CSC 411 Lecture 13:t-SNE

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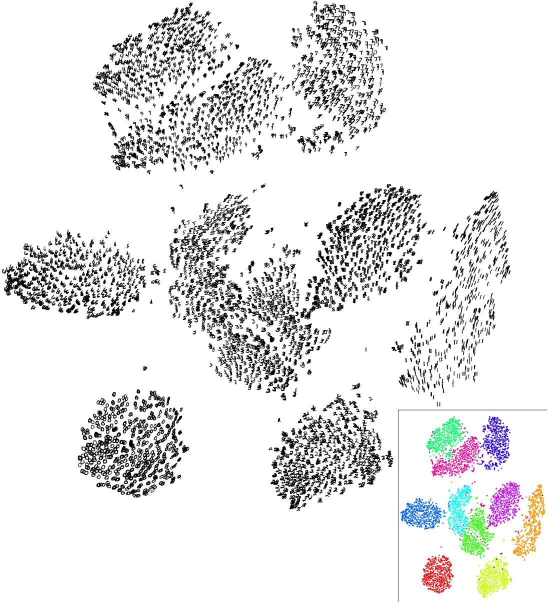
Today

- SNE - Stochastic Neighbor Embedding
- t-SNE
- KL divergence

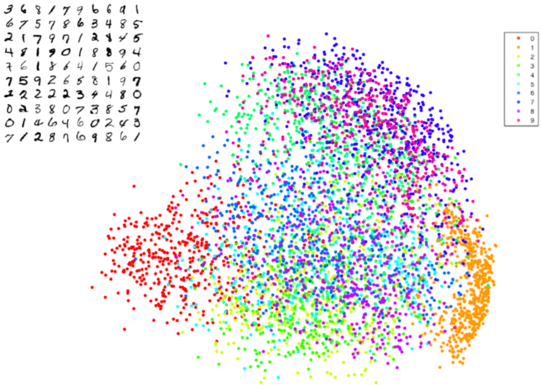
Local embedding

- t-SNE is an alternative dimensionality reduction algorithm.
- PCA tries to find a global structure
  - Low dimensional subspace
  - Can lead to local inconsistencies
    - Far away point can become nearest neighbors
- t-SNE tries to perserve local structure
  - Low dimensional neighborhood should be the same as original neighborhood.
- Unlike PCA almost only used for visualization
  - No easy way to embed new points

tSNE 2 dimensions embedding for MNIST



PCA 2 dimensions embedding for MNIST



Stochastic Neighbor Embedding (SNE)

SNE basic idea:

- "Encode" high dimensional neighborhood information as a distribution
- Intuition: Random walk between data points.
  - High probability to jump to a close point
- Find low dimensional points such that their neighborhood distribution is similar.
- How do you measure distance between distributions?
  - Most common measure: KL divergence

Neighborhood Distributions

- Consider the neighborhood around an input data point $\mathbf{x}_i \in \mathbb{R}^d$
- Imagine that we have a Gaussian distribution centered around $\mathbf{x}_i$
- Then the probability that $\mathbf{x}_i$ chooses some other datapoint $\mathbf{x}_j$ as its neighbor is in proportion with the density under this Gaussian
- A point closer to $\mathbf{x}_i$ will be more likely than one further away

Probabilities P_{ij}

The $i \to j$ probability (should be familiar from A1Q2), is the probability that point $\mathbf{x}_i$ chooses $\mathbf{x}_j$ as its neighbor

$$P_{j|i} = \frac{\exp\left(-||\mathbf{x}^{(i)} - \mathbf{x}^{(j)}||^2/2\sigma_i^2\right)}{\sum_{k \neq i} \exp\left(-||\mathbf{x}^{(i)} - \mathbf{x}^{(k)}||^2/2\sigma_i^2\right)}$$

With $P_{i|i} = 0$

- The parameter σ_i sets the size of the neighborhood
  - Very low σ_i - all the probability is in the nearest neighbor.
  - Very high σ_i - Uniform weights.
- Here we set σ_i differently for each data point
- Results depend heavily on σ_i - it defines the neighborhoods we are trying to preserve.
- Final distribution over pairs is symmetrized: $P_{ij} = \frac{1}{2N}(P_{i|j} + P_{j|i})$
  - Pick i (or j) uniformly and then "jump" to j (i) acording to $P_{j|i}$ ($P_{i|j}$)

Perplexity

- For each distribution $P_{j|i}$ (depends on σ_i) we define the perplexity
  - $perp(P_{j|i}) = 2^{H(P_{j|i})}$ where $H(P) = -\sum_i P_i \log(P_i)$ is the entropy.
- If P is uniform over k elements - perplexity is k.
  - Smooth version of k in kNN
  - Low perplexity = small σ^2
  - High perplexity = large σ^2
- Define the desired perplexity and set σ_i to get that (bisection method)
- Values between 5-50 usually work well
- Important parameter - different perplexity can capture different scales in the data
- If your interested - try $A1Q2$ which a fixed perplexity instead (let me know how it worked)!

Perplexity

[Pic credit: https://distill.pub/2016/misread-tsne/]

SNE objective

- Given $\mathbf{x}^{(1)}, .., \mathbf{x}^{(N)} \in \mathbb{R}^D$ we define the distribution P_{ij}
- Goal: Find good embedding $\mathbf{y}^{(1)}, .., \mathbf{y}^{(N)} \in \mathbb{R}^d$ for some $d < D$ (normally 2 or 3)
- How do we measure an embedding quality?
- For points $\mathbf{y}^{(1)}, .., \mathbf{y}^{(N)} \in \mathbb{R}^d$ we can define distribution Q similarly the same (notice no σ_i^2 and not symmetric)

$$Q_{ij} = \frac{\exp\left(-||\mathbf{y}^{(i)} - \mathbf{y}^{(j)}||^2\right)}{\sum_k \sum_{l \neq k} \exp\left(-||\mathbf{y}^{(l)} - \mathbf{y}^{(k)}||^2\right)}$$

- Optimize Q to be close to P
  - Minimize KL-divergence
- The embeddings $\mathbf{y}^{(1)}, .., \mathbf{y}^{(N)} \in \mathbb{R}^d$ are the parameters we are optimizing.
  - How do you embed a new point? No embedding function!

KL divergence

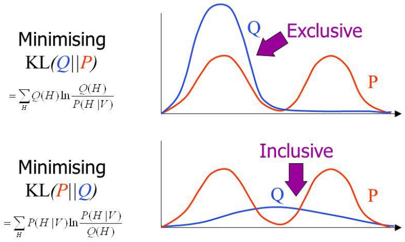
Measures distance between two distributions, P and Q:

$$KL(Q||P) = \sum_{ij} Q_{ij} \log \left(\frac{Q_{ij}}{P_{ij}} \right)$$

- Not a metric function - not symmetric!
- Code theory intuition: If we are transmitting information that is distributed according to P, then the optimal (lossless) compression will need to send on average $H(P)$ bits.
- What happens you expect P (and design your compression accordingly) but the actual distribution is Q?
  - will send on average $H(Q) + KL(Q||P)$
  - $KL(Q||P)$ is the "penalty" for using wrong distribution

KL Properties

- $KL(Q||P) \geq 0$ and zero only when $Q = P$ (a.s)
- $KL(Q||P)$ is a convex function.
- if $P_{ij} = 0$ but $Q_{ij} > 0$ then $KL(Q||P) = \infty$



[Pic credit: `https://timvieira.github.io/blog/post/2014/10/06/kl-divergence-as-an-objective-function/`]

SNE algorithm

- We have P, and are looking for $\mathbf{y}^{(1)}, .., \mathbf{y}^{(N)} \in \mathbb{R}^d$ such that the distribution Q we infer will minimize $L(Q) = KL(P||Q)$ (notice Q on right, uncommon).
- Note that $KL(P||Q) = \sum_{ij} P_{ij} \log\left(\frac{P_{ij}}{Q_{ij}}\right) = -\sum_{ij} P_{ij} \log\left(Q_{ij}\right) + const$
- Can show that $\frac{\partial L}{\partial \mathbf{y}^{(i)}} = \sum_j (P_{ij} - Q_{ij})(\mathbf{y}^{(i)} - \mathbf{y}^{(j)})$
- Not a convex problem! No guarantees, can use multiple restarts.
- Main issue - crowding problem.

Crowding Problem

- In high dimension we have more room, points can have a lot of different neighbors
- In 2D a point can have a few neighbors at distance one all far from each other - what happens when we embed in 1D?
- This is the "crowding problem" - we don't have enough room to accommodate all neighbors.
- This is one of the biggest problems with SNE.
- t-SNE solution: Change the Gaussian in Q to a heavy tailed distribution.
    - if Q changes slower, we have more "wiggle room" to place points at.

t-SNE

t-Distributed Stochastic Neighbor Embedding

- Student-t Probability density $p(x) \propto (1 + \frac{x^2}{v})^{-(v+1)/2}$
  - for $v = 1$ we get $p(x) \propto \frac{1}{1+x^2}$
- Probability goes to zero much slower then a Gaussian.
- Can show it is equivalent to averaging Gaussians with some prior over σ^2
- We can now redefine Q_{ij} as

$$Q_{ij} = \frac{(1 + ||\mathbf{y}_i - \mathbf{y}_j||^2)^{-1}}{\sum_k \sum_{l \neq k} (1 + ||\mathbf{y}_k - \mathbf{y}_l||^2)^{-1}}$$

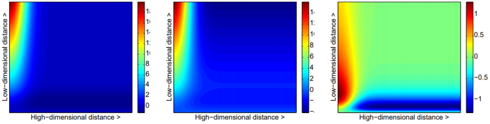
- We leave P_{ij} as is!

t-SNE gradients

- Can show that the gradients of t-SNE objective are

$$\frac{\partial L}{\partial \mathbf{y}^{(i)}} = \sum_j (P_{ij} - Q_{ij})(\mathbf{y}^{(i)} - \mathbf{y}^{(j)})(1 + ||y_i - y_j||^2)^{-1}$$

  - Compare to the SNE gradients: $\frac{\partial L}{\partial \mathbf{y}^{(i)}} = \sum_j (P_{ij} - Q_{ij})(\mathbf{y}^{(i)} - \mathbf{y}^{(j)})$



(a) Gradient of SNE. (b) Gradient of UNI-SNE. (c) Gradient of t-SNE.

- Both repulse close dissimilar points and attract far similar points, but the $t - SNE$ has a smaller attraction term to solve crowding.

[Image credit: "Visualizing Data using t-SNE"]

Algorithm

Algorithm 1: Simple version of t-Distributed Stochastic Neighbor Embedding.

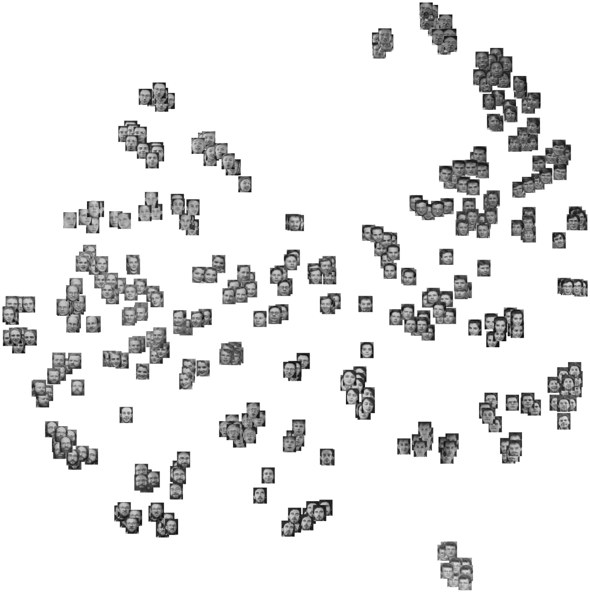
Data: data set $\mathcal{X} = \{x_1, x_2, ..., x_n\}$,
cost function parameters: perplexity $Perp$,
optimization parameters: number of iterations T, learning rate η, momentum $\alpha(t)$.
Result: low-dimensional data representation $\mathcal{Y}^{(T)} = \{y_1, y_2, ..., y_n\}$.
begin
  compute pairwise affinities $p_{j|i}$ with perplexity $Perp$ (using Equation 1)
  set $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$
  sample initial solution $\mathcal{Y}^{(0)} = \{y_1, y_2, ..., y_n\}$ from $\mathcal{N}(0, 10^{-4} I)$
  for t=1 **to** T **do**
    compute low-dimensional affinities q_{ij} (using Equation 4)
    compute gradient $\frac{\delta C}{\delta \mathcal{Y}}$ (using Equation 5)
    set $\mathcal{Y}^{(t)} = \mathcal{Y}^{(t-1)} + \eta \frac{\delta C}{\delta \mathcal{Y}} + \alpha(t) \left(\mathcal{Y}^{(t-1)} - \mathcal{Y}^{(t-2)} \right)$
  end
end

[Slide credit: "Visualizing Data using t-SNE"]

CNN features example

[Image credit: http://cs.stanford.edu/people/karpathy/cnnembed/]

CNN features example



[Image credit: https://lvdmaaten.github.io/tsne/]

Recap

- t-SNE is a great way to visualize data
- Helps understand "black-box" algorithms like DNN.
- Reduced "crowding problem" with heavey tailed distribution.
- Non-convex optimization - solved by GD with momentum.
- Less suitable for SGD (think about the parameters), some alternative speedups exists ("Barnes-Hut t-SNE").
- Great extra resource: `https://distill.pub/2016/misread-tsne/`