Visualizing High Dimensional Data using Parallelized t-SNE Dimensionality Reduction

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Input and Output

$$x = \{x_1, x_2, x_3, \dots, x_N\}$$

$$x_i \in \mathbb{R}^H$$

$$y = \{y_1, y_2, y_3, \dots, y_N\}$$

$$y_i \in \mathbb{R}^2$$



Example input $x_i \in \mathbb{R}^{784}$

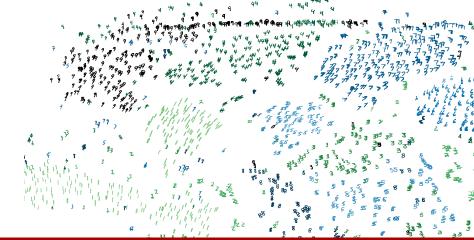
$$x_1 = 3, x_2 = 3, x_3 = 3, \dots$$

Example for $y_i \in \mathbb{R}^2$



The t-SNE Algorithm How? Implementation Hogwild Parallelization Math Barnes-Hut Approxi

Example



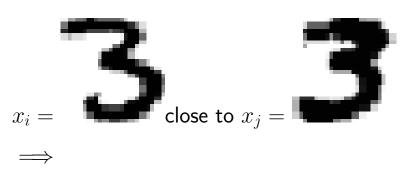
The t-SNE Algorithm

Student's t-Distributed

Stochastic

Neighbor Embedding

Neighbor Embedding



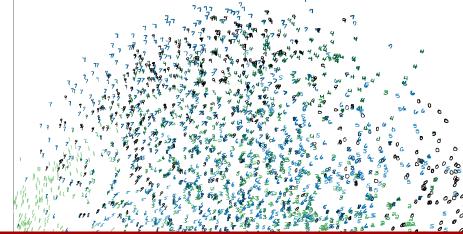
 y_i close to y_j

Algorithm Pseudocode 1

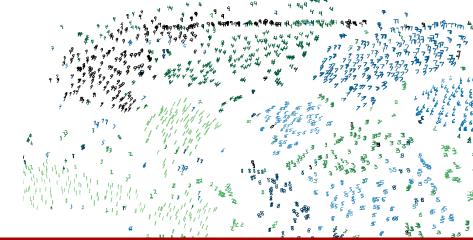
van der Maaten and Hinton 2008 [Journal of Machine Learning]

- 1. Guess y.
- 2. Iteratively improve y.

The t-SNE Algorithm How? Implementation Hogwild Parallelization Math Barnes-Hut Approxi



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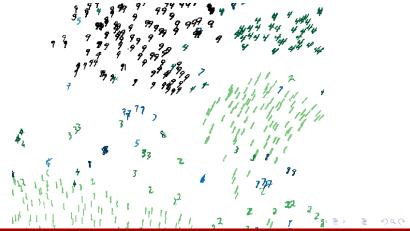
N-Body System

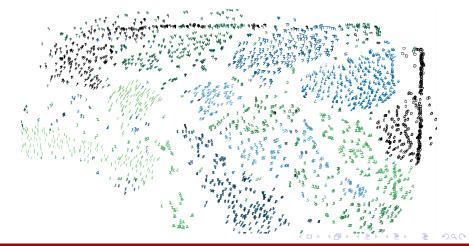
van der Maaten 2014 [Journal of Machine Learning]

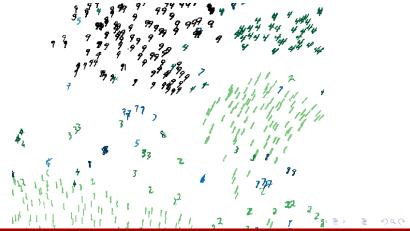
Connected by springs



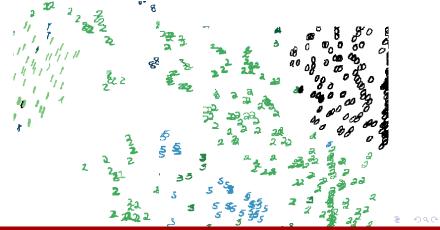
Spring strength
$$\sim \mathsf{dist}_1(x_i, x_j) - \mathsf{dist}_2(y_i, y_j)$$











```
http://infohost.nmt.edu/~hrivera/
hpc/mnist.mp4
```

My Code

```
hr@v580 > cloc tsne.c matrix.c
                         code
Language
              comment
C + OpenMP
              216
                         470
O(n^2/p)
```

Algorithm Pseudocode 2

```
1 P = N x N matrix
2 P[i,j] = probability that x[i] neighbors x[j]
3 y[i] = random 2D vector from -1E-4 to 1E-4
4 for t=1..T
5 for i=1..N
6  Qy = N x N matrix
7 Qy[i,j] = probability that y[i] neighbors y[j]
8 y[i] = y[i] - gradient of KL(P, Qy)
```

Parallelized using Hogwild GD

```
Niu, Recth, Re, Wright 2011

for t=1..T

parallel for i=1..N shared(P, Qy, y)

Qy = N x N matrix

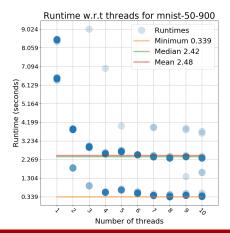
Qy[i,j] = probability that y[i] neighbors y[j]

y[i] = y[i] - gradient of KL(P, Qy)
```

Best if sparse



Performance Increase



How? (part 2)

van der Maaten and Hinton 2008 [Journal of Machine Learning]

Compute the pairwise similarities of x, $P \in \mathbb{R}^{N \times N}$.

Guess y, compute pairwise similarities $Q(y) \in \mathbb{R}^{N \times N}$.

Must minimize difference between P and Q(y).

Minimize Difference Using

Gradient Descent

Kullbach-Leibler divergence: diff of P, Q.

$$\begin{split} KL(P,Q) &= \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} P_{ij} \log \frac{P_{ij}}{Q_{ij}} \\ y_i^{\text{improved}} &= y_i - \frac{\delta}{\delta y_i} KL(P,Q(y)) \end{split}$$

Equations

$$P_{j|i}(x) = \frac{\exp(-\|x_i - x_j\|^2 / 2\sigma_i^2)}{\sum_{k=1, k \neq i}^{N} \exp(-\|x_i - x_k\|^2 / 2\sigma_i^2)}$$

$$P_{ij} = (P_{j|i} + P_{i|j}) / 2N$$

$$Q_{ij}(y) = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{\sum_{k=1}^{N} \sum_{l=1, l \neq k}^{N} (1 + \|y_k - y_l\|^2)^{-1}}$$

Equations

$$KL(P,Q) = \sum_{i=1,j\neq i}^{N} P_{ij} \log \frac{P_{ij}}{Q_{ij}}$$
$$\frac{\delta}{\delta y_i} KL(P,Q(y)) = \sum_{j\neq i}^{N} 4(P_{ij} - Q_{ij})$$
$$(y_i - y_j)Q_{ij}Z$$

Barnes-Hut Approximation

Group distant nodes

Questions?