|$ in $[0, \infty].$
Given $u, v : X \to [0, \infty] \xrightarrow{\psi} [0, 1]^{op}$, set
 $C(u, v) = C(\psi \cdot u, \psi \cdot v)$
 $= \sum_{x \in X} [e^{-u(x)}(v(x) - u(x)) + e^{-u(x)^*}(v(x)^* - u(x)^*)].$

For $u, v : X \to [0, \infty]$, C(u, v) is the **cross entropy** from v to u.

ep-metric spaces

An extended pseudo-metric space (**ep-metric space**) (X, D) is a set X and a function $D: X \times X \to [0, \infty]$ such that

- 1) D(x, x) = 0, 2) D(x, y) = D(y, x), 3) $D(x, z) \le D(x, y) + D(y, z)$.
- Can have distinct x, y such that D(x, y) = 0 ("pseudo").
- Can have u, v such that $D(u, v) = \infty$ ("extended").

Example: Every metric space (Y, d) is an ep-metric space:

$$Y \times Y \xrightarrow{d} [0,\infty) \subset [0,\infty].$$

A morphism $f : (X, d_X) \to (Y, d_Y)$ of ep-metric spaces is a function $f : X \to Y$ such that

 $d_Y(f(x), f(y)) \le d_X(x, y)$ (compresses distance, "non-expanding").

 $ep - \underline{Met}$ is the category of ep-metric spaces and their morphisms.

Cocompleteness (Spivak [7])

(X, d) an ep-metric space and $p: X \to Y$ a surjective function. For $x, y \in Y$ set

$$D(x,y) = \inf_{P} \sum_{i=0}^{k} d(x_i, y_i)$$

"Polygonal path" P: pairs (x_i, y_i) , $0 \le i \le k$, in X with $x = p(x_0)$, $p(y_i) = p(x_{i+1})$, $y = p(y_k)$.

Quotient map $p:(X,d) \rightarrow (Y,D)$ satisfies universal property.

Lemma 2.

 $ep - \underline{Met}$ is cocomplete (has all small colimits).

Underlying set is colimit in sets: $\sqcup_i (X_i, d_i)$ has $D(x, y) = d_i(x, y)$ if x, y in some X_i , $D(x, y) = \infty$ otherwise.

Coequalizers (or pushouts) given by quotient construction.

Vietoris-Rips complex

- (X, d_X) a finite **ep-metric space**, $d_X : X \times X \to [0, \infty]$. $s \in [0, \infty]$:
- 1) If X totally ordered (has a listing), then $V_s(X)$ has *n*-simplices $x_0 \le x_1 \le \cdots \le x_n$ with $d_X(x_i, x_j) \le s$ for all i, j.

 $V(X): s \mapsto V_s(X), s \in [0,\infty]$ is Vietoris-Rips system for X.

Simplicial fuzzy set: $V_*(X)$ is a simplicial sheaf of monomorphisms on $[0, \infty]^{op}_+$.

2) $P_s(X)$ is the poset of all subsets $\sigma \subset X$ such that $d_X(x, y) \leq s$ for all $x, y \in \sigma$.

 $P_s(X)$ is the poset of non-degenerate simplices of $V_s(X)$.

Nerve $BP_s(X)$ is the **barycentric subdivision** of $V_s(X)$. There is a natural weak equivalence $\gamma : BP_s(X) \xrightarrow{\simeq} V_s(X)$, $s \in [0, \infty]$.

NB: Poset const. $BP_s(X)$ does not use a total ordering on X.

The nerve construction

The **nerve** BC of a category C is a simplicial set with *n*-simplices BC_n given by the set of strings of arrows

 $a_0 \rightarrow a_1 \rightarrow \cdots \rightarrow a_n$

of length *n* in *C*, equivalently functors $\underline{n} \rightarrow C$, where

 $\underline{n} = \{0, 1, \ldots, n\},\$

with the obvious poset structure.

Composition with the functors $\theta : \underline{m} \to \underline{n}$ defines the simplicial set structure of *BC*.

Examples: 1) $B\underline{n} = \Delta^n$, the standard *n*-simplex in simplicial sets.

2) BG = K(G, 1) for a group G, classifies principal G-bundles in the homotopy category.

BC is also called the **classifying space** of C.

Comments

1) The systems $s \mapsto H_p BP_s(X) \cong H_p V_s(X)$ (coefficients in a field) define persistent homology for (X, d).

2) The sets $\pi_0 BP_s(X) \cong \pi_0 V_s(X)$ are clusters for (X, d).

Hierarchy $\Gamma(X, d)$: a tree with vertices (s, [x]), $[x] \in \pi_0 BP_s(X)$, and edges $(s, [x]) \rightarrow (t, [x])$ with $s \leq t$. Typical source of hierarchical clustering algorithms.

3) $\pi BP_s X$ is fundamental groupoid of $BP_s(X)$.

There are isomorphisms $\pi_0 BP_s(X) \cong \pi_0 \pi BP_s(X)$ so the system $s \mapsto \pi_0 \pi BP_s(X)$ "computes" clusters and hierarchies of clusters.

4) One cares most about $\varinjlim_{s < \infty} BP_s(X)$, which is a disjoint union of **global components**, each of which consists of simplices having edges of finite length.

Each global component is contractible, and has a Vietoris-Rips filtration in the usual sense.

Stability

Theorem 3 (Rips stability).

Suppose $i : X \subset Y$ are finite ep-metric spaces such that $d_H(X, Y) < r$. There is a homotopy commutative diagram

 $P_{s}(X) \xrightarrow{\sigma} P_{s+2r}(X)$ $i \downarrow \xrightarrow{\theta} \qquad \qquad \forall i$ $P_{s}(Y) \xrightarrow{\sigma} P_{s+2r}(Y)$

Corollary 4 (Stability for persistence invariants).

Same assumptions as Theorem 1. There are commutative diagrams

$$\begin{array}{c} H_k(V_s(X)) \xrightarrow{\sigma} H_k(V_{s+2r}(X)) \\ \downarrow & \downarrow \\ H_k(V_s(Y)) \xrightarrow{\sigma} H_k(V_{s+2r}(Y)) \end{array}$$

There is a corresponding statement for π_0 (clusters).

Stability: sketch proof

 $y \in Y$: there is $\theta(y) \in X$ st. $d(y, \theta(y)) < r$ (from $d_H(X, Y) < r$). $x \in X$: $\theta(x) = x$.



 $\sigma = \{y_1, \dots, y_k\} \text{ in } P_s(Y), \text{ then}$ $\sigma \cup \theta(\sigma) = \{y_1, \dots, y_k, \theta(y_1), \dots, \theta(y_k)\} \in P_{s+2r}(Y)$

and there are homotopies (natural transformations)

$$\sigma \subseteq \sigma \cup \theta(\sigma) \supseteq \theta(\sigma).$$

between poset morphisms $P_s(Y) \rightarrow P_{s+2r}(Y)$.

"Fuzzy graph" for (X, d_X)

Graph $\Gamma_*(X)$ has elts of X as vertices, and edges $\{x, y\}$ with $x \neq y$ and $d_X(x, y) < \infty$. $\Gamma_s(X)$ has edges $\{x, y\}$ with $d_X(x, y) \leq s$. $\check{C}(X)$ is **Čech groupoid**: X = objects, and there is a morphism $x \to y$ iff $d_X(x, y) < \infty$. $B\check{C}(X)_s$: $d_X(x, y) \leq s$. There are bijections

$$\pi_0 \Gamma_s(X) \xleftarrow{\cong} \pi_0 N \operatorname{sk}_1 B\check{C}(X)_s \xrightarrow{\cong} \pi_0 B\check{C}(X)_s,$$

natural in s: $s \leq t$ induces inclusion $B\check{C}(X)_s \subset B\check{C}(X)_t$.

Functor $\check{C}(X)_s \to \pi BP_s(X)$ (fund groupoid) takes a morphism $x \to y$ to the composite $\{x\} \to \{x, y\} \leftarrow \{y\}$

Theorem 5.

There are bijections

$$\pi_0\Gamma_s(X) \xleftarrow{\cong} \pi_0 N \operatorname{sk}_1 B\check{C}(X)_s \xrightarrow{\cong} \pi_0 B\check{C}(X)_s \xrightarrow{\cong} \pi_0 \pi B P_s(X).$$

The unoriented fuzzy graph $\Gamma_*(X)$ computes clusters for (X, d_X) .

Z = simplicial set.

 $N \operatorname{sk}_1 Z = \operatorname{sk}_0 Z \cup (\sqcup_{\sigma:\Delta^1 \to Z, \ d_0 \sigma \neq d_1 \sigma} \Delta^1) \to Z, \ \pi_0 ext{-isomorphism}.$

Boundary of a simplex $\sigma : \Delta^1 \to Z$: $\partial \sigma = \{ d_0 \sigma, d_1 \sigma \}.$

 $\Gamma(Z)$ is unoriented graph with vertices Z_0 with edges given by boundaries $\{d_0\sigma, d_1\sigma\}$ for $\sigma: \Delta^1 \to Z$ with $d_0\sigma \neq d_1\sigma$.

$$\pi_0\Gamma(Z)=Z_0/\sim,$$

where $x \sim y$ if $\{x, y\}$ is an edge, generates an equiv relation \sim . There are bijections

$$\pi_0 \Gamma(Z) \xleftarrow{\cong} \pi_0 N \operatorname{sk}_1 Z \xrightarrow{\cong} \pi_0 Z,$$

natural wrt inclusions $Z \subset Z'$ of simplicial sets.

Singular functor S

Spivak [7]: There is an adjoint pair of functors $\operatorname{Re}: s\operatorname{Set}^{[0,\infty]} \leftrightarrows ep - \operatorname{Met}: S$ $S(Y,d)_{s,n} = \operatorname{functions} \phi: \{0,1,\ldots,n\} \to Y \text{ with}$ $d(\phi(i),\phi(j)) \leq s, \text{ for } (Y,d) \text{ in } ep - \operatorname{Met} (\text{"bags of words"}).$

$$S(X,d)_s = B\check{C}(X)_s$$
 (!!)

For (X, d) a totally ordered finite ep-metric space, there is a canonical map of systems (functors)

$$\eta: V(X,d)_s \to S(X,d)_s.$$

 η takes the simplex $x_0 \le x_1 \le \cdots \le x_n$ to the sequence (x_0, x_1, \dots, x_n) .

Theorem 6 ([3]).

The map $\eta: V(X,d)_s \to S(X,d)_s$ is a weak equivalence of simplicial sets, for each s.

UMAP complex

 $(X, d_X) =$ finite data set, or finite ep-metric space ... but very big.

1) Choose **neighbourhood set** N_x , $x \in X$. Set $U_x = \{x\} \sqcup N_x \subset X$.

e.g. $N_x = k$ nearest neighbours if X is totally ordered, has metric (if you can find them — there are algorithms).

2) Set
$$(U_x, D_x) = \bigvee_{y \in N_x} (\{x, y\}, d_y)$$
 in ep – Met.
 $d_y(x, y) > 0$ is a **weight**.

3) Extend to an ep-metric D_x on X by setting $D_x(y, z) = \infty$ if either y or z is outside of U_x .

4) We have inclusions $X \subset V(X, D_x)$, $x \in X$ (X discrete). Form the iterated pushout

$$V(X, N) = \bigvee_{x \in X} V(X, D_x) \simeq \bigvee_X S(X, D_x).$$

BP(X, N) = V(X, N) is "the" **UMAP complex** — a simplicial presheaf on $[0, \infty]^{op}_+$, simp. fuzzy set with coefficients in $[0, \infty]^{op}$.

Given (X, d_X) and (X, D_x) as above, form the wedge sum

$$(X,D) = \vee_{x \in X} (X,D_x)$$

in ep-metric spaces.

 (X, D_x) is the realization of $V(X, D_x)$ for each x [3], so (X, D) is the realization of the UMAP complex V(X, N).

Theorem 7 (Excision for π_0).

 $V(X, N) = \lor_x V(X, D_x) \rightarrow V(X, D)$ induces a bijection

$$\pi_0 V(X, N)_s \xrightarrow{\cong} \pi_0 V(X, D)_s, 0 \le s < \infty.$$

Corollary 8.

There are bijections

 $\pi_0\Gamma(X,D)_s\cong\pi_0V(X,D)_s\cong\pi_0V(X,N)_s,\ 0\leq s<\infty.$

UMAP algorithm: Dimension reduction I

 (X, d_X) finite ep-metric space, X totally ordered, |X| = n. ep-metric space (X, D) constructed from neighbours N_X as above. Assume that (X, D) is **connected**: $D(x, y) < \infty$ for all $x, y \in X$.

• Unoriented weighted graph: $\Gamma(X) = \Gamma_*(X, D)$.

Find a node embedding $p : X \subset \mathbb{R}^d$ with d small:

- Weight matrix $W = (a_{i,j})$, with $a_{i,j} = D(x_i, x_j)$ for $i \neq j$,
- Diagonal matrix $D = (d_{i,i})$ with $d_{i,i} = \sum_{i \neq j} D(x_i, x_j)$.
- L = W D is the weighted Laplacian for the graph $\Gamma(X)$.

Find orthonormal basis of eigenvectors $\{w_1, \ldots, w_N\}$ for L.

Lemma 9.

There is a basis for \mathbb{R}^n consisting of vectors $\overline{e}_i = e_i + \delta_i w_1$, with all δ_i small, such the images $p(\overline{e}_i)$ are distinct.

Corollary 10.

Suppose that $V = \langle w_1, ..., w_d \rangle \subset \mathbb{R}^n$. Then the projection $p : \mathbb{R}^n \to \mathbb{R}^d \cong V$ onto V restricts to an injective function $\overline{e}_i \mapsto p(\overline{e}_i)$.

NB: The number d is usually 2 or 3 in practice, and is bounded above by the rank of L.

Set $y_i = p(\overline{e}_i) \in \mathbb{R}^d$.

Optimisation

We have a graph (Y, E) with vertices y_i , and edges $[y_i, y_j]$ with weights $d(y_i, y_j)$ given by distance.

Adjust vertices of (Y, E) by minimizing cross entropy:

 $w_X: X \times X \to [0,\infty], \ (x,y) \mapsto D(x,y), \ w_Y: X \times X \to [0,\infty], \ (x,y) \mapsto d(p(x),p(y)).$

$$C(w_X, w_Y) = \sum_{x,y} [e^{-w_X(x,y)}(w_X(x,y) - w_Y(x,y)) + e^{-w_X(x,y)^*}(w_X(x,y)^* - w_Y(x,y)^*)]$$

Suggestion: Minimise

$$(w_X(x,y) - w_Y(x,y))^2, (w_X(x,y)^* - w_Y(x,y)^*)^2$$

by moving the y_i (stochastic gradient descent).

One finishes with a graph (Y, E), $X = Y \subset \mathbb{R}^d$, which is "optimally close" to (X, D).

We're not done:

Write $(Y, E)_s$ for the subgraph of (Y, E) with vertices $Y = X \subset \mathbb{R}^d$ and edges $[x, y] \in E$ (in $\Gamma(X)$) with $d(x, y) \leq s$.

- We have clusters $\pi_0(Y, E)_s$ and a hierarchy $\Gamma(Y, E)$.
- $\Gamma(Y, E)$ is a tree with objects (s, [x]) with $[x] \in \pi_0(Y, E)_s$, and morphisms $(s, [x]) \rightarrow (t, [x])$ with $s \leq t$.

Michael Barr.

Fuzzy set theory and topos theory. Canad. Math. Bull., 29(4):501–508, 1986.

- Dinabandhu Bhandari and Nikhil R. Pal. Some new information measures for fuzzy sets. Inform. Sci., 67(3):209–228, 1993.
 - J.F. Jardine.

Metric spaces and homotopy types. Preprint, http://uwo.ca/math/faculty/jardine/, 2020.

 Leland McInnes and John Healy.
 UMAP: Uniform Manifold Approximation and Projection for Dimension Reduction.
 CoRR, abs/1802.03426, 2018.

 Leland McInnes, John Healy, and James Melville.
 Umap: Uniform Manifold Approximation and Projection for Dimension Reduction.
 Preprint, arXiv: 1802.03426 [stat.ML], 2020.

Claude E. Shannon. A mathematical theory of communication. *Bell Syst. Tech. J.*, 27(3):379–423, 1948.

D.I. Spivak. Metric realization of fuzzy simplicial sets. Preprint, 2009.

Homotopies

A natural transformation h between functors $f, g: C \rightarrow D$ is a diagram of functors



where $1 = \{0 \le 1\}$, $i_{\epsilon}(a) = (a, \epsilon)$. $B(C \times 1) \cong BC \times B1 = BC \times \Delta^1$

