IGSSE 13.05: ExaNIML

An Exascale Library for Numerically Inspired Machine Learning

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Introduction

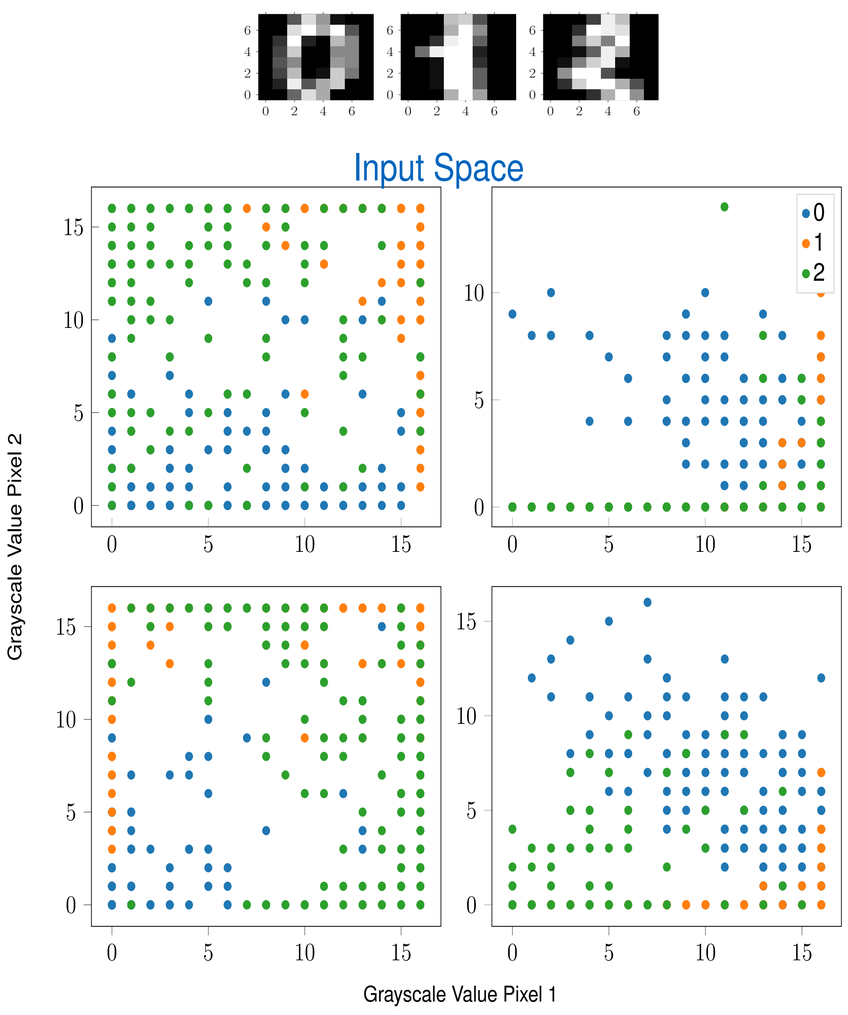
Problem

- Significant gap between machine learning (ML) peers and high-performance computing
- ML is consuming an increasing portion of supercomputer usage $\rightarrow$ we need adequate software!
- In ExaNIML we want to implement ML software that allows transition to exascale systems

Goal

- Classification on full kernel space
  - High-dimensional[1]
  - Expensive
- Classification on lower-dimensional manifold
  - Find lower-dimensional structure
  - Define clusters and surfaces
  - Use sparse grids[2] to define approximations on the manifold

Scientific Computing for Machine Learning



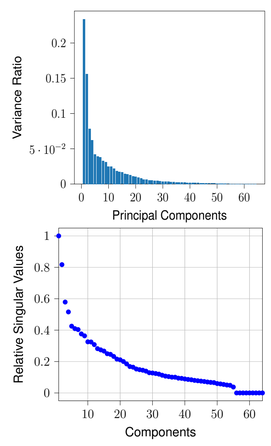
Many more dimensions... (here: 64)

Classification on Input space

Machine Learning

- (Kernel) support vector machine (SVM)
- Kernel density estimation *or* sparse grids density estimation
- Neural network

Goal 1



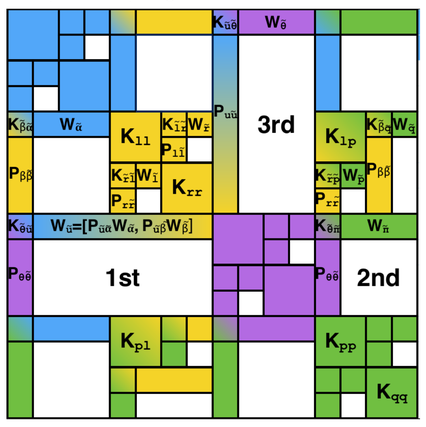
Manifold Learning Algorithms

- (Kernel) principal component Analysis (uses SVD)
- Isomap algorithm
- Hessian local eigenmaps, ...

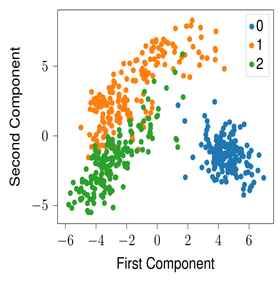
Goal 2

Inhouse code GOFMM[1]

- Hierarchically off-diagonal low-rank
- Speeds up algebraic operations



Hierarchical compression can be used for Goal 1, 2, and 3



Classification on Component Space

- Here forced to 2D manifold (plotting)
- Classification on lower dimensional manifold

$\rightarrow$ Sparse grid classification[3]

Goal 3

Codes

- For manifold algorithms: scikit-learn
- For neural networks: TensorFlow

Conclusion

- Method design
  - Run prominent models from current machine learning peers
  - Combine models with **hierarchical** kernel and **sparse grid** methods
- Library design
  - **Community/reproducibility:** ExaNIML library for others to play

References

[1] C. D. Yu, S. Reiz, and G. Biros, "Distributed-memory hierarchical compression of dense SPD matrices," in *Proceedings of the International Conference for High Performance Computing, Networking, Storage, and Analysis*, SC '18, (Piscataway, NJ, USA), pp. 15:1–15:15, IEEE Press, 2018.

[2] H.-J. Bungartz and M. Griebel, "Sparse grids," *Acta numerica*, vol. 13, pp. 147–269, 2004.

[3] B. Peherstorfer, D. Pflüge, and H.-J. Bungartz, "Density estimation with adaptive sparse grids for large data sets," in *Proceedings of the 2014 SIAM international conference on data mining*, pp. 443–451, SIAM, 2014.