CSC 2535: 2013
Lecture 11

Non-linear dimensionality reduction

Geoffrey Hinton

Dimensionality reduction: Some Assumptions

- High-dimensional data often lies on or near a much lower dimensional, curved manifold.
- A good way to represent data points is by their low-dimensional coordinates.
- The low-dimensional representation of the data should capture information about high-dimensional pairwise distances.

The basic idea of non-parameteric dimensionality reduction

- Represent each data-point by a point in a lower dimensional space.
- Choose the low-dimensional points so that they optimally represent some property of the data-points (e.g. the pairwise distances).
  – Many different properties have been tried.
- Do not insist on learning a parametric "encoding" function that maps each individual data-point to its low-dimensional representative.
- Do not insist on learning a parametric "decoding" function that reconstructs a data-point from its low dimensional representative.

Two types of dimensionality reduction

- Global methods assume that all pairwise distances are of equal importance.
  - Choose the low-D pairwise distances to fit the high-D ones (using magnitude or rank order).

- Local methods assume that only the local distances are reliable in high-D.
  - Put more weight on modeling the local distances correctly.

Linear methods of reducing dimensionality

- PCA finds the directions that have the most variance.
  - By representing where each datapoint is along these axes, we minimize the squared reconstruction error.
  - Linear autoencoders are equivalent to PCA

- Multi-Dimensional Scaling arranges the low-dimensional points so as to minimize the discrepancy between the pairwise distances in the original space and the pairwise distances in the low-D space.

Metric Multi-Dimensional Scaling

- Find low dimensional representatives, y, for the high-dimensional data-points, x, that preserve pairwise distances as well as possible.
- An obvious approach is to start with random vectors for the y's and then perform steepest descent by following the gradient of the cost function.
- Since we are minimizing squared errors, maybe this has something to do with PCA?
  - If so, we don't need an iterative method to find the best embedding.

$$Cost = \sum_{i<j} (d_{ij} - \hat{d}_{ij})^2$$

$$d_{ij} = \| x_i - x_j \|^2$$

$$\hat{d}_{ij} = \| y_i - y_j \|^2$$

Converting metric MDS to PCA

- If the data-points all lie on a hyperplane, their pairwise distances are perfectly preserved by projecting the high-dimensional coordinates onto the hyperplane.
  - So in that particular case, PCA is the right solution.
- If we "double-center" the data, metric MDS is equivalent to PCA.
  - Double centering means making the mean value of every row and column be zero.
  - But double centering can introduce spurious structure.

Other non-linear methods of reducing dimensionality

- Non-linear autoencoders with extra layers are much more powerful than PCA but they can be slow to optimize and they get different, locally optimal solutions each time.

- Multi-Dimensional Scaling can be made non-linear by putting more importance on the small distances. A popular version is the Sammon mapping:

$$Cost = \sum_{i\,j} \left(\frac{\| \mathbf{x}_i \overset{\substack{\text{high-D}\\\text{distance}\\\Downarrow}}{-} \mathbf{x}_j \| - \| \mathbf{y}_i \overset{\substack{\text{low-D}\\\text{distance}\\\Downarrow}}{-} \mathbf{y}_j \|}{\| \mathbf{x}_i - \mathbf{x}_j \|} \right)^2$$

- Non-linear MDS is also slow to optimize and also gets stuck in different local optima each time.

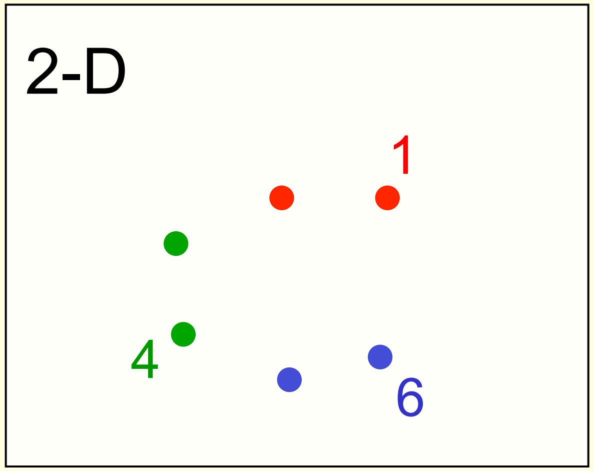
Problems with Sammon mapping

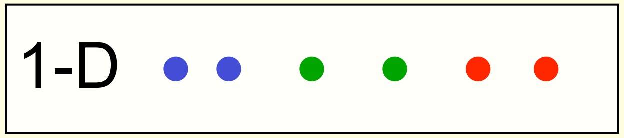
- It puts too much emphasis on getting very small distances exactly right.
- It produces embeddings that are circular with roughly uniform density of the map points.

IsoMap: Local MDS without local optima

- Instead of only modeling local distances, we can try to measure the distances along the manifold and then model these intrinsic distances.
  - The main problem is to find a robust way of measuring distances along the manifold.
  - If we can measure manifold distances, the global optimisation is easy: It's just global MDS (i.e. PCA)

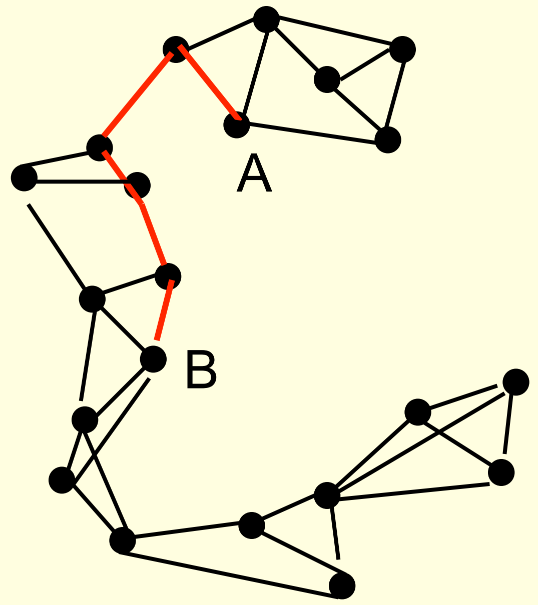
If we measure distances along the manifold, d(1,6) > d(1,4)



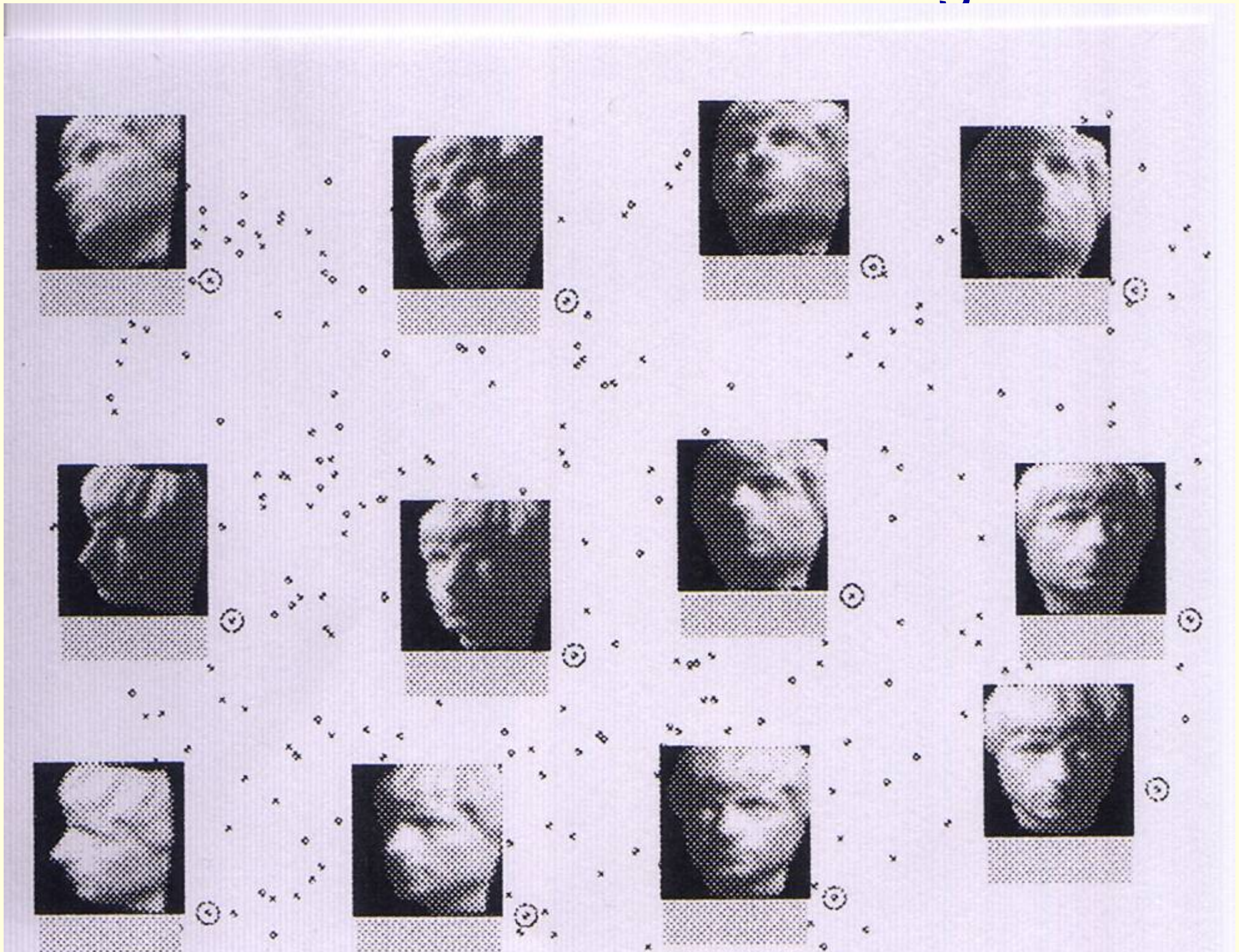


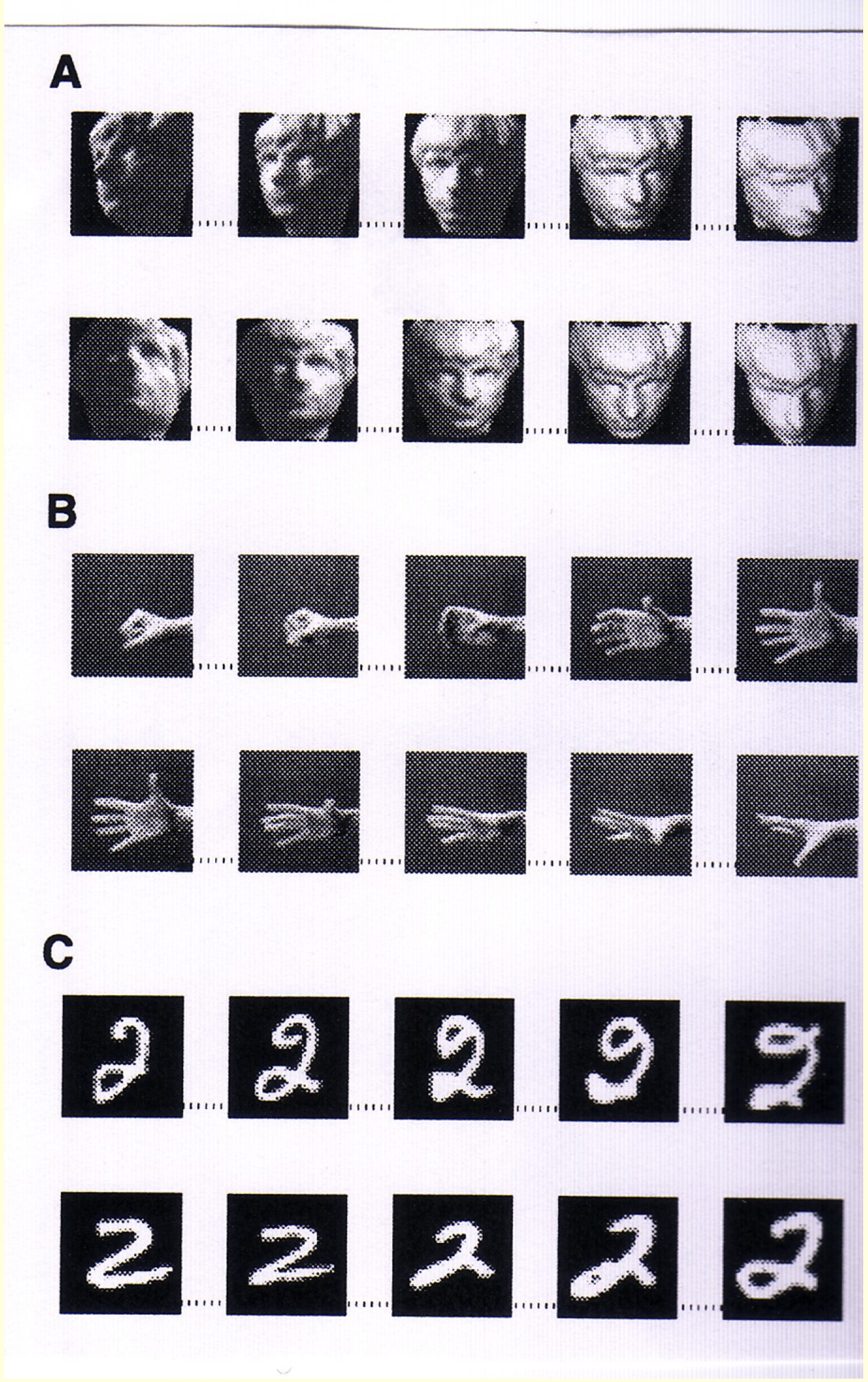
How Isomap measures intrinsic distances

- Connect each datapoint to its K nearest neighbors in the high-dimensional space.
- Put the true Euclidean distance on each of these links.
- Then approximate the manifold distance between any pair of points as the shortest path in this “neighborhood graph”.



Using Isomap to discover the intrinsic manifold in a set of face images





Linear methods cannot interpolate properly between the leftmost and rightmost images in each row.

This is because the interpolated images are NOT averages of the images at the two ends.

Isomap does not interpolate properly either because it can only use examples from the training set. It cannot create new images.

But it is better than linear methods.

Maps that preserve local geometry

- The idea is to make the local configurations of points in the low-dimensional space resemble the local configurations in the high-dimensional space.
- We need a coordinate-free way of representing a local configuration.
- If we represent a point as a weighted average of nearby points, the weights describe the local configuration.

$$\mathbf{x}_i \approx \sum_j w_{ij} \mathbf{x}_j$$

Finding the optimal weights

- This is easy.
- Minimize the squared “construction” errors subject to the sum of the weights being 1.

$$Cost = \sum_i \| \mathbf{x}_i - \sum_{j \varepsilon N(i)} w_{ij} \mathbf{x}_j \|^2, \qquad \sum_{j \varepsilon N(i)} w_{ij} = 1$$

- If the construction is done using less neighbors than the dimensionality of x, there will generally be some construction error
  - The error will be small if there are as many neighbors as the dimensionality of the underlying noisy manifold.

A sensible but inefficient way to use the local weights

- Assume a low-dimensional latent space.
  - Each datapoint $\mathbf{x}_i$ has latent coordinates $\mathbf{y}_i$.
- Find a set of latent points that minimize the construction errors produced by a two-stage process:
  - 1. First use the latent points to compute the local weights that construct $\mathbf{y}_i$ from its neighbors.
  - 2. Use those weights to construct the high-dimensional coordinates of a datapoint $\mathbf{x}_i$ from the high-dimensional coordinates of its neighbors.
- Unfortunately, this is a hard optimization problem.
  - Iterative solutions are expensive because they must repeatedly measure the construction error in the high-dimensional space.

Local Linear Embedding: A less sensible but more efficient way to use local weights

- Instead of using the the latent points plus the other datapoints to construct each held-out datapoint, do it the other way around.
- Use the datapoints to determine the local weights, then try to construct each latent point from its neighbors.
  - Now the construction error is in the low-dimensional latent space.
- We only use the high-dimensional space once to get the local weights.
  - The local weights stay fixed during the optimization of the latent coordinates.
  - This is a much easier search.

The convex optimization

$$Cost = \sum_i \| \mathbf{y}_i - \sum_{j \varepsilon N(i)} \overset{\text{fixed weights}}{\overset{\downarrow}{w_{ij}}} \mathbf{y}_j \|^2$$

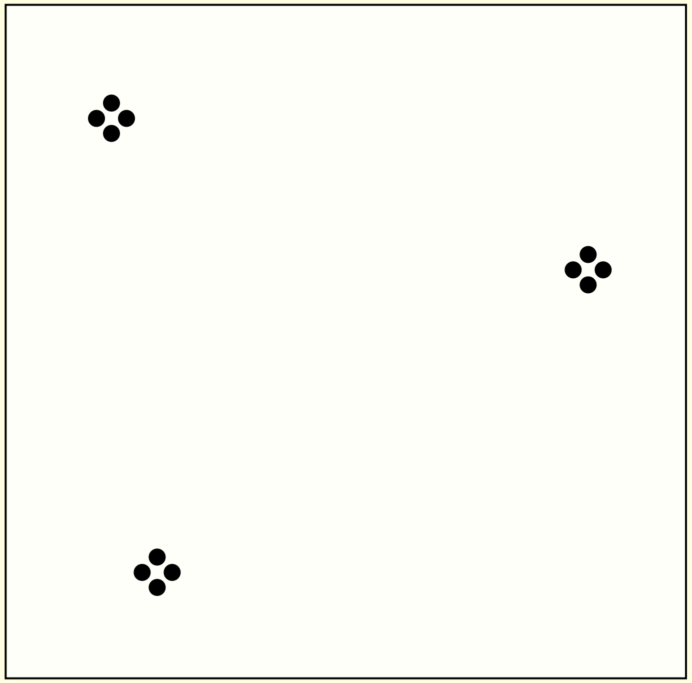
- Find the y’s that minimize the cost subject to the constraint that the y’s have unit variance on each dimension.
  - Why do we need to impose a constraint on the variance?

The collapse problem

- If all of the latent points are identical, we can construct each of them perfectly as a weighted average of its neighbors.
  - The root cause of this problem is that we are optimizing the wrong thing.
  - But maybe we can fix things up by adding a constraint that prevents collapse.
- Insist that the latent points have unit variance on each latent dimension.
  - This helps a lot, but sometimes LLE can satisfy this constraint without doing what we really intend.

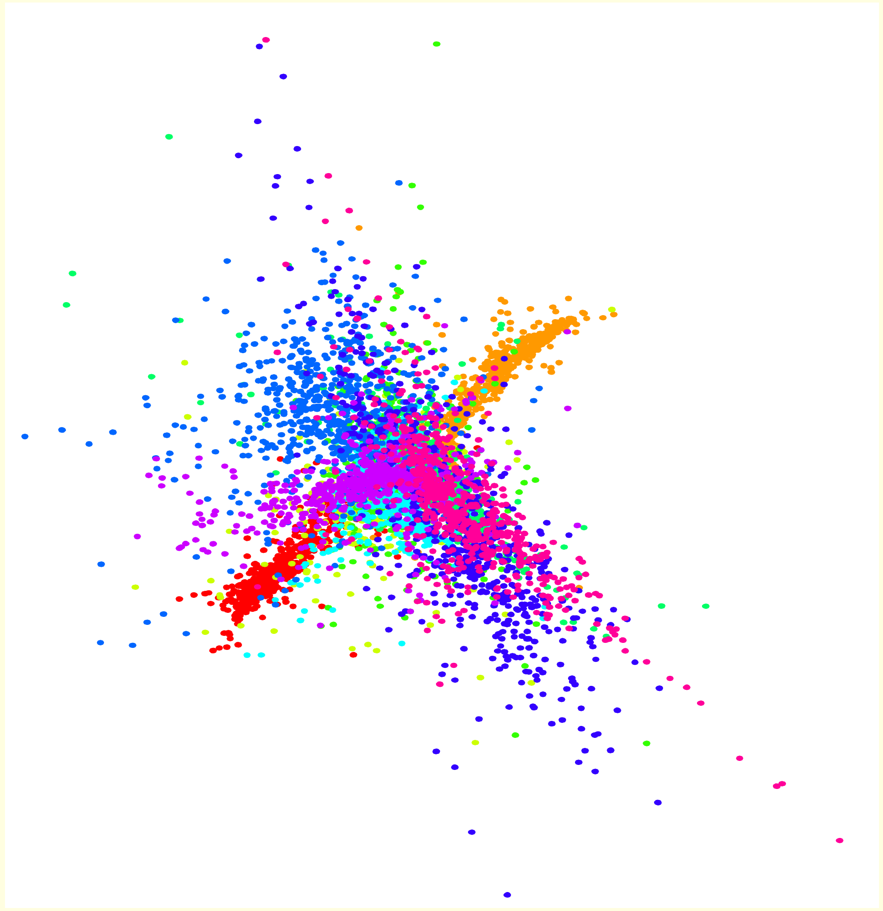
Failure modes of LLE

- If the neighborhood graph has several disconnected pieces, we can satisfy the unit variance constraint and still have collapses.
- Even if the graph is fully connected, it may be possible to collapse all the densely connected regions and satisfy the variance constraint by paying a high cost for a few outliers.



A typical embedding found by LLE

- LLE embeddings often look like this.
- Most of the data is close to the center of the space.
- A few points are far from the center to satisfy the unit variance constraint.



A comment on LLE

- It has two very attractive features
  - 1. The only free parameters are the dimensionality of the latent space and the number of neighbors that are used to determine the local weights.
  - 2. The optimization is convex so we don't need multiple tries and we don't need to fiddle with optimization parameters.
- It has one bad feature:
  - It is not optimizing the right thing!
  - One consequence is that it does not have any incentive to keep widely separated datapoints far apart in the low-dimensional map.

Maximum Variance Unfolding

- This fixes one of the problems of LLE and still manages to be a convex optimization problem.
- Use a few neighbors for each datapoint and insist that the high-dimensional distances between neighbors are exactly preserved in the low-dimensional space.
  - This is like connecting the points with rods of fixed lengths.
- Subject to the rigid rods connecting the low-dimensional points, maximize their squared separations.
  - This encourages widely separated datapoints to remain separated in the low-dimensional space.

How to solve many problems in AI

- 1. Map from the data domain to a domain of feature vectors in which the important relationships can be modeled by linear operations.
- 2. Do some linear operations.
- 3. Map the answer back to the data domain.

Modeling relational data

- Suppose we have a set of facts of the form ARB
  - i.e. The relation R maps A to B as in Allan has-mother Beatrice
- We could model the facts using matrix algebra.
  - Learn a vector for each object
  - Learn a matrix for each relation
  - The aim is to make A*R=B
- This doesnt work because all the vectors learn to be zero.
  - We need A*R to be closer to B than to C.

A discriminative cost function

$$p_{B|AR} = \frac{e^{\|AR-B\|^2}}{\sum_C e^{\|AR-C\|^2}}$$

Applying the idea to dimensionality reduction

- 0. Compute a big probability table that contains the probability that each high-dimensional data-point , i, would pick another data-point , j, as its "neighbor".
- 1. Use a learned look-up table to convert each high-dimensional data-point to a 2-D feature vector.
- 2. Multiply by the identity matrix.
- 3. Compare the resulting 2-D feature vector with all the other 2-D feature vectors to get a predicted distribution over data-points in the original data-space.
- Learn the look-up tables so that the probabilities computed in the 2-D space match the probabilities computed in the original space.

A probabilistic version of local MDS

- It is more important to get local distances right than non-local ones, but getting infinitessimal distances right is not infinitely important.
  - All the small distances are about equally important to model correctly.
  - Stochastic neighbor embedding has a probabilistic way of deciding if a pairwise distance is “local”.

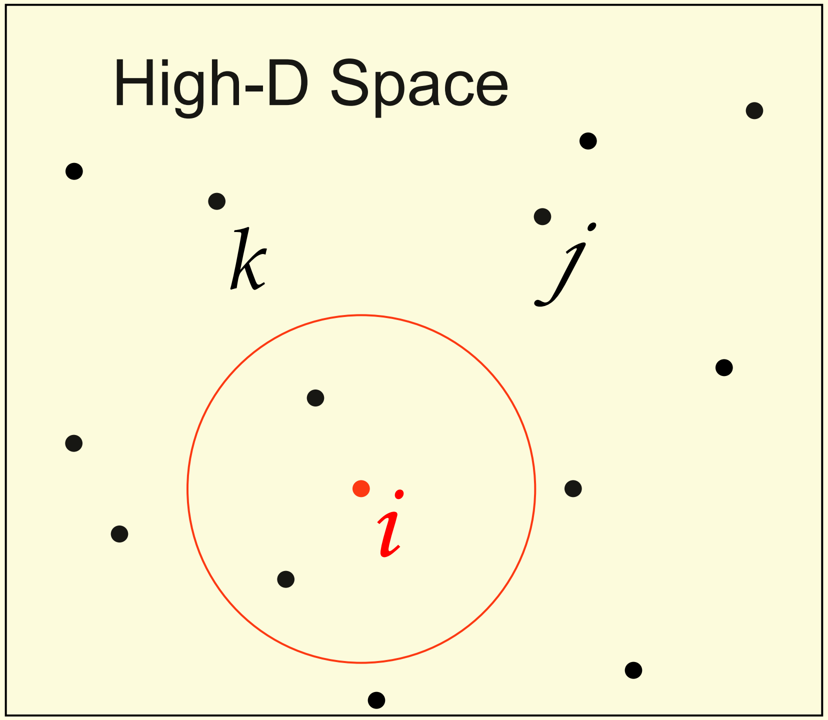
Stochastic Neighbor Embedding

- First convert each high-dimensional similarity into the probability that one data point will pick the other data point as its neighbor.
- To evaluate a map:
  - Use the pairwise distances in the low-dimensional map to define the probability that a map point will pick another map point as its neighbor.
  - Compute the Kullback-Leibler divergence between the probabilities in the high-dimensional and low-dimensional spaces.

A probabilistic local method

- Each point in high-D has a conditional probability of picking each other point as its neighbor.

- The distribution over neighbors is based on the high-D pairwise distances.
  - If we do not have coordinates for the datapoints we can use a matrix of dissimilarities instead of pairwise distances.



$$p_{j|i} = \frac{e^{-d_{ij}^2 / 2\sigma_i^2}}{\sum_k e^{-d_{ik}^2 / 2\sigma_i^2}}$$

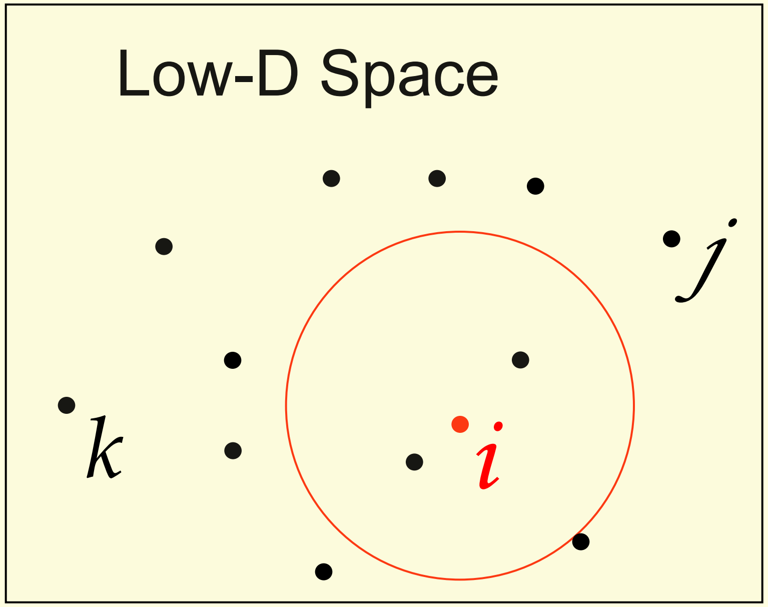
probability of picking j given that you start at i

Throwing away the raw data

- The probabilities that each points picks other points as its neighbor contains all of the information we are going to use for finding the manifold.
  - Once we have the probabilities $p_{j|i}$ we do not need to do any more computations in the high-dimensional space.
  - The input could be "dissimilarities" between pairs of datapoints instead of the locations of individual datapoints in a high-dimensional space.

Evaluating an arrangement of the data in a low-dimensional space

- Give each datapoint a location in the low-dimensional space.
  - Evaluate this representation by seeing how well the low-D probabilities model the high-D ones.



$$q_{j|i} = \frac{e^{-d_{ij}^2}}{\sum_k e^{-d_{ik}^2}}$$

probability of picking j given that you start at i

The cost function for a low-dimensional representation

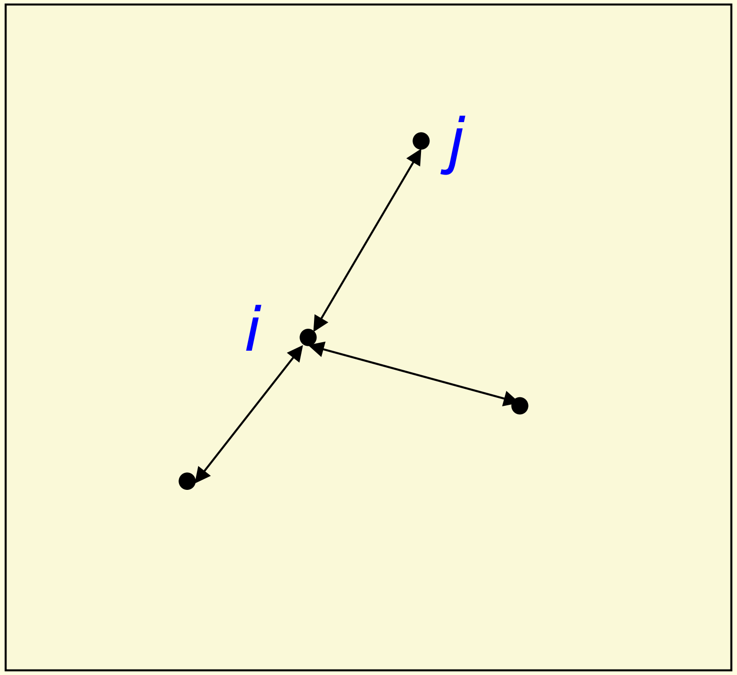
$$Cost = \sum_i KL(P_i \,||\, Q_i) = \sum_i \sum_j p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}$$

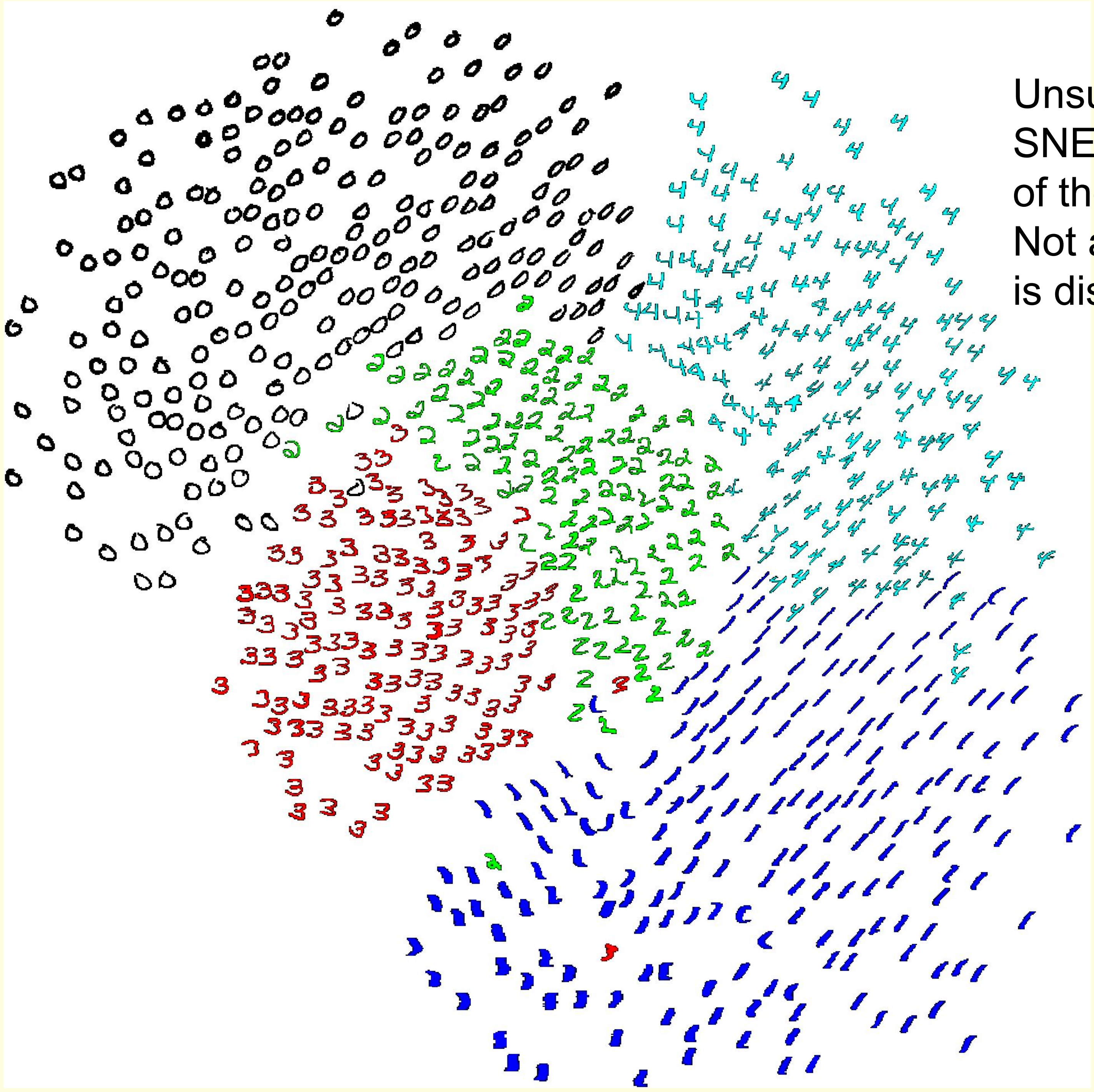
- For points where p_{ij} is large and q_{ij} is small we lose a lot.
  - Nearby points in high-D really want to be nearby in low-D
- For points where q_{ij} is large and p_{ij} is small we lose a little because we waste some of the probability mass in the Q_i distribution.
  - Widely separated points in high-D have a mild preference for being widely separated in low-D.

The forces acting on the low-dimensional points

$$\frac{\partial Cost}{\partial \mathbf{y}_i} = 2\sum_j (\mathbf{y}_j - \mathbf{y}_i)(p_{j|i} - q_{j|i} + p_{i|j} - q_{i|j})$$

- Points are pulled towards each other if the p's are bigger than the q's and repelled if the q's are bigger than the p's





Unsupervised SNE embedding of the digits 0-4. Not all the data is displayed

Picking the radius of the gaussian that is used to compute the p's

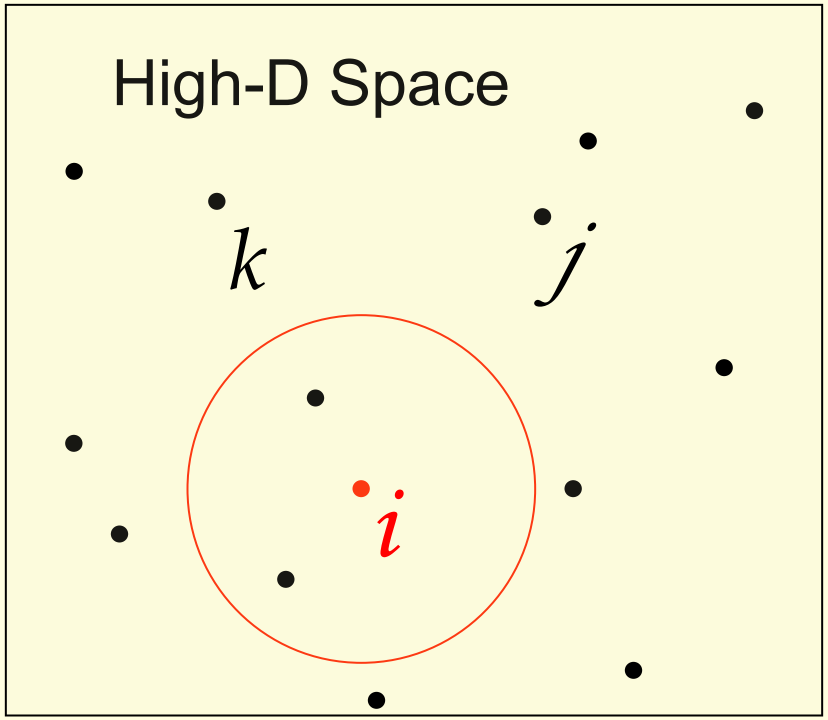
- We need to use different radii in different parts of the space so that we keep the effective number of neighbors about constant.
- A big radius leads to a high entropy for the distribution over neighbors of i.
- A small radius leads to a low entropy.
- So decide what entropy you want and then find the radius that produces that entropy.
- Its easier to specify 2^entropy
  - This is called the perplexity
  - It is the effective number of neighbors.

Symmetric SNE

- There is a simpler version of SNE which seems to work about equally well.
- Symmetric SNE works best if we use different procedures for computing the p's and the q's
  - This destroys the nice property that if we embed in a space of the same dimension as the data, the data itself is the optimal solution.

Computing the p’s for symmetric SNE

- Each high dimensional point, i, has a conditional probability of picking each other point, j, as its neighbor.
- The conditional distribution over neighbors is based on the high-dimensional pairwise distances.



$$p_{j|i} = \frac{e^{-d_{ij}^2 / 2\sigma_i^2}}{\sum_k e^{-d_{ik}^2 / 2\sigma_i^2}}$$

probability of picking j given that you start at i

Turning conditional probabilities into pairwise probabilities

To get a symmetric probability between i and j we sum the two conditional probabilities and divide by the number of points (points are not allowed to choose themselves).

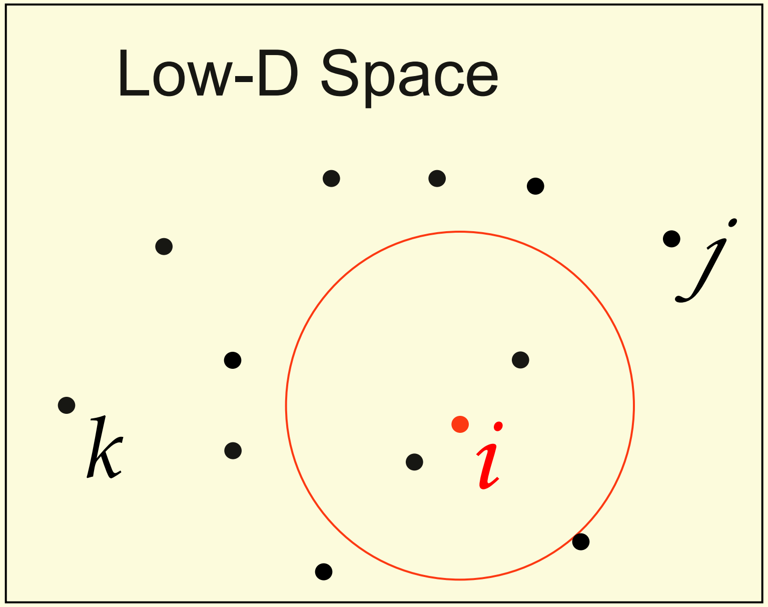
joint probability of picking the pair i,j $\longrightarrow$ $$p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$$

This ensures that all the pairwise probabilities sum to 1 so they can be treated as probabilities.

$$\sum_{i,j} p_{ij} = 1$$

Evaluating an arrangement of the points in the low-dimensional space

- Give each data-point a location in the low-dimensional space.
  - Define low-dimensional probabilities symmetrically.
  - Evaluate the representation by seeing how well the low-D probabilities model the high-D affinities.



$$q_{ij} = \frac{e^{-d_{ij}^2}}{\sum_{k<l} e^{-d_{kl}^2}}$$

The cost function for a low-dimensional representation

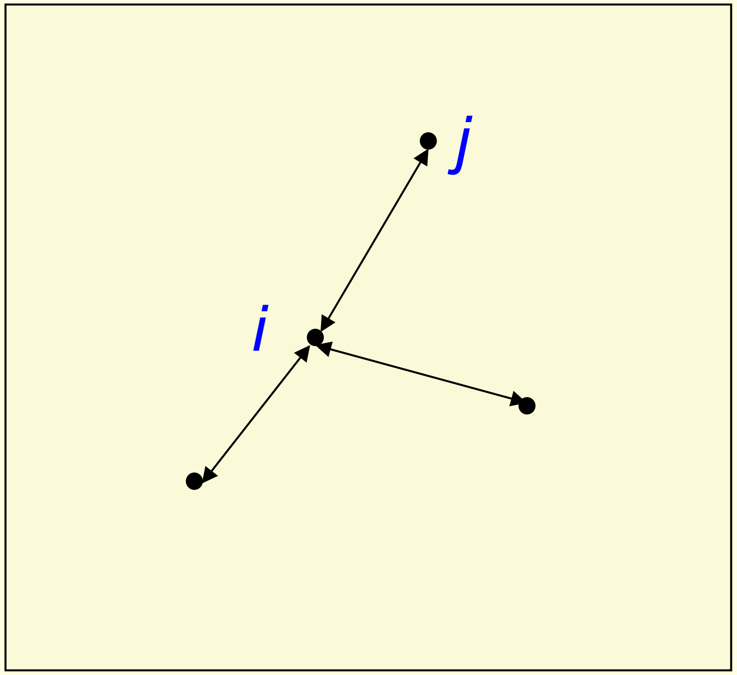
$$Cost = KL(P \| Q)| = \sum_{i<j} p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

- It's a single KL instead of the sum of one KL for each datapoint.

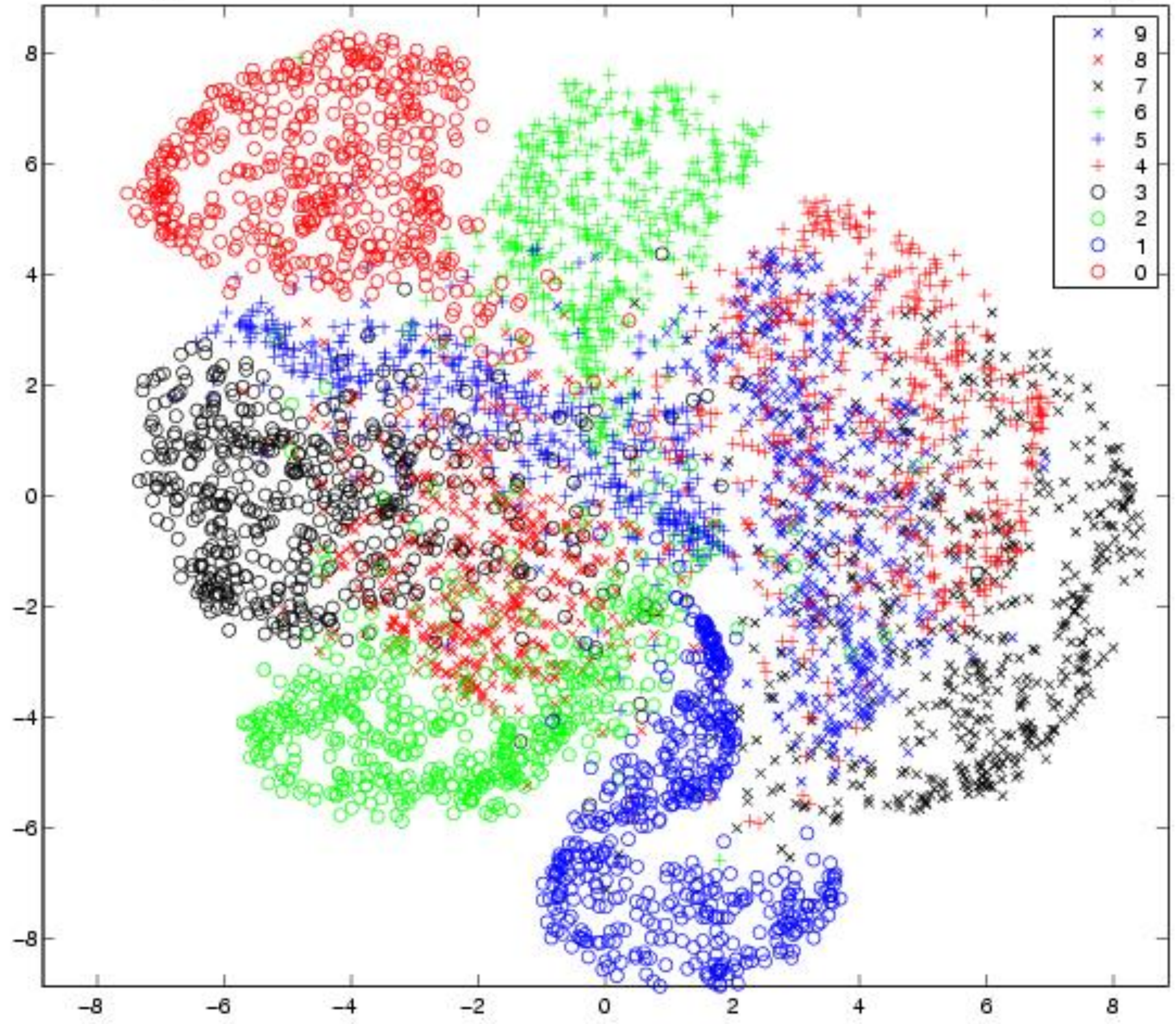
The forces acting on the low-dimensional points

$$\frac{\partial KL(P\|Q)}{\partial \mathbf{y}_i} = 2\sum_j (\mathbf{y}_i \overset{\substack{\text{extension}\\ \downarrow}}{-} \mathbf{y}_j)\,(p_{ij} \overset{\substack{\text{stiffness}\\ \downarrow}}{-} q_{ij})$$

- Points are pulled towards each other if the p's are bigger than the q's and repelled if the q's are bigger than the p's
  - Its equivalent to having springs whose stiffnesses are set dynamically.



SNE applied to 30−dimensional PCA codes of 5000 MNIST digits



Optimization methods for SNE

- We get much better global organization if we use annealing.
  - Add Gaussian noise to the y locations after each update.
  - Reduce the amount of noise on each iteration.
  - Spend a long time at the noise level at which the global structure starts to form from the hot plasma of map points.
- It also helps to use momentum (especially at the end).
- It helps to use an adaptive global step-size.

More optimization tricks for SNE

- Anneal the perplexity.
  - This is expensive because it involves computing distances in the high-dimensional data-space.
- Dimension decay
  - Use additional dimensions to avoid local optima, then penalize the squared magnitudes of the map points on the extra dimensions.
    - Turn up the penalty coefficient until all of the map points have very small values on those extra dimensions.
- Neither of these tricks is a big win in general.

A more interesting variation that uses the probabilistic foundation of SNE

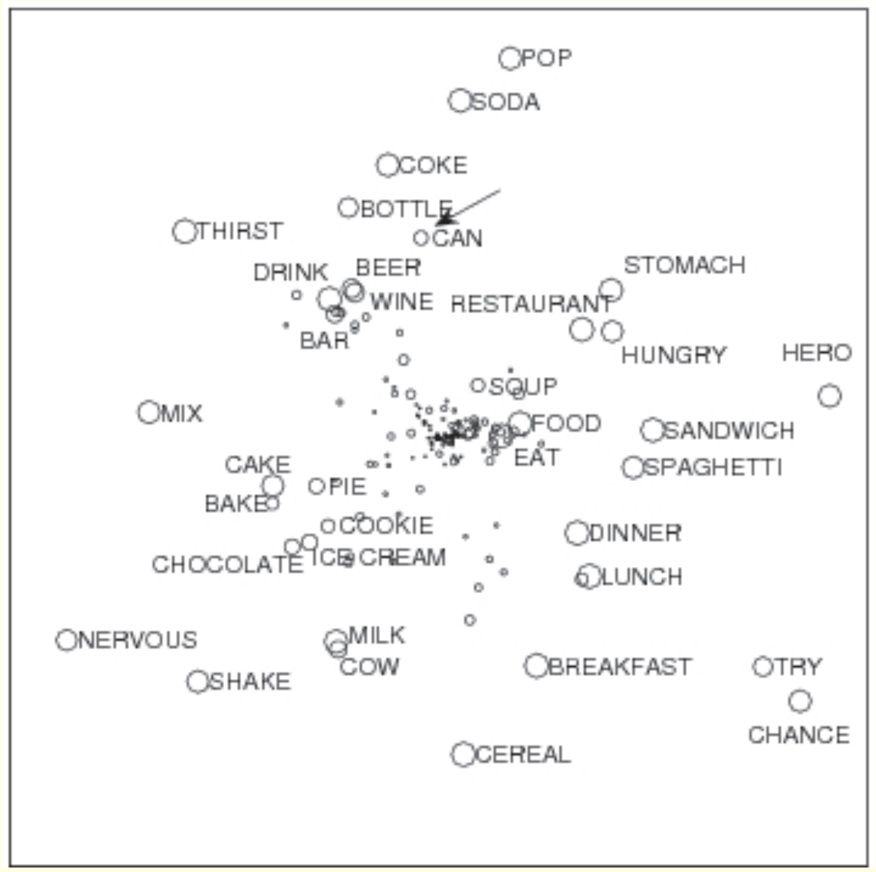
- All other dimensionality reduction methods assume that each data point is represented by ONE point in the map.
- But suppose we had several different maps.
  - Each map has a representative of each datapoint and the representative has a mixing proportion.
  - The overall qij is a sum over all maps

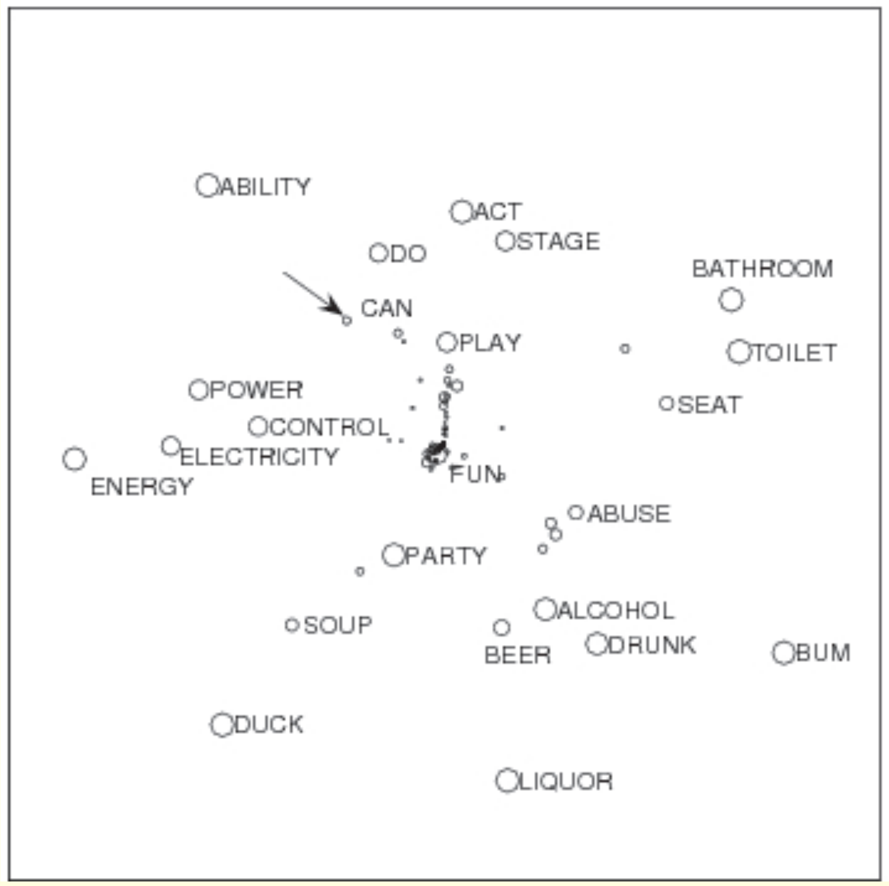
$$q_{ij} = \sum_m q_{ij}^m \qquad q_{ij}^m = \frac{\pi_i^m \pi_j^m \exp(-d_{ij}^m)}{Z}$$

A nice dataset for testing “Aspect maps”

- Give someone a word and ask them to say the first other word they associate with it.
  - Different senses of a word will have different associations and so they should show up in different aspect maps.

Two of the 50 aspect maps for the Florida word association data





The relationship between aspect maps and clustering

- If we force all of the locations in each map to be the same, it’s a form of spectral clustering!
- Putting a point into a map is not just based on the affinities it has to the other points in the map.
  - It depends on whether it can find a location in the map that allows it to mathc the pattern of affinities.
  - It has a very abstract resemblance to mixtures of experts vs ordinary mixtures.

A weird behaviour of aspect maps

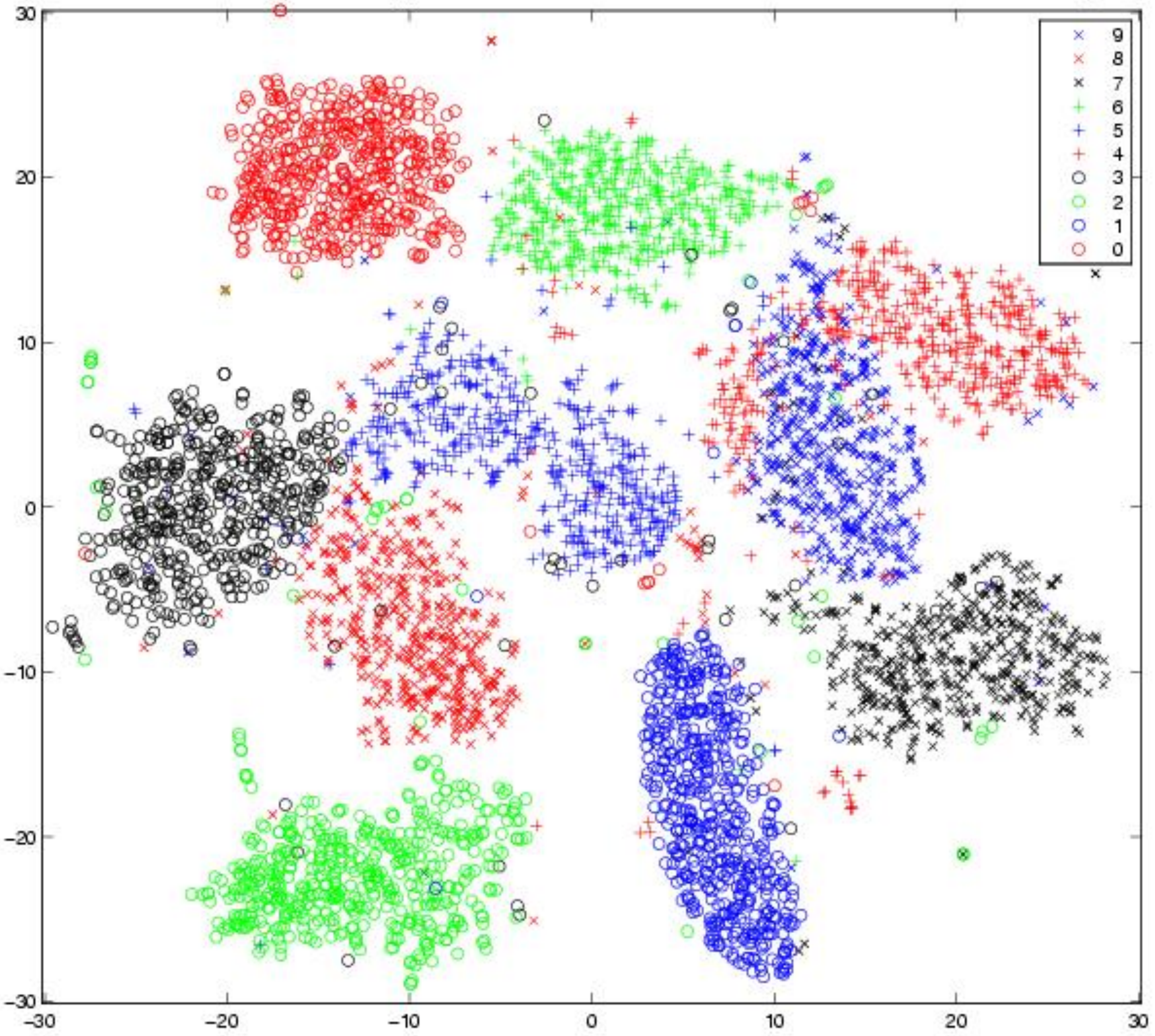
- If we use just 2 aspect maps, one of them collapses all of the map points to the same location.
  - Its trying to tell us something!
- It wants to use a uniform background probability for all pairs

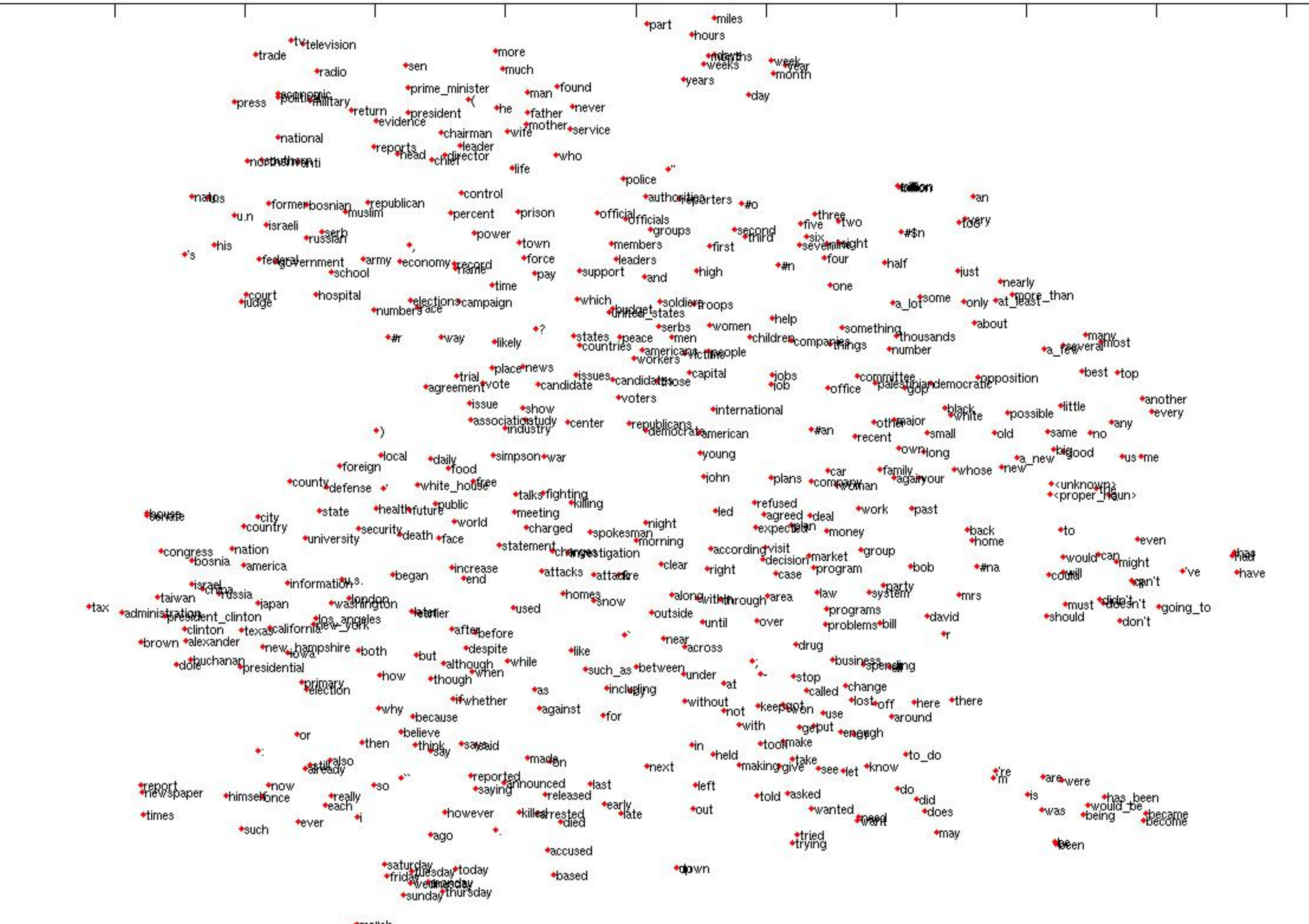
$$q_{ij} = \pi_1 \, q_{ij}^1 + \frac{1-\pi_1}{N^2}$$

Why SNE does not have gaps between classes

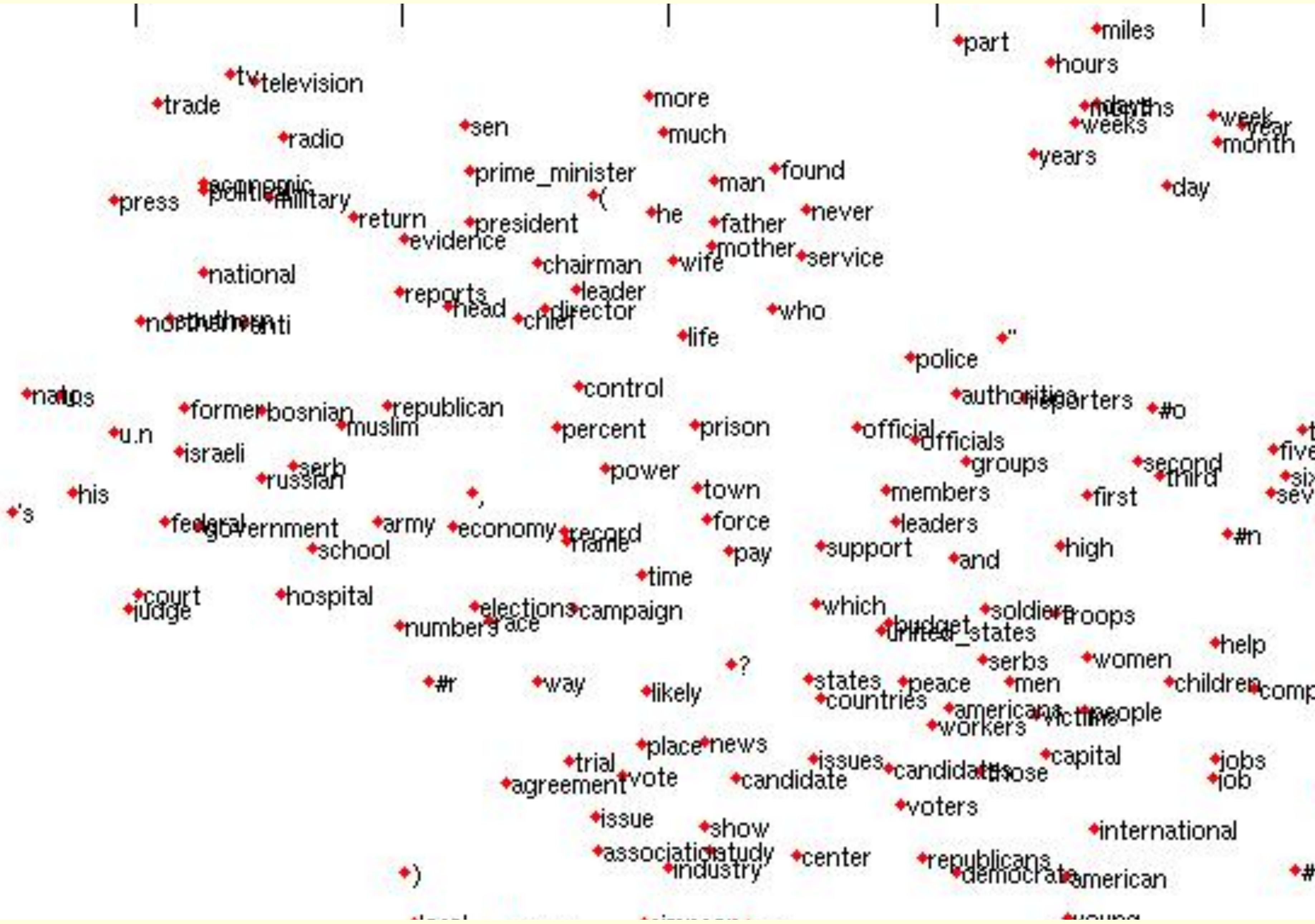
- In the high-dimensional space there are many pairs of points that are moderately close to each other.
  - The low-D space cannot model this. It doesn't have enough room around the edges.
- So there are many pij's that are modeled by smaller qij's.
  - This has the effect of lots of weak springs pulling everything together and crushing different classes together in the middle of the space.
- A uniform background model eliminates this effect and allows gaps between classes to appear.
  - It is quite like Maximum Variance Unfolding

SNE then UNI–SNE applied to 30–D PCA codes of 5000 MNIST digits

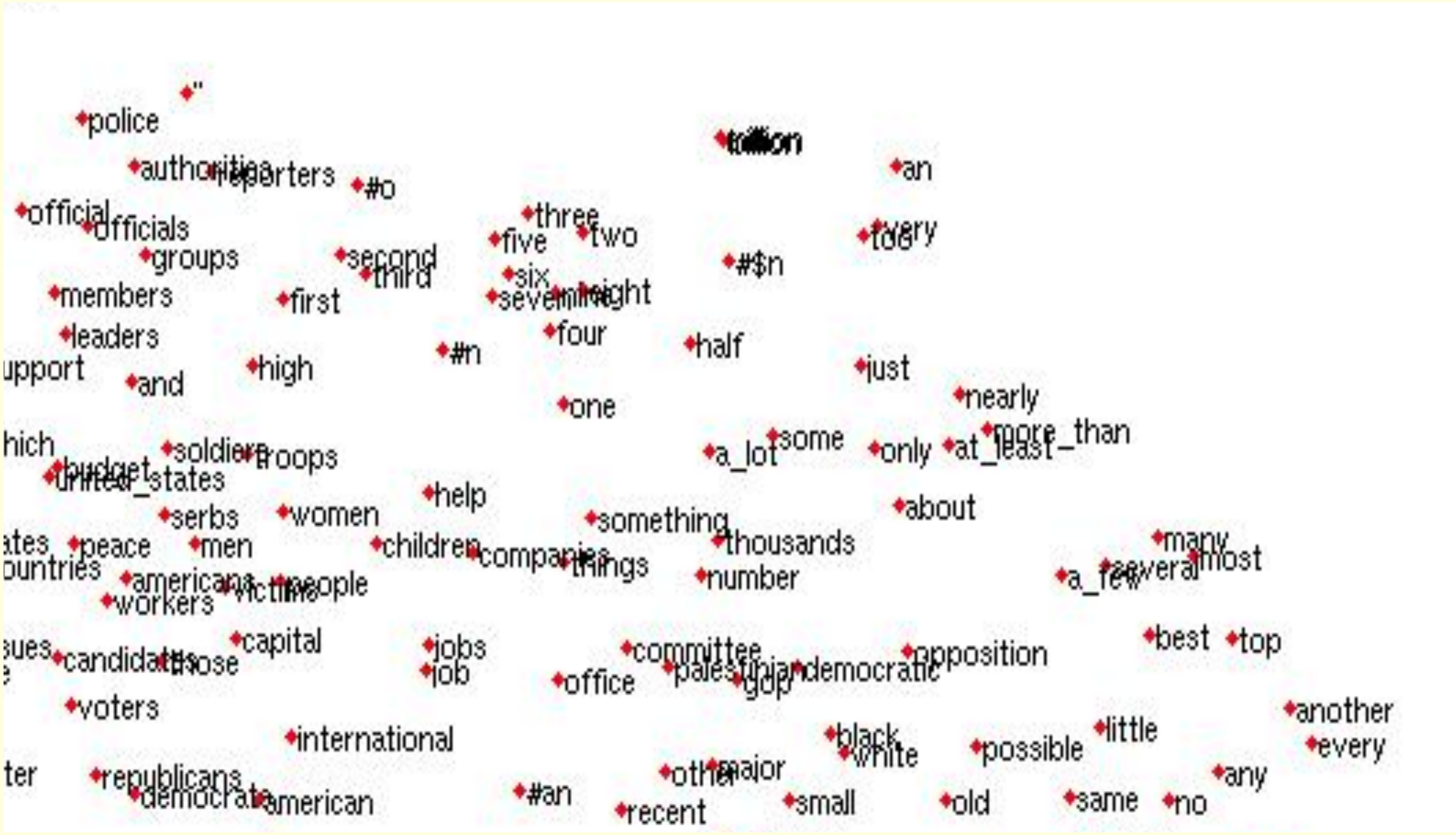


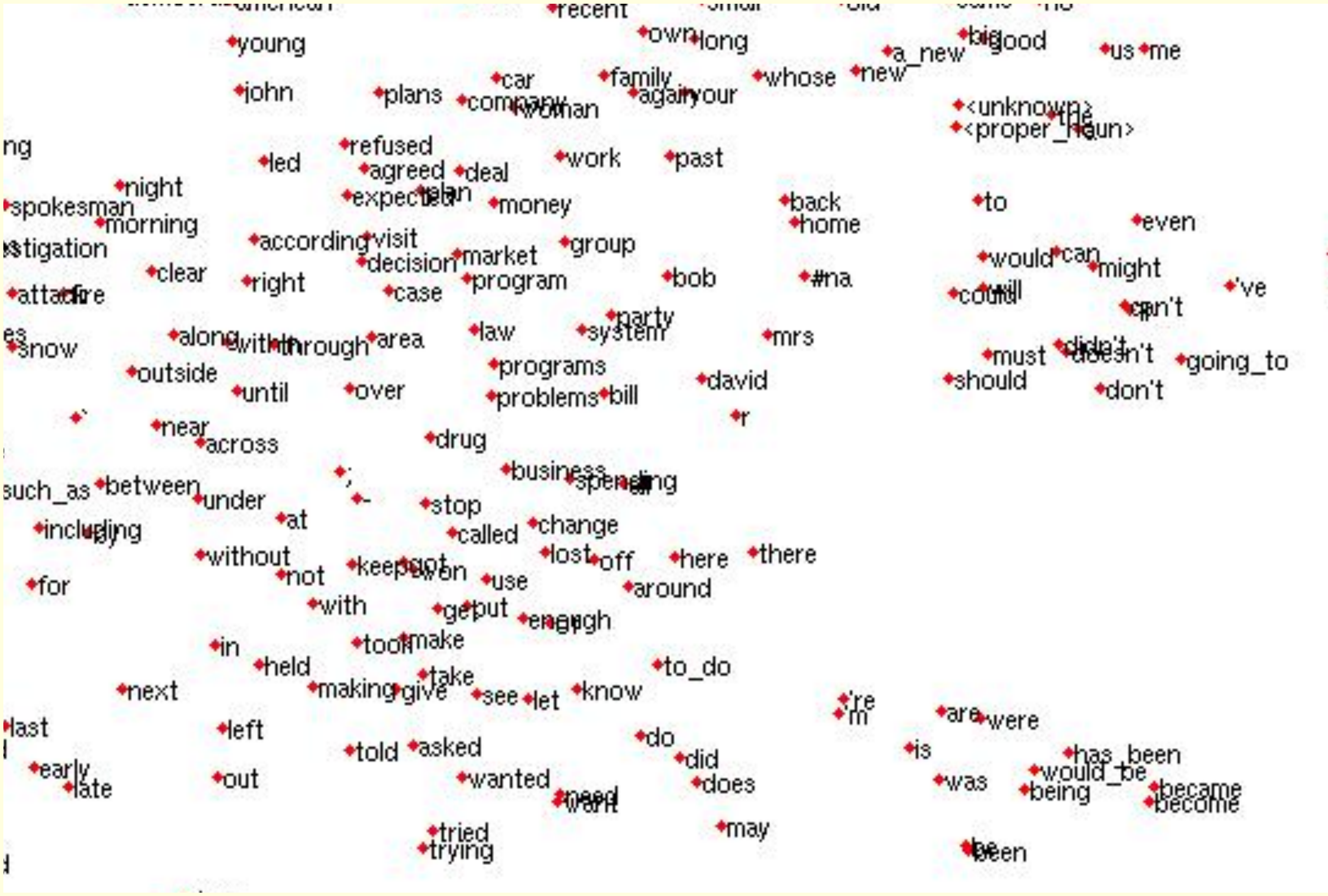


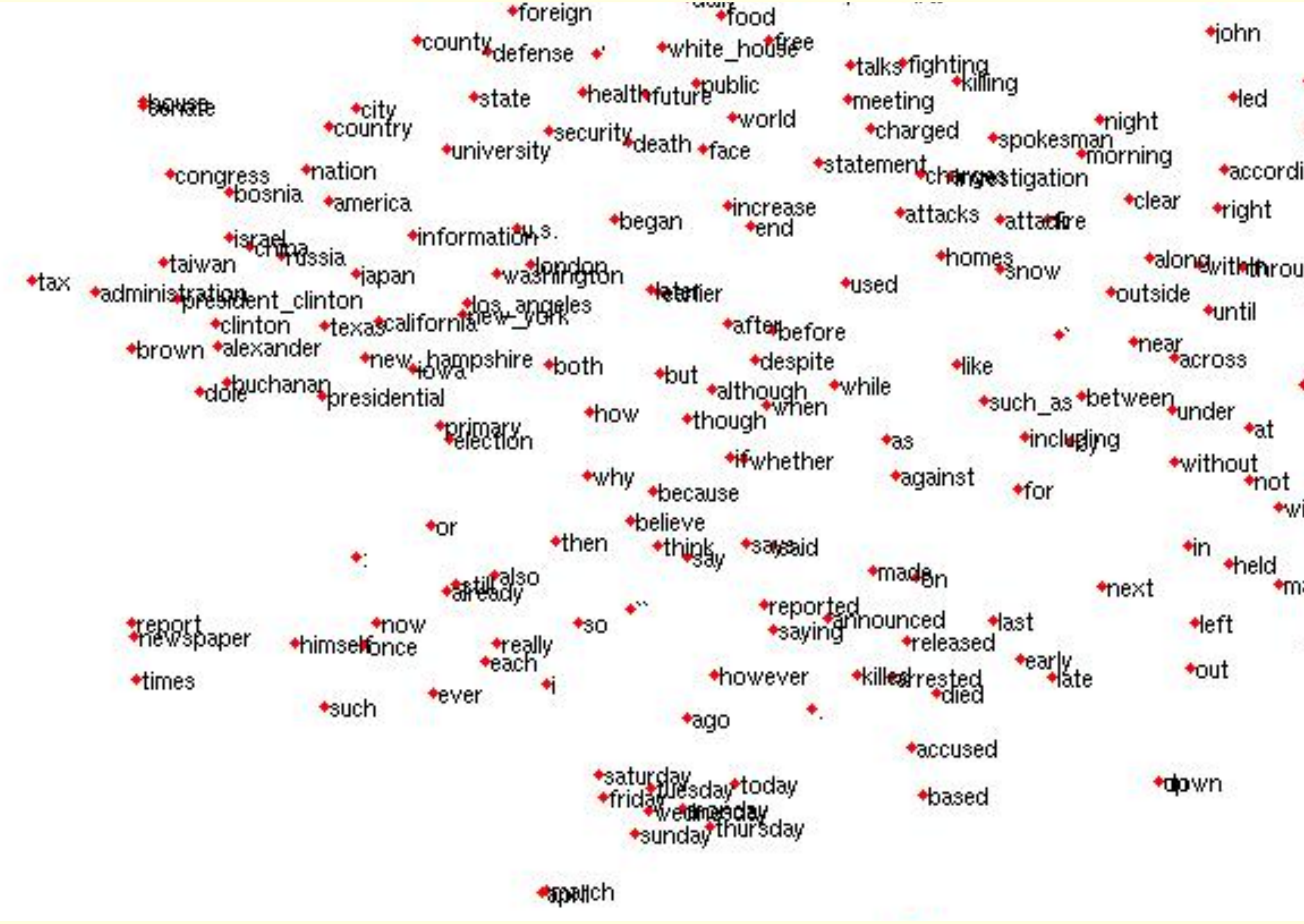
part
miles
hours
months
weeks
week
year
month
years
day
tv
television
trade
radio
sen
more
much
prime_minister
man
found
press
economic
political
military
return
evidence
president
(
he
father
never
mother
wife
service
national
chairman
leader
reports
head
chief
director
who
life
northern
southern
anti
police
"
billion
trillion
an
authorities
reporters
#o
control
nato
us
former
bosnian
republican
muslim
percent
prison
official
officials
u.n
israeli
serb
russian
power
groups
three
two
five
six
seven
eight
#$n
every
too
his
's
,
town
members
second
third
first
federal
government
army
economy
record
name
force
leaders
school
pay
support
and
high
#n
four
half
just
time
court
judge
hospital
elections
campaign
race
numbers
which
budget
united_states
soldiers
troops
one
nearly
a_lot
some
only
at_least
more_than
help
something
#r
way
likely
?
states
countries
peace
serbs
men
women
children
companies
things
thousands
number
about
americans
workers
victims
people
many
several
most
a_few
place
news
trial
agreement
vote
candidate
issues
candidates
those
capital
jobs
job
office
committee
palestinian
gop
democratic
opposition
best
top
issue
show
association
study
industry
center
voters
international
republicans
democrats
american
black
white
possible
little
another
every
other
major
recent
#an
small
old
same
no
any
)
simpson
war
local
daily
food
young
own
long
big
good
us
me
a_new
new
whose
foreign
car
company
woman
family
against
your
county
defense
'
white_house
free
john
plans
<unknown>
<proper_noun>
talks
fighting
killing
health
future
public
refused
agreed
deal
work
past
house
senate
city
country
state
meeting
night
expected
plan
money
back
home
to
even
security
death
face
charged
spokesman
morning
university
statement
charges
investigation
according
visit
decision
market
group
has
had
congress
nation
bosnia
america
clear
right
program
bob
#na
would
can
might
could
will
've
have
increase
end
attacks
attack
fire
case
israel
china
russia
information
u.s.
began
party
system
can't
won't
taiwan
homes
snow
along
with
through
area
law
mrs
must
didn't
doesn't
going_to
tax
administration
president_clinton
japan
washington
london
later
earlier
used
outside
programs
david
should
don't
clinton
texas
california
los_angeles
new_york
after
before
until
over
problems
bill
r
brown
alexander
new_hampshire
iowa
both
despite
near
across
drug
dole
buchanan
presidential
but
although
while
like
such_as
between
under
business
spending
primary
election
how
though
when
as
including
during
at
;
-
stop
called
change
why
if
whether
because
against
for
without
not
keep
got
won
lost
off
here
there
use
around
with
get
put
enough
or
believe
think
say
says
said
then
:
in
held
took
make
to_do
also
still
already
made
on
next
making
give
take
see
let
know
're
'm
are
were
report
newspaper
now
so
`
reported
announced
saying
last
left
himself
once
really
each
released
is
told
asked
do
did
has_been
times
i
however
killed
arrested
died
early
late
out
wanted
need
want
does
was
would_be
being
became
become
such
ever
ago
.
tried
trying
may
be
been
accused
saturday
tuesday
friday
wednesday
monday
today
thursday
sunday
based
up
down



miles
part
hours
months
weeks
week
year
month
years
day
tv
television
trade
radio
sen
more
much
prime_minister
found
man
economic
political
military
press
return
president
(
he
father
never
evidence
mother
wife
service
chairman
national
leader
reports
head
director
chief
who
northern
southern
anti
life
"
police
control
nato
us
former
bosnian
republican
muslim
authorities
reporters
#o
u.n
percent
prison
official
officials
israeli
serb
russian
power
groups
second
third
five
six
town
members
first
his
,
's
federal
government
army
economy
record
name
force
leaders
school
support
and
high
#n
pay
time
court
judge
hospital
elections
campaign
which
soldiers
troops
budget
united_states
number
race
help
serbs
women
?
#r
way
likely
states
peace
men
children
countries
americans
people
victims
workers
place
news
trial
issues
capital
jobs
job
agreement
vote
candidate
candidates
those
voters
issue
show
international
association
study
center
republicans
industry
democrats
american
)


"
police
authorities
reporters
#o
trillion
an
official
officials
three
two
five
very
too
groups
second
third
six
#$n
members
first
seven
nine
eight
leaders
four
#n
half
upport
and
high
just
one
nearly
hich
soldiers
troops
a_lot
some
only
at_least
more_than
budget
united_states
help
serbs
women
something
about
ates
peace
men
children
companies
thousands
many
ountries
things
number
a_few
several
most
americans
victims
people
workers
sues
candidates
those
capital
jobs
job
committee
office
palestinian
democratic
gop
opposition
best
top
voters
another
international
black
white
possible
little
every
ter
republicans
democrats
american
#an
other
major
recent
small
old
same
no
any


american
recent
young
own
long
a_new
big
good
us
me
john
plans
car
company
woman
family
again
your
whose
new
<unknown>
the
<proper_noun>
refused
led
agreed
deal
work
past
night
spokesman
expected
plan
money
back
home
to
even
morning
according
visit
decision
market
group
would
can
might
clear
right
case
program
bob
#na
could
will
've
can't
attack
fire
party
along
with
through
area
law
system
mrs
must
didn't
doesn't
going_to
snow
outside
programs
david
should
don't
until
over
problems
bill
near
across
drug
r
business
spending
such_as
between
under
at
stop
including
called
change
without
not
keep
got
on
use
lost
off
here
there
for
around
with
get
put
enough
in
took
make
held
take
to_do
next
making
give
see
let
know
're
'm
are
were
last
left
do
did
is
has_been
early
late
told
asked
wanted
need
want
does
was
would_be
being
became
become
out
may
tried
trying
be
been


foreign
food
john
county
defense
white_house
free
talks
fighting
killing
house
senate
city
state
health
future
public
meeting
led
country
security
world
charged
night
university
death
face
spokesman
morning
congress
nation
statement
charges
investigation
according
bosnia
america
increase
clear
right
began
end
attacks
attack
fire
israel
china
russia
information
u.s.
homes
along
with
through
taiwan
london
snow
tax
japan
washington
later
earlier
used
outside
administration
president_clinton
los_angeles
until
clinton
texas
california
new_york
after
before
brown
alexander
near
across
new_hampshire
both
despite
like
iowa
but
while
buchanan
although
such_as
between
dole
presidential
when
under
how
though
at
primary
election
including
as
if
whether
without
why
against
not
because
for
believe
or
then
think
says
said
in
say
held
:
made
on
also
still
already
next
``
reported
report
now
so
announced
last
left
newspaper
himself
once
really
saying
released
each
early
out
times
however
killed
arrested
late
i
died
ever
such
ago
.
accused
saturday
tuesday
today
up
down
friday
wednesday
monday
based
sunday
thursday
april
march

From UNI-SNE to t-SNE

- Laurens van der Maaten started experimenting on UNI-SNE and we soon realised that it was easier to replace the mixture of a Gaussian and a uniform by an infinite mixture of Gaussians:

$$q_{ij} \propto \frac{1}{1 + d_{ij}^2}$$

- By using a Gaussian to compute p_{ij} and a heavy-tailed student's t to compute q_{ij} we partially compensate for the different rates of growth of volume as you move away from a point in 2-D and in N-D.

t-SNE

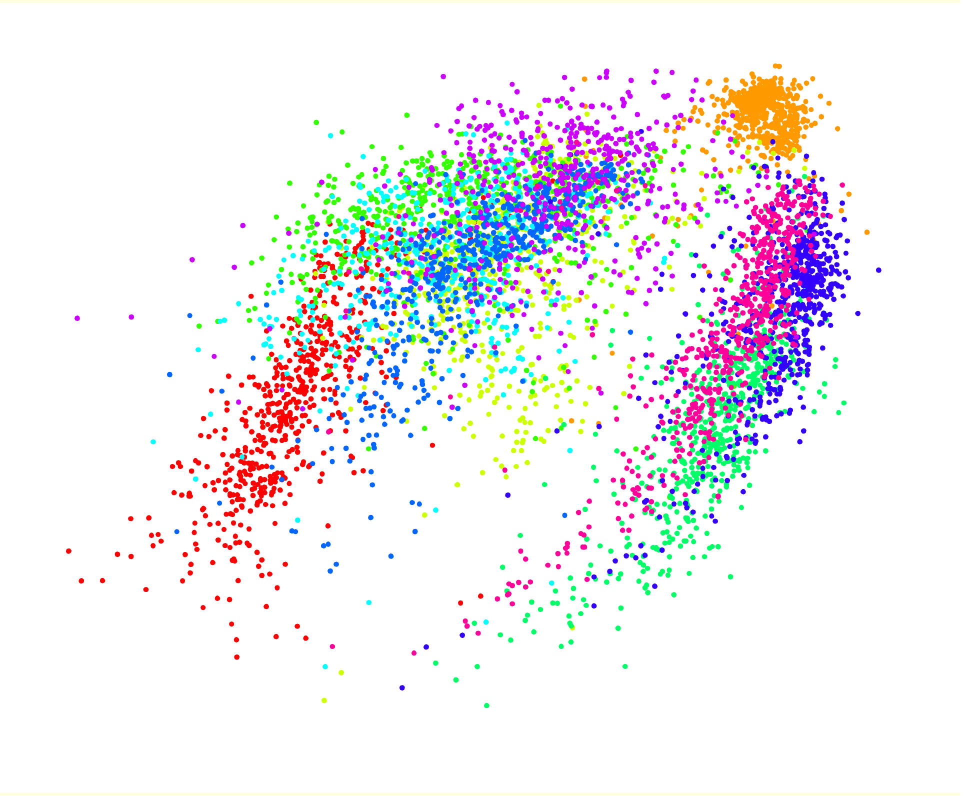
- Instead of using a gaussian plus a uniform, why not use gaussians at many different spatial scales?
  - This sounds expensive, but if we use an infinite number of gaussians, its actually cheaper because we avoid exponentiating.

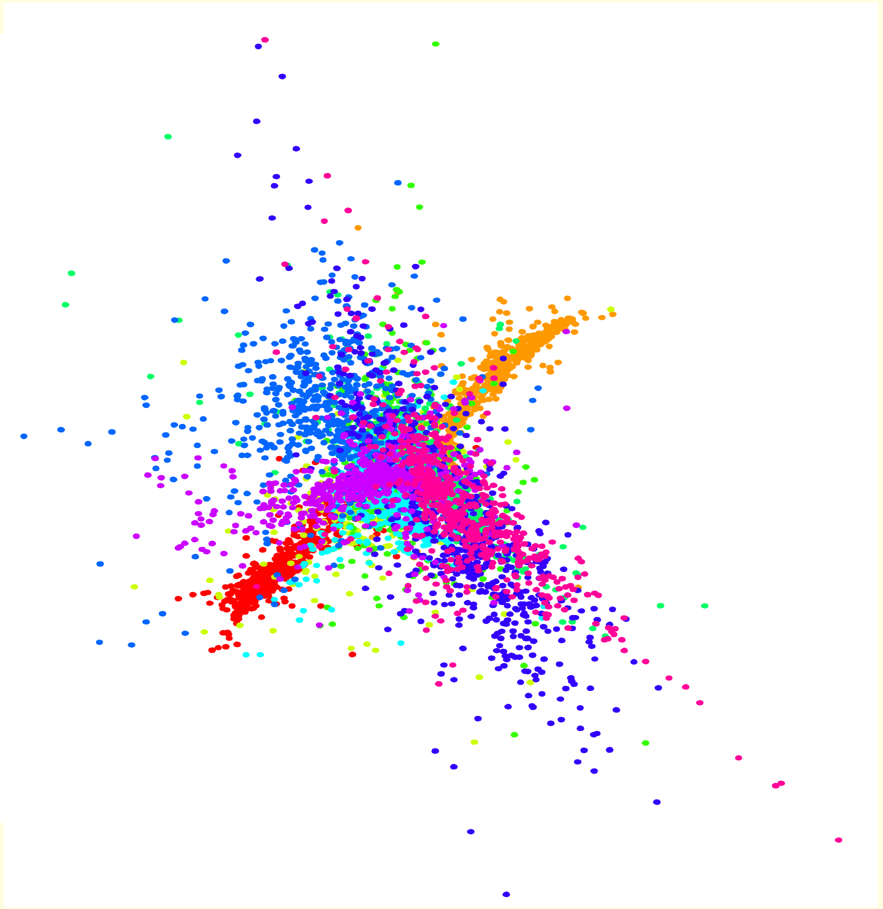
$$q_{ij} \propto \frac{1}{1+d_{ij}^2}$$

Optimization hacks

- Reputable hack: Introduce a penalty term that keeps all the map-points close together.
  - Then gradually relax the penalty to break symmetry slowly.
- Disreputable hack: Allow the probabilities to add up to 4.
  - This causes the map-points to curdle into small clusters leaving lots of space for clusters to move past each other.
  - Then make the probabilities add up to 1.

Two other state-of-the-art dimensionality reduction methods on the 6000 MNIST digits

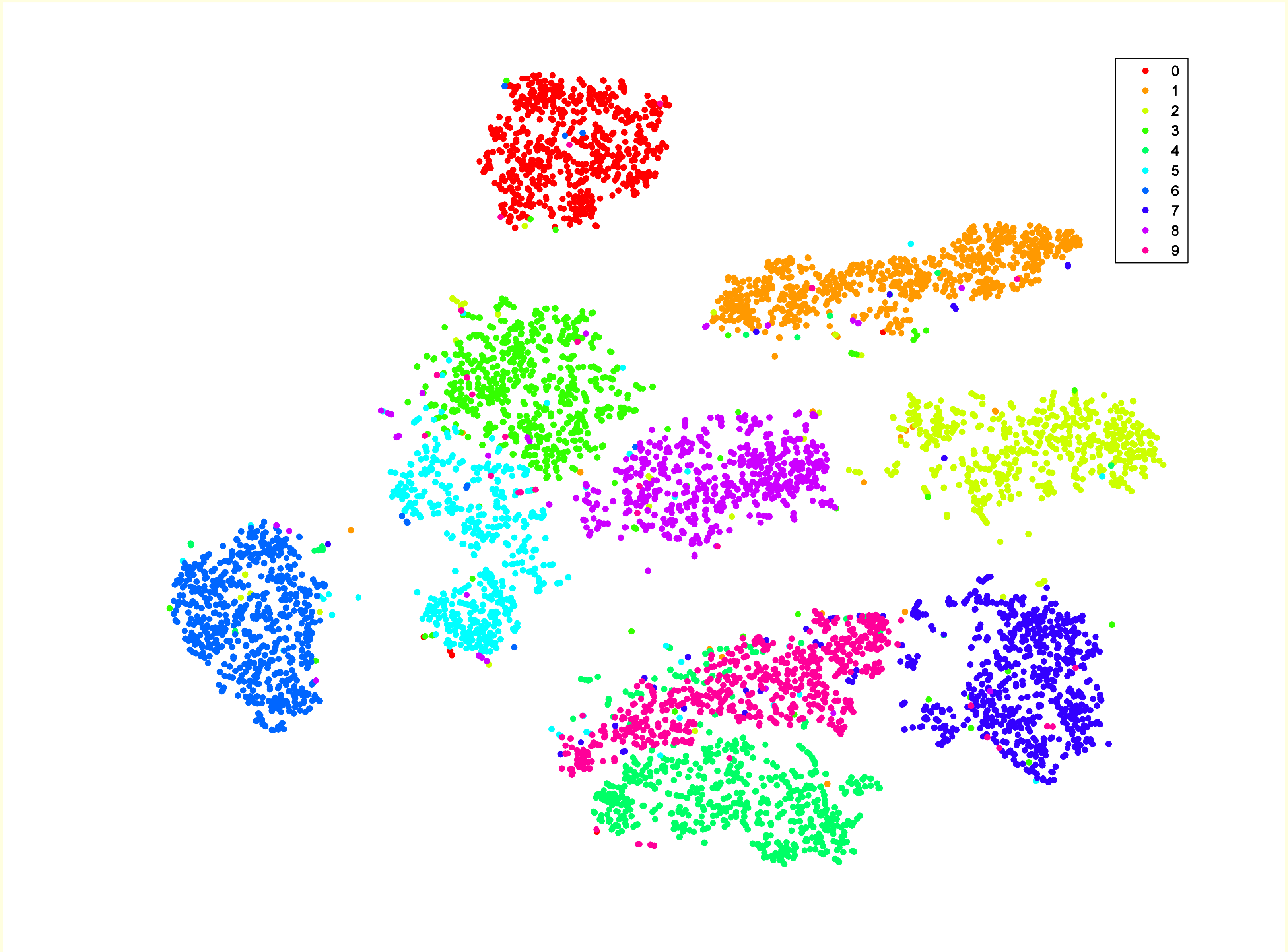




Isomap

Locally Linear Embedding

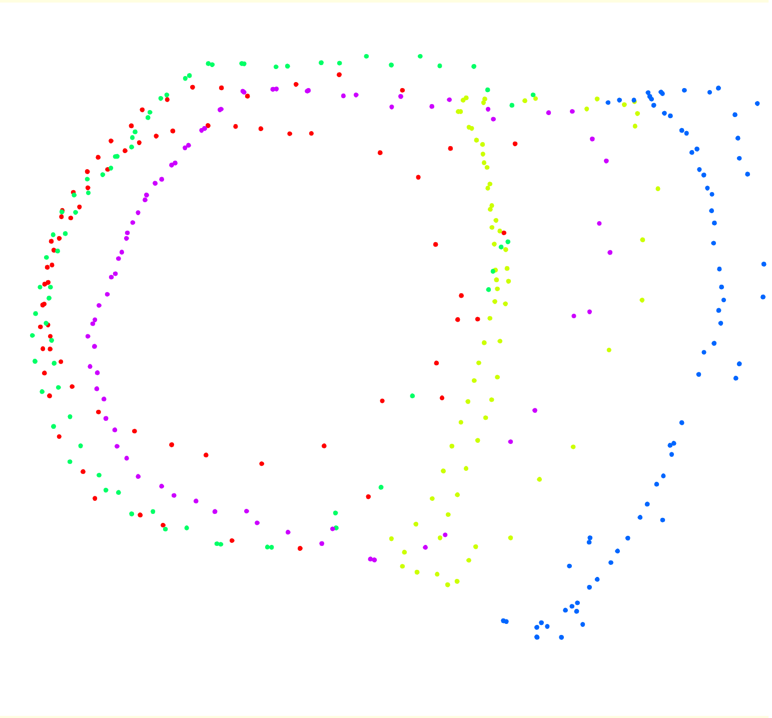
t-SNE on the 6000 MNIST digits

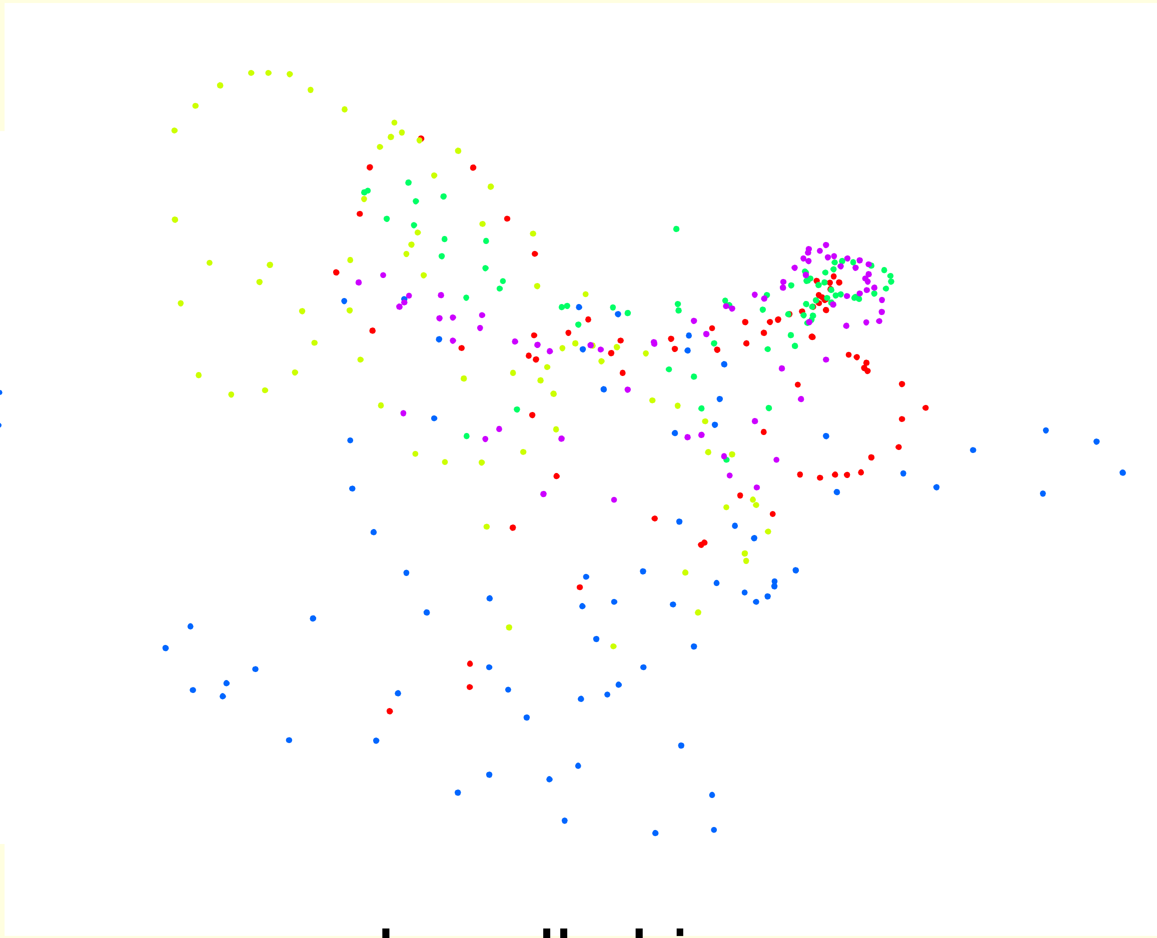


The COIL20 dataset

Each object is rotated about a vertical axis to produce a closed one-dimensional manifold of images.

Isomap & LLE for COIL20 dataset

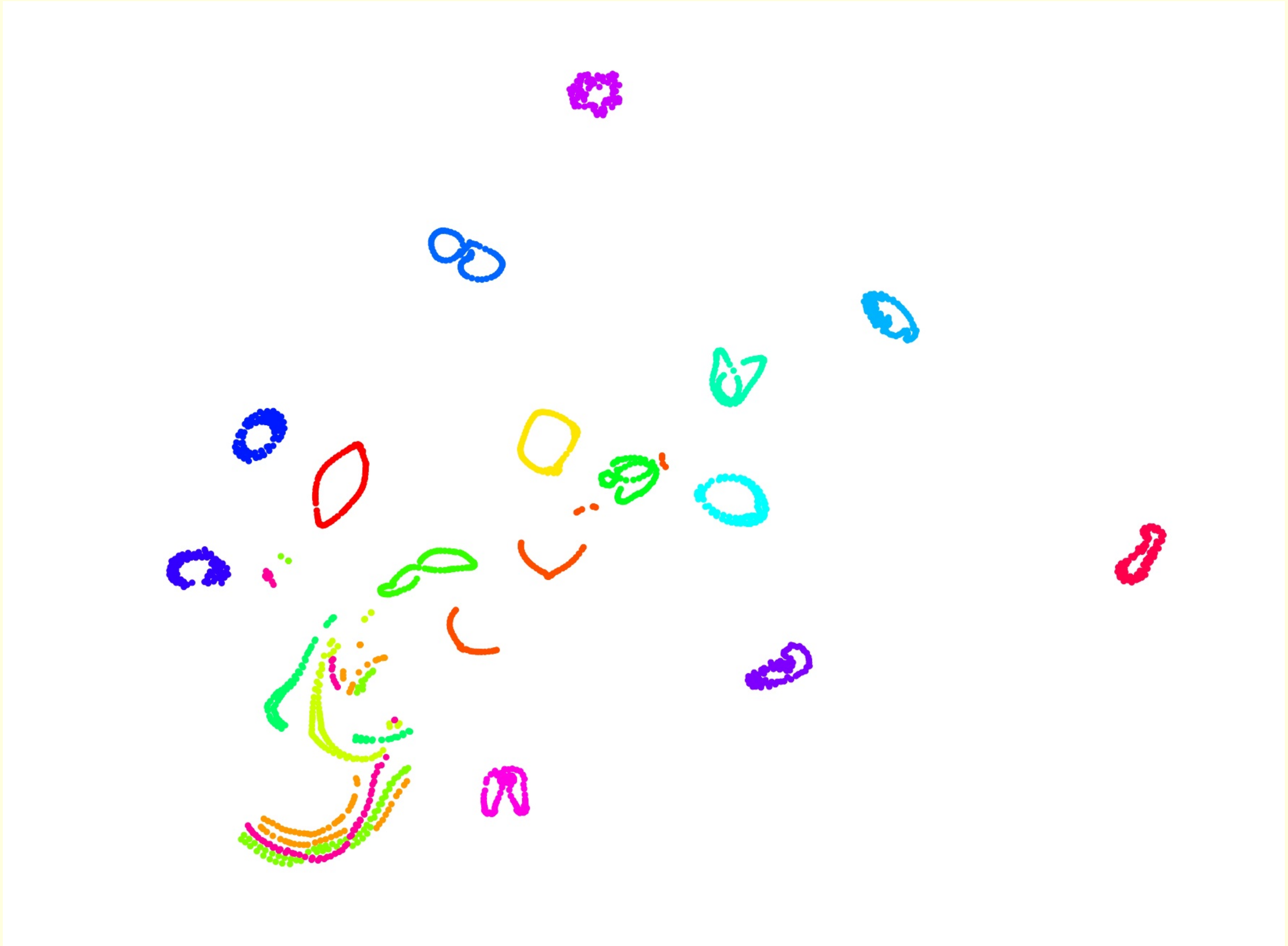




Isomap

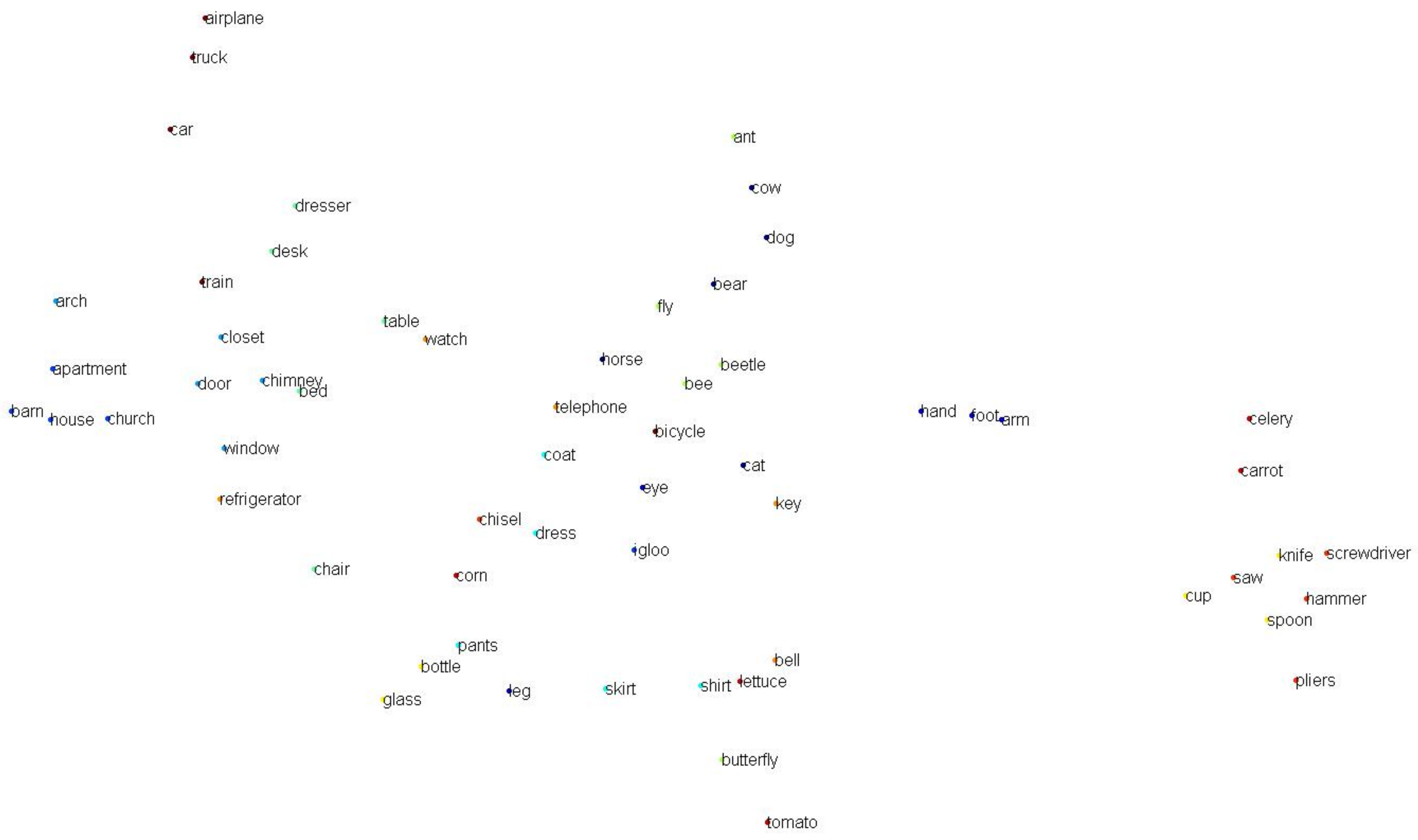
Locally Linear Embedding

t-SNE for COIL20 dataset



Show the map of 2000 English words produced by Joseph Turian using t-SNE on the feature vectors learned by Colobert and Weston (ICML 2008)

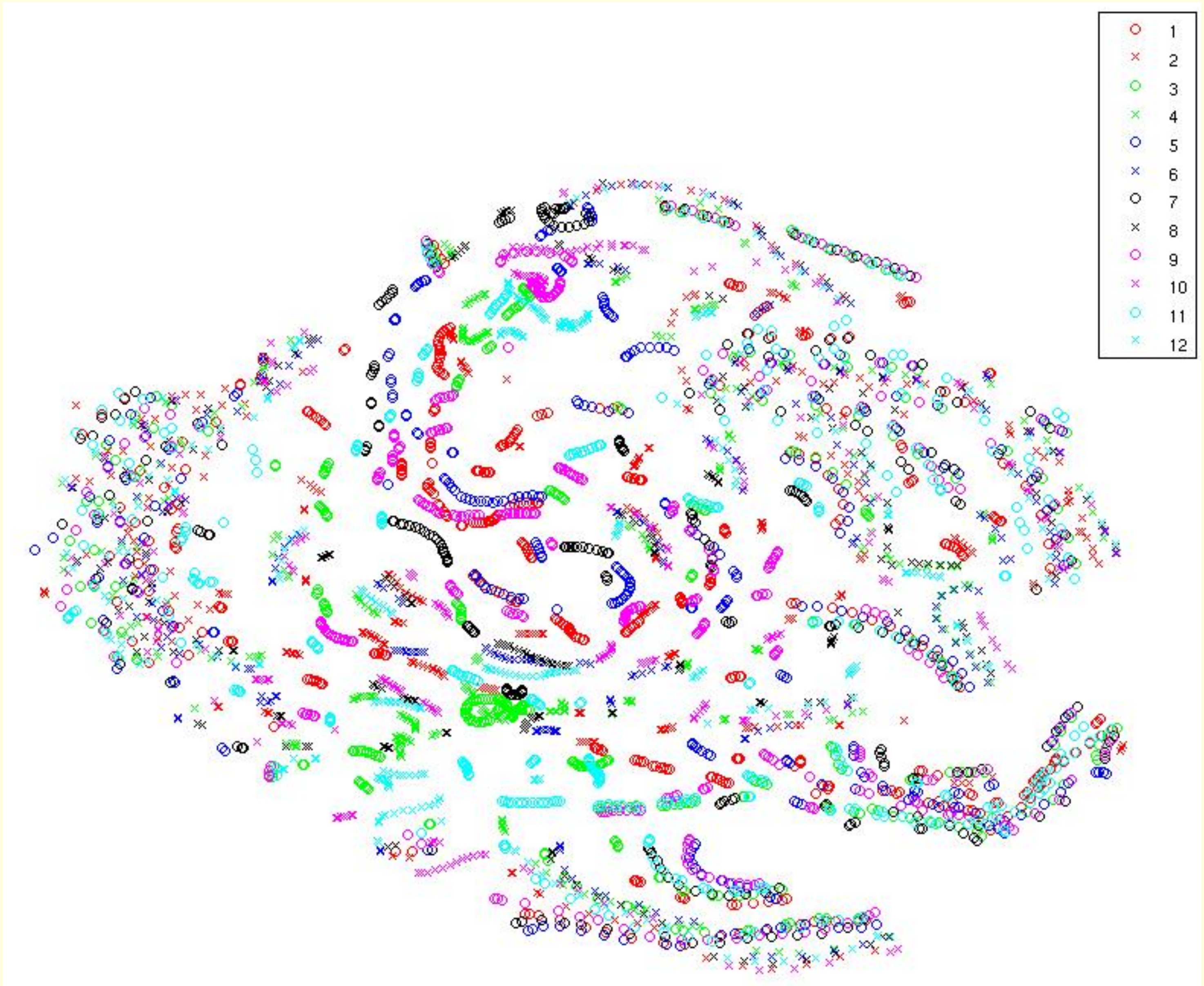
Using t-SNE to see what you are thinking



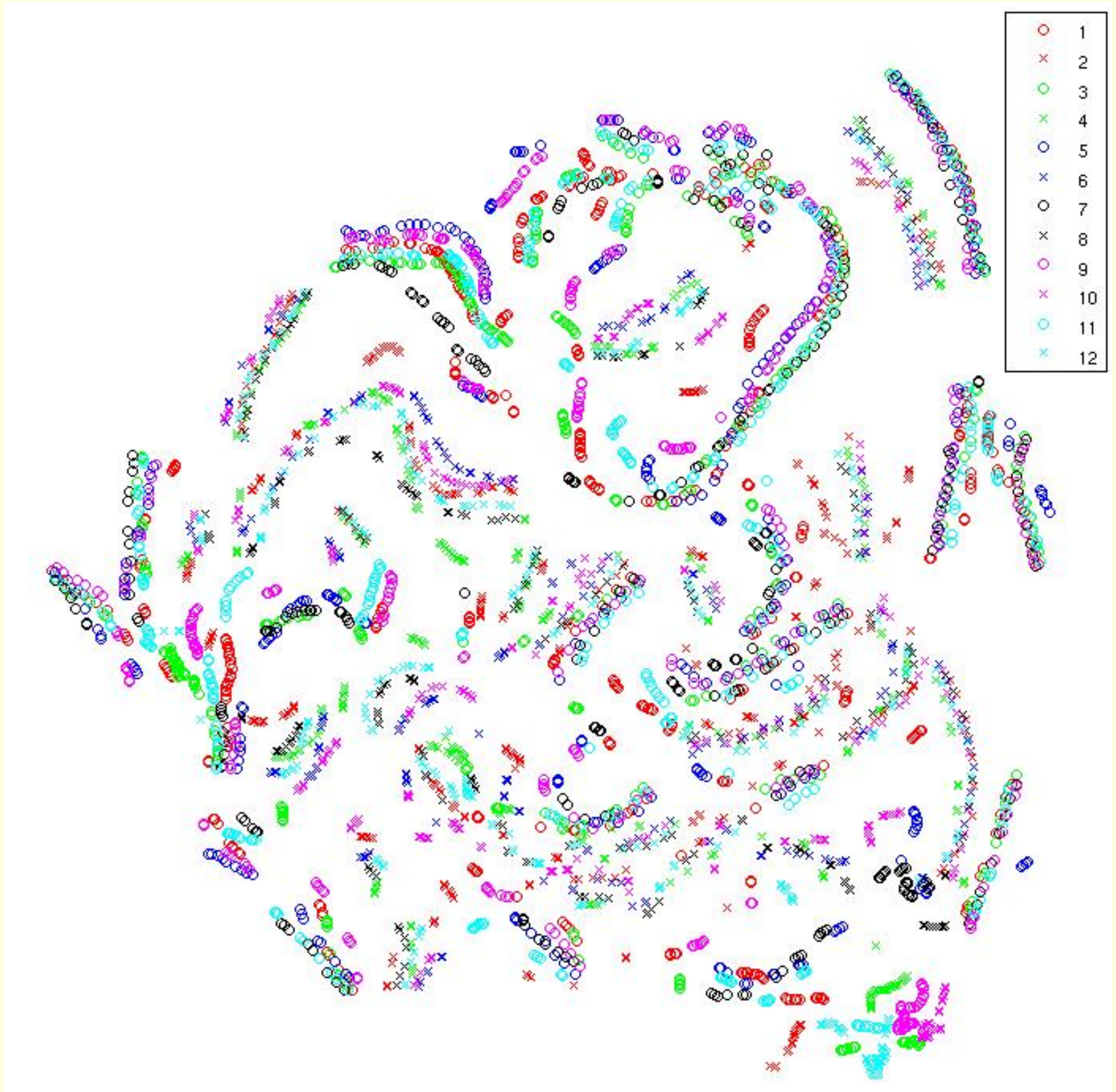
Using t-SNE to see how a DBN that recognizes phonemes deals with speaker variation

- Current speech recognizers try to preprocess the input to eliminate differences between speakers.
- We get very good performance from a DBN without doing this.
  - Its very difficult to improve the DBN by adding speaker information.
- Maybe the DBN is using its hidden layers to get rid of speaker variation .
  - This would explain why speaker information is not much help.

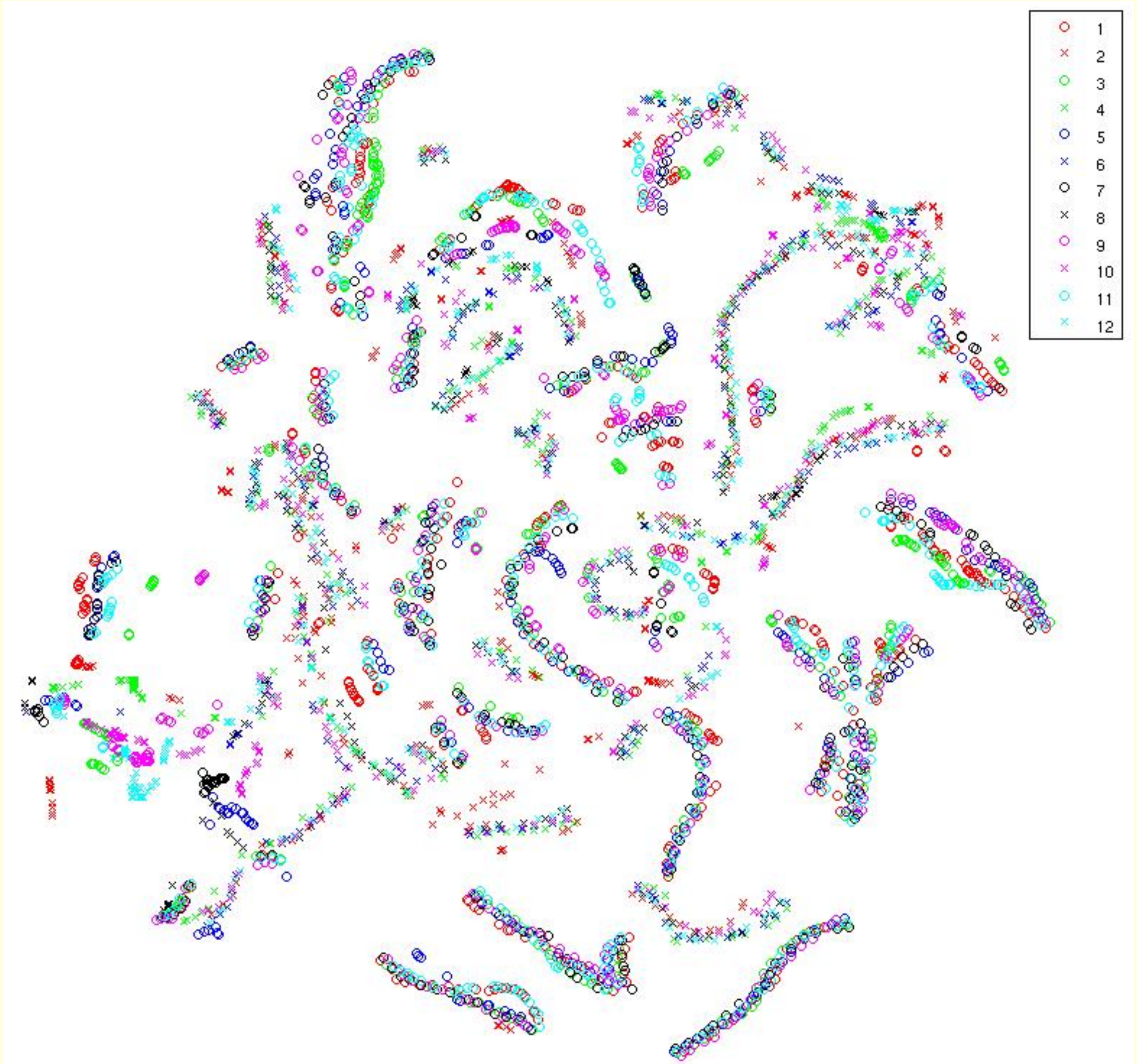
t-SNE applied to windows of 15 input frames for 6 speakers saying two sentences



t-SNE applied to the first hidden layer



t-SNE applied to the 8th hidden layer



Some recent developments

- Miguel Carreira-Perpinan (ICML 2010) showed that the original SNE cost function can be rewritten so that it is equivalent to Laplacian Eigenmaps with an extra repulsion term that spreads out the map points (like in MVU).

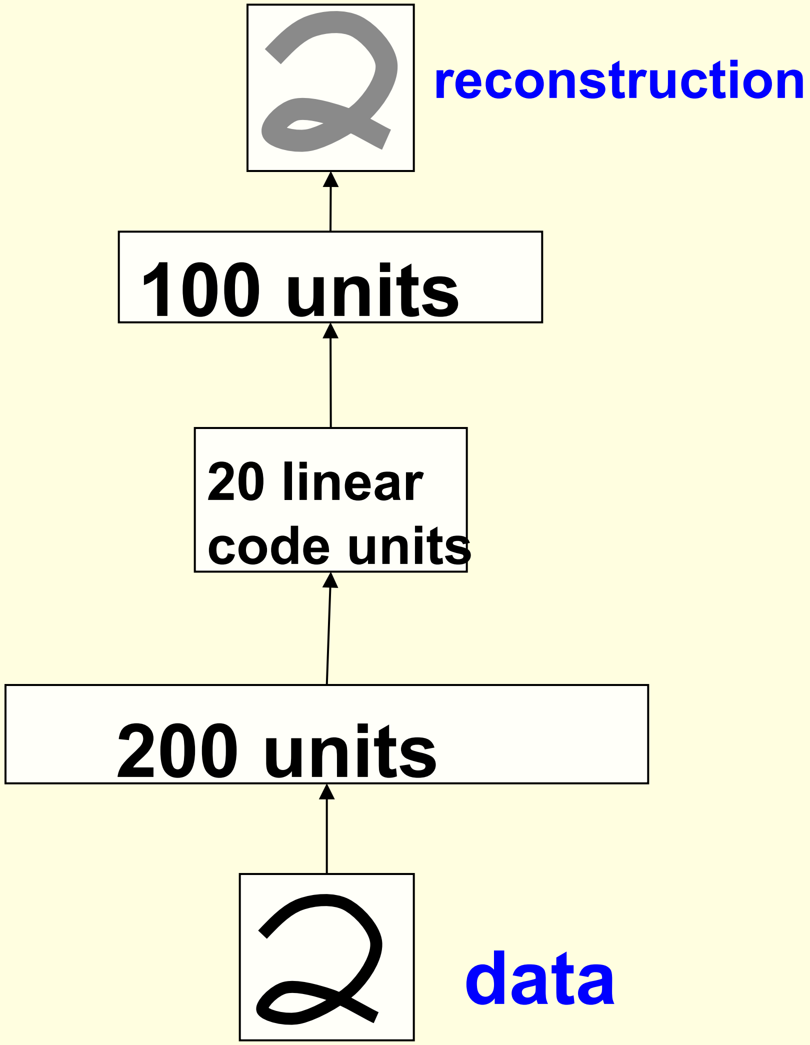
- This led to a much faster optimization method. The fast code is now on the t-SNE webpage.

Combining non-parametric dimensionality reduction with neural networks

- If we have a smooth objective function that assigns a value to a set of codes, we can backpropagate its derivatives through a feedforward neural net.
  - The neural net is like the "encoder" part of an autoencoder.
- We could combine this objective function with the objective of getting good reconstructions from the codes.

Evaluating the codes found by an autoencoder

- Use 3000 images of handwritten digits from the USPS training set.
  - Each image is 16x16 and fairly binary.
- Use a highly non-linear autoencoder
  - Use logistic output units and linear code units.

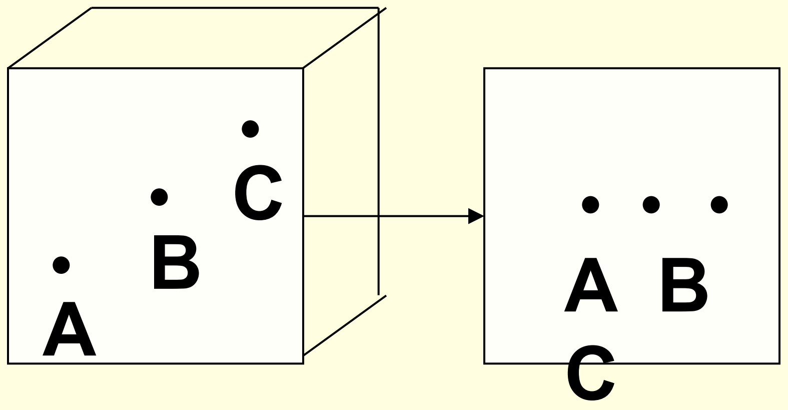


Does code space capture the structure of the data?

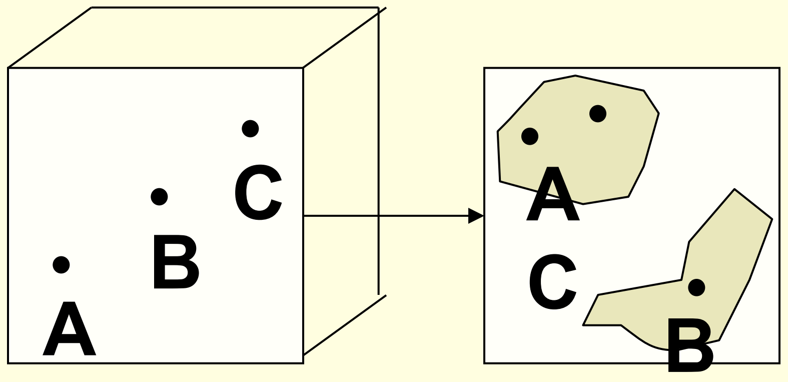
- We would like the code space to model the underlying structure of the data.
  - Digits in the same class should get closer together in code space.
  - Digits of different classes should get further apart.
- We can use k nearest neighbors to see if this happens.
  - Hold out each image in turn and try to label it by using the labels of its k nearest neighbors.
- In pixel space we get 5.9% errors. In code space we get about 12% errors. Why doesn't it work?

How it goes wrong

- PCA is not powerful enough to really mangle the data.



- Non-linear auto-encoders can fracture a manifold into many different domains.
  - This can lead to very different codes for nearby data-points.

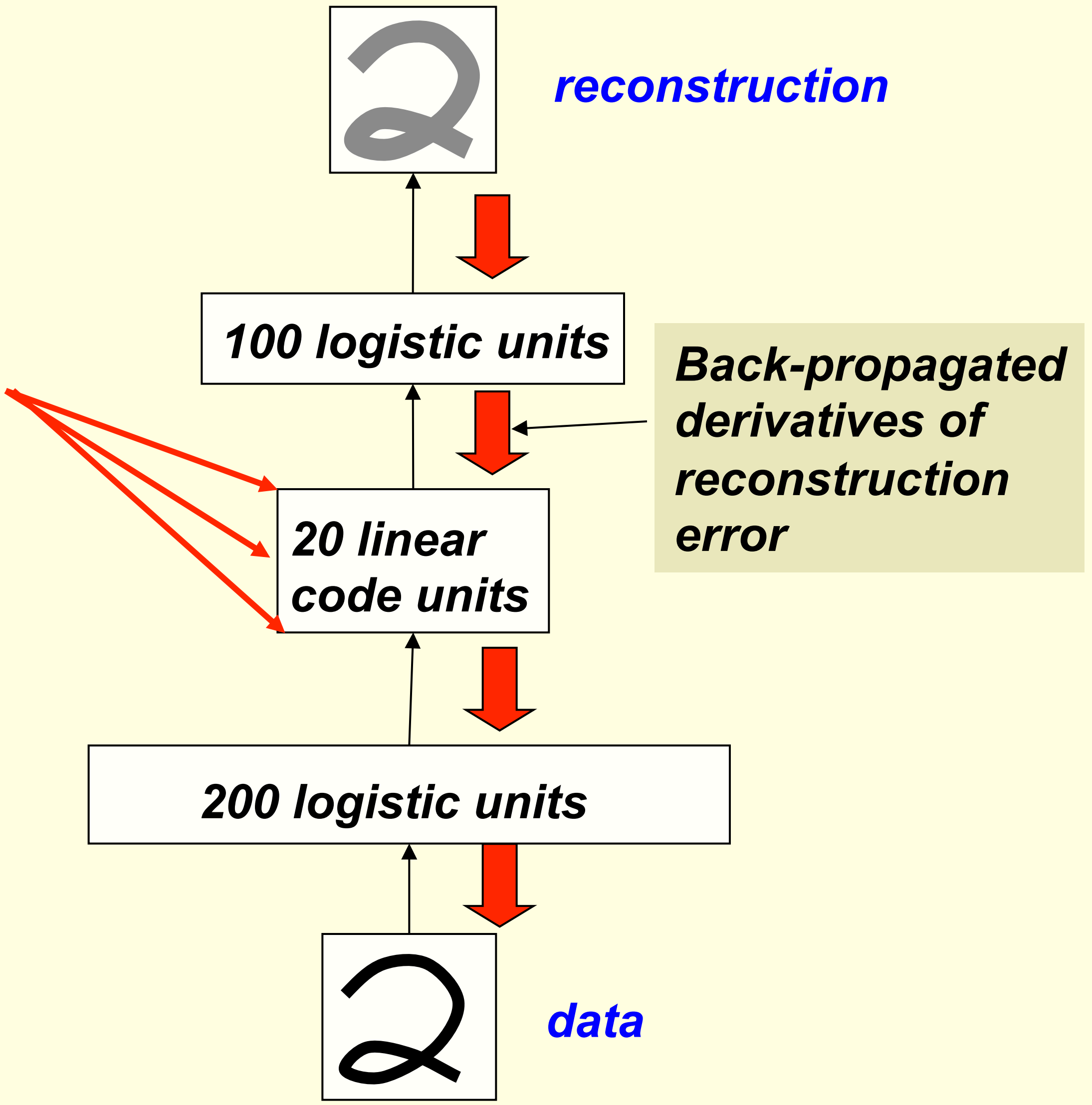


How to fix it

- We need a regularizer that will make it costly to fracture the manifold.
  - There are many possible regularizers.
- Stochastic neighbor embedding can be used as a regularizer.
  - Its like putting springs between the codes to prevent the codes for similar datapoints from being too far apart.

How the gradients are combined

Forces generated by springs attaching this code to the codes for all the other data-points. The stiffness of each spring is dynamically set to be: $p_{ij} - q_{ij}$

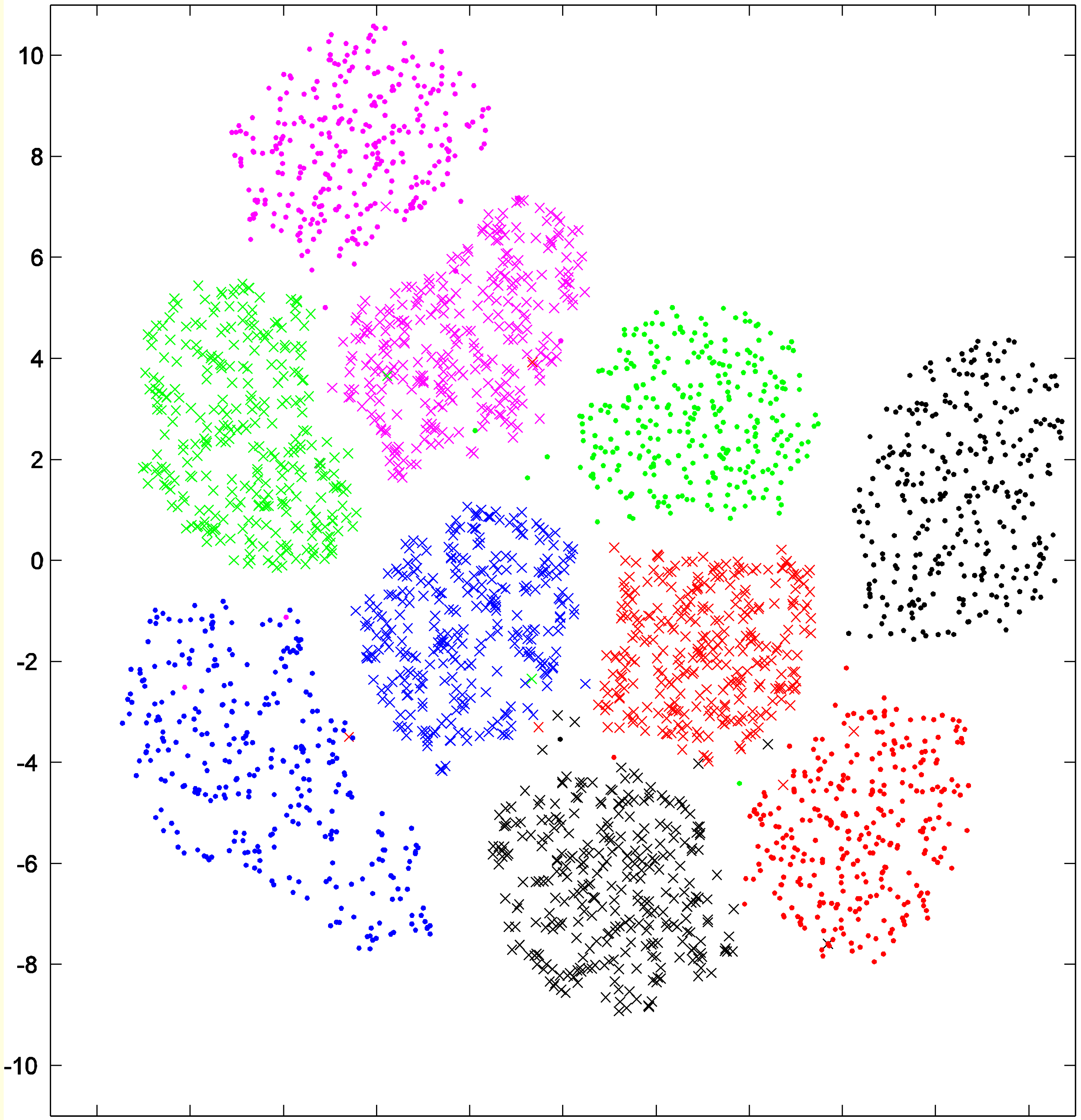


How well does it work?

- Instead of rising from 5.9% to 12%, the hold-one-out KNN error falls to about 2%
  - The strength of the regularizer must be chosen sensibly.
  - The SNE regularizer alone gives about 4.5% hold-one-out KNN errors.
- Can we visualize the codes that are produced using the regularizer?

Learning codes with some pairwise information about labels

- If we pair each digit with another of the same class, there are very nice category boundaries between digits.


10
8
6
4
2
0
-2
-4
-6
-8
-10

A more efficient version

- The derivatives that come from the autoencoder will stop the codes from all collapsing to a point.
  - So we don't need the quadratically expensive normalization term that is used in computing the qij's
- We should be able to just add attractive forces between codes that correspond to similar inputs.
  - The similarity could be measured in the input space or it could be based on extra information (e.g. identity of class labels).

Non-linear Neighborhood Components Analysis (Salakhutdinov and Hinton, 2007)

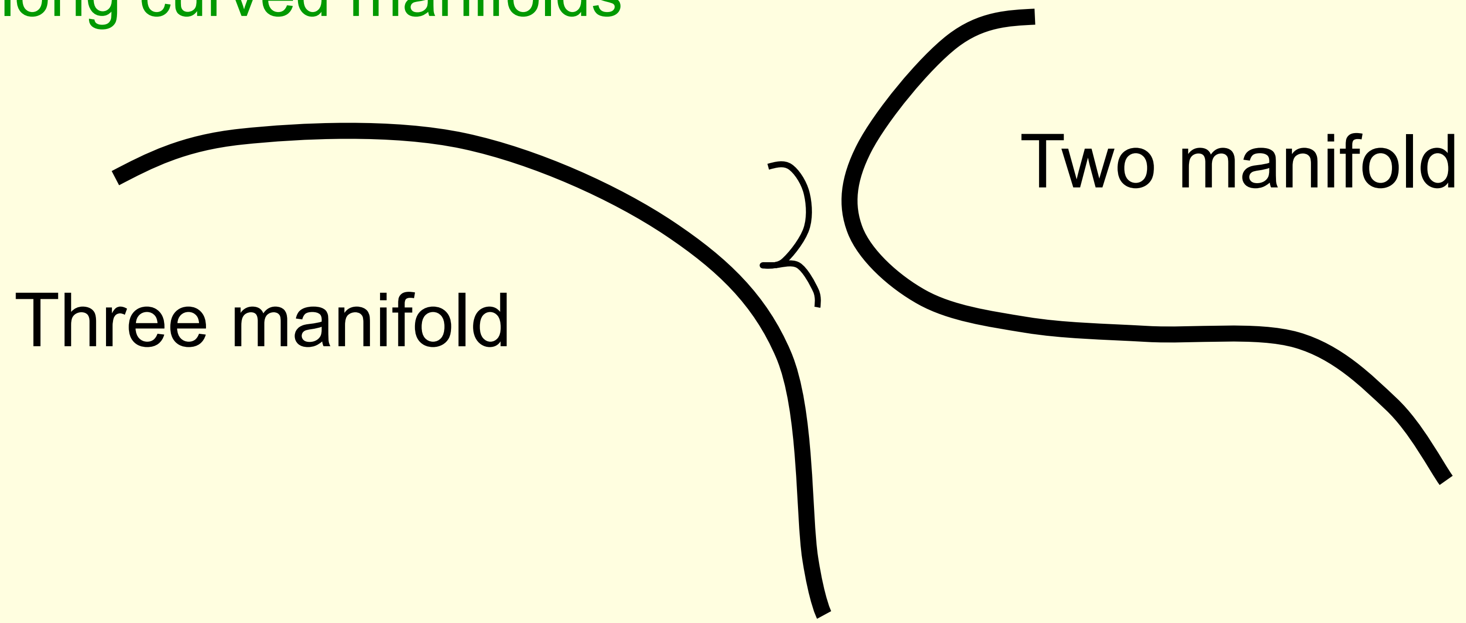
- Use a feed forward neural net to learn codes that make nearest neighbor classification work well.
- In code space, we can predict the class of a point by summing the probabilities assigned to other points of that class when we use the stochastic neighbor probabilities.

$$p(class(i) = c) = \sum_{j \in c} p_{j|i}$$

- So we do gradient ascent in the log probabilities of getting the correct class for each point when it is held-out

What NNCA achieves

- Linear Discriminant Analysis tries to find a projection of the data that makes each point be close to other points of the same class and far from other points of different classes.
  - This is a bad objective function if the classes form long curved manifolds



NCA

- NCA is the linear version of NNCA. It aims to find projections in which each datapoint is close to some other datapoints of the same class and not too close to datapoints of other classes.
  - This does not force all points of the same class to be similar.
  - But it can allow manifolds to become disconnected.