Review of "Towards a comprehensive visualization of structure in large scale data sets"

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March 3, 2022

This work proposes a parallelized Barnes-Hut t-Stochastic neighbouring Embedding (t-SNE), named pt-SNE, for high-dimensional data visualization. The main contribution of pt-SNE is two-folded: (1) breaking the computational limitations of t-SNE under the large neighbourhood setting with large perplexity (ppx); (2) simplifying the parameterization setup in t-SNE. Here are the comments.

Comments:

- 1. In line 256, page 10, high sensitivity to ppx is one of the main features of pt-SNE, which may help to reveal the higher level structure in data. However, the high sensitivity of pt-SNE may need extra computational resources and time to find a desired visualization with proper ppx while previous t-SNE methods (e.g. FIt-SNE) are robust to ppx. Also, the chunk&mix protocol introduces extra parameters for parallelization. Therefore, it is unclear whether the tuning process of pt-SNE is indeed simplified compared to other methods, especially when the local structure with small ppx is of interest.
- 2. In line 209, page 9, authors point out that the ppxs in pt-SNE and FIt-SNE are not equivalent due to the chunk&mix protocol. A larger ppx should be applied for pt-SNE to achieve similar visualization as FIt-SNE. However, authors do not provide a way to judge whether two methods are at the same "perplexity level" with different ppxs. Therefore, the fairness of the comparisons between FIt-SNE and pt-SNE in Figure 4 (e) (f) and Figure 6 (e) (f) are suspicious. Because the performances in two methods may not be comparable with the same ppx, and thus the comparisons of accuracy and time may be unfair.
- 3. Authors implement the experimental comparisons (Figures 3, 4, 5, 6) merely between FIt-SNE and pt-SNE. More discussions or experimental comparisons with MultiCore t-SNE (Ulyanov, 2016) and UMAP (McInnes et al., 2018) should be added. Specifically, MultiCore t-SNE is a multicore modification of Barnes-Hut t-SNE, and MultiCore t-SNE should be the most competitive method with pt-SNE in terms of computation. The UMAP is believed to preserve the global structure better than t-SNE, and it would be interesting to see the comparison between the global structures found by UMAP and pt-SNE.
- 4. Typo: Should there have an expectation over i for the second term $KL(p_{i|\cdot}, q_{i|\cdot})$ in the right hand side of equation (1)?

Given these limitations, I would be hesitant to decide that this paper is suitable for the venue.

References

McInnes, L., Healy, J., and Melville, J. (2018). Umap: Uniform manifold approximation and projection for dimension reduction. arXiv preprint arXiv:1802.03426.

Ulyanov, D. (2016). Multicore-tsne. https://github.com/DmitryUlyanov/Multicore-TSNE.