Topology Preservation II: The Lattice Strikes Back

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About Data-driven Lattices...

What’s new?

Previously...

- Topology lattice predefined
- Based on some “intuition”/idea for the data
- In the best case scenario:
  - You know the data topology
  - You select the nicest lattice shape to preserve it

But life is cruel

Usually no idea beforehand about data topology (or not much)
About Data-driven Lattices…

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About Data-driven Lattices . . .

What’s new?

So, what about trying to infer a topology from the data itself?
Ideally, then:

- Unconstrained embedding
- More adaptive

Now how do we do this?

Lattice is in fact a graph built from the data:

- Vertices: data points
- Edges: neighbourhood relationships
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Lattice is in fact a graph built from the data:
- Vertices: data points
- Edges: neighbourhood relationships
Outline

1. Creating these graphs
2. Locally Linear Embedding (LLE)
3. Laplacian Eigenmap (LE)
Creating these graphs

As seen before... We just want to connect neighbouring points of the space.

Two main situations:
- Data not quantized
- Data quantized

And two color figures to divert you...

(a) Sine example  
(b) Spiral example
$K$-rule - Does not exactly work well on the examples. . .

The $K$-rule

- Find the $K$ closest points

- Choosing incorrectly $K$ may lead to “wrong” neighbours
- And hence, edges issues
The \( K \)-rule

- Find the \( K \) closest points

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Creating these graphs

Data not quantized
Data quantized

*K-rule - Does not exactly work well on the examples... (2)

Edges and neighbours issues, for example

(c) Sine example

(d) Spiral example
\( \epsilon \)-rule - Funny results also…

- Each point gets connected to points within an \( \epsilon \) radius ball (centered on the considered point)
  - But then… Isolated points may have no neighbours (or “wrong” ones)
  - Hard to evaluate a proper \( \epsilon \) (more than \( K \)) in practice
  - Results are OK when data is uniformly distributed
    - Too dense \( \implies \) Too many edges
    - Too sparse \( \implies \) Disconnected points
Creating these graphs
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$\epsilon$-rule - Funny results also…

$\epsilon$-rule

- Each point gets connected to points within an $\epsilon$ radius ball (centered on the considered point)
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ε-rule - Funny results also...

**ε-rule**

- Each point gets connected to points within an ε radius ball (centered on the considered point)
- But then... Isolated points may have no neighbours (or “wrong” ones)
- Hard to evaluate a proper ε (more than K) in practice
- Results are OK when data is uniformly distributed
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\(\epsilon\)-rule - Funny results also...

\(\epsilon\)-rule

- Each point gets connected to points within an \(\epsilon\) radius ball (centered on the considered point)
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Creating these graphs

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$\epsilon$-rule - Funny results also... (2)

(e) Sine example

(f) Spiral example
Creating these graphs

Data not quantized

Data quantized

\( \tau \)-rule - Slightly better...

\( \tau \)-rule

Two points \( \mathbf{y}(i) \) and \( \mathbf{y}(j) \) are connected if

\[
\min_j \| \mathbf{y}(i) - \mathbf{y}(j) \| \leq \tau \min_i \| \mathbf{y}(j) - \mathbf{y}(i) \| \quad \text{and} \quad d_j \leq \tau d_i \quad \text{(similarity cond.)}
\]

(1)

\[
\| \mathbf{y}(i) - \mathbf{y}(j) \| \leq \tau d_i \quad \text{or} \quad \| \mathbf{y}(j) - \mathbf{y}(i) \| \leq \tau d_j \quad \text{(neighborhood cond.)}
\]

(2)

Behaves almost like the \( \epsilon \)-rule but with an implicit radius (in \( \tau \))
Creating these graphs
Data not quantized
Data quantized

\( \tau \)-rule - Slightly better... (2)

(g) Sine example
(h) Spiral example
Creating these graphs

Data not quantized

Data quantized

Data rule: let’s be serious

Why not use the information of the quantization for the graph building?

Data rule

- for each point \( y(i) \)
- compute the \( K \) closest prototypes \( c(j_1), \ldots, c(j_K) \)
- Each pair \( c(j_s), c(j_t) \) has to follow the two conditions to be connected:
  - "Condition of the ellipse": \( d(y(i), c(j_s)) + d(y(i), c(j_t)) < C_1 d(c(j_s), c(j_t)) \) (3)
  - "Condition of the circle": \( d(y(i), c(j_s)) < C_2 d(y(i), c(j_t)) \) and \( d(y(i), c(j_t)) < C_2 d(y(i), c(j_s)) \) (4)
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(j) Spiral example
Creating these graphs

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Histogram rule exists also...

(k) Sine example
(l) Spiral example
Locally Linear Embedding (LLE)

Ideas behind...

- While SOM and GTM try to preserve neighbouring points close, we work on angles with LLE

- LLE uses conformal mapping to preserve local angles

- This is somewhat related to preserving distances: aims at preserving the local scalar product properties
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Locally Linear Embedding (LLE)

A little algorithm...

**LLE algorithm**

1. **Determine which angles to take into account**
   - Select neighbours for each point using a previous graph building technique (mostly $K$ closest or $\epsilon$ ball)

2. **Then, replace each data point with a linear combination of the selected neighbours**

3. **Local geometry of manifold characterized by these linear coefficients.**

4. **Reconstruction error measured by**

   \[
   E(W) = \sum_{i=1}^{N} \left\| y(i) - \sum_{j \in \mathcal{N}(i)} w_{i,j} y(j) \right\|_2^2
   \]  
   \(5\)

   With $\mathcal{N}(i)$ the set of neighbours of $y(i)$ and $w_{i,j}$ the coefficients of the $N \times N$ matrix $W$ of weights.
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A little algorithm... (2)

To compute the $w_{i,j}$, $E(W)$ is minimized under two constraints

- Points are reconstructed solely from their neighbours:
  
  \[ w_{i,j} = 0 \ \forall \ j \notin N(i) \]

- Rows of $W$ sum to one:
  \[ \sum_{j=1}^{N} w_{i,j} = 1 \]

Nice thing lies here

- Obtained $w_{i,j}$ verify invariance to rotations, scalings and translations of the associated point $y(i)$ and its neighbours

- Hence, weights characterize intrinsic geometric properties of the considered neighbourhood of the manifold

- Hopefully, these geometric properties are also valid in a lower $P$-dimensional representation.
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A little algorithm... (3)

- Coordinates in this $P$-dimensional space are found by minimizing the embedding cost function

$$
\Phi(\hat{X}) = \sum_{i=1}^{N} \left\| \hat{x}(i) - \sum_{j \in N(i)} w_{i,j} \hat{x}(j) \right\|^2
$$

(6)

- Error calculated in the embedding space, this time, and $w_{i,j}$ fixed
- Details of the calculation omitted. Use an EVD on a certain matrix $M = (I - W)^T (I - W)$ to minimize $\Phi(\hat{X})$ and find the coordinates in the $P$-dimensional space
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Locally Linear Embedding (LLE)

Looks rather nice

Smooth, correct embedding, except for a crushed face on the open box
Advantages and some other things...

• Assumes that data linear locally, not globally

• Manifold can be mapped to a plane using a conformal mapping

• Elegant for the mind and simple in the ideas

• Sticks to an eigensolver for the hardest part (and matrix often sparse, which makes things easier)
Laplacian Eigenmap (LE)

Ideas behind...

- Also going for a local approach to the problem of NLDR

- This time, minimization of neighbouring distances within the graph, with constraints (avoids the trivial case)

- Relies on the idea that the data set $Y = \{\ldots, \mathbf{y}(i), \ldots, \mathbf{y}(j), \ldots\}_{1 \leq i, j \leq M}$ contains a sufficiently large number $N$ of points on a smooth $P$-dimensional manifold

- If $N$ large enough, manifold can be represented by a graph $G = (V_N, E)$

- Again, neighbourhood relationships determined using $K$-ary neighbourhoods or $\epsilon$-balls
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What’s done in practice... 

Some steps of LE

- Map $Y$ to a set of low dimensional points $X = \{\ldots, x(i), \ldots, x(j), \ldots\}_{1 \leq i, j \leq N}$ keeping same neighbourhood relationships, under the constraint of minimizing

$$E_{LE} = \frac{1}{2} \sum_{i,j=1}^{N} ||x(i) - x(j)||_2^2 w_{i,j}$$

(7)

with $w_{i,j} = 0$ if $y(i)$ and $y(j)$ not neighbours, and $0 \leq w_{i,j}$ otherwise.

- Most often, $w_{i,j}$ follow a Gaussian kernel, or more simply, $w_{i,j} = 1$ if $y(i)$ and $y(j)$ are neighbours

- Thus, minimizing $E_{LE}$ means that if $y(i)$ and $y(j)$ are close to each other, then $x(i)$ and $x(j)$ should be as well
Laplacian Eigenmap (LE)

What’s done in practice...

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$$E_{LE} = \frac{1}{2} \sum_{i,j=1}^{N} ||x(i) - x(j)||^2_w$$

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What’s done in practice. . . (2)

With some calculations, criterion reduces to

\[ E_{LE} = \text{tr}(XLX^T) \]  

(8)

with \( L = \mathbf{W} - \mathbf{D} \) being the weighted Laplacian matrix of the graph \( G \),

and \( \mathbf{D} \) diagonal with \( d_{i,j} = \sum_{j=1}^{N} w_{i,j} \)

Problem ends up to an EVD of \( L \) and keep the \( P \) “lowest” eigenvectors.
Laplacian Eigenmap (LE)

Algorithm in a big nutshell...

**LE algorithm**

1. Determine neighbourhoods ($K$-ary or $\epsilon$-balls)
2. Build the graph (and determine adjacencies)
3. Build matrix $W$ (using kernel or...)
4. Compute $D$ matrix (diagonal, sums of weights rowwise)
5. Compute $L$, Laplacian matrix of $W$: $L = W - D$
6. Normalize the Laplacian matrix
7. Compute its EVD and do some operations on eigenvectors to obtain the embedding

But again, life is cruel...

Parameters controlling the graph ($K$ or $\epsilon$) are very sensitive and require great care
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3. Build matrix $W$ (using kernel or...)
4. Compute $D$ matrix (diagonal, sums of weights rowwise)
5. Compute $L$, Laplacian matrix of $W$: $L = W - D$
6. Normalize the Laplacian matrix
7. Compute its EVD and do some operations on eigenvectors to obtain the embedding

But again, life is cruel...

Parameters controlling the graph ($K$ or $\epsilon$) are very sensitive and require great care
Laplacian Eigenmap (LE)

Algorithm in a big nutshell...

**LE algorithm**

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Not-so-bad-but-not-so-good...

Swiss roll has third (spiral) dimension crushed and box is OK except for one crushed dimension again
Finally, for LE...

- LE has few parameters (once kernel for weights $W$ is chosen): $K$ or $\epsilon$
- But parameters have a "dramatic" influence on results
- Apparently much nicer for clustering than dimensionality reduction
- Minimizing distances may lead to degenerate solutions (all in one point or such)
Conclusion

A small conclusion on these two methods...

- LLE has sexy and seducing ideas and concepts
- Not so hard on the calculation part
- Rather ok results (box crushed is “usual” unfortunately)

- LE is definitely not meant for dimension reduction
- Seriously, the book says so!
- Used for clustering, more
- You may as well forget this one, I guess

And now, for the end of the show...
Antti takes on with Isotop
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