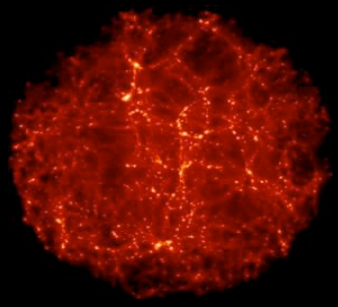
Machine Learning on Massive Datasets



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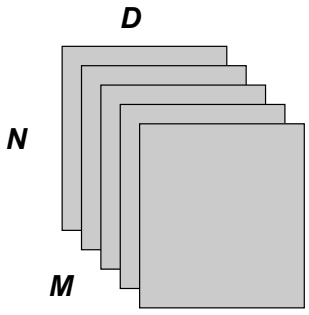
FASTlab: Fundamental Algorithmic and Statistical Tools

The problem: big datasets



Could be large:
N *(#data),* ***D*** *(#features),* ***M*** *(#models)*

What we'd like

Allow users to apply all the state-of-the-art statistical methods…

….with orders-of-magnitude more computational efficiency

Core methods of statistics / machine learning / mining

- **Querying:** nearest-neighbor **O(N),** spherical range-search **O(N),** orthogonal range-search **O(N),** contingency table
- **Density estimation:** kernel density estimation **O(N^2),** mixture of Gaussians **O(N)**
- **Regression:** linear regression **O(D^3),** kernel regression **O(N^2),** Gaussian process regression **O(N^3)**
- **Classification:** nearest-neighbor classifier **O(N^2)**, nonparametric Bayes classifier **O(N^2)**, support vector machine
- **Dimension reduction:** principal component analysis **O(D^3)**, non-negative matrix factorization, kernel PCA **O(N^3)**, maximum variance unfolding **O(N^3)**
- **Outlier detection:** by robust L_2 estimation, by density estimation, by dimension reduction
- **Clustering:** k-means **O(N)**, hierarchical clustering **O(N^3),** by dimension reduction
- **Time series analysis:** Kalman filter **O(D^3),** hidden Markov model, trajectory tracking
- **2-sample testing:** n-point correlation **O(N^n)**
- **Cross-match:** bipartite matching **O(N^3)**

5 main computational bottlenecks:

Aggregations, GNPs, graphical models, linear algebra, optimization

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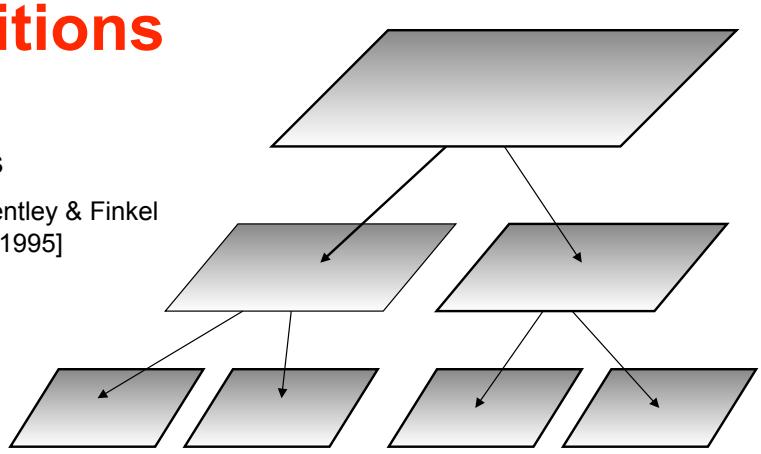
How can we compute these efficiently?

Multi-scale

Decompositions

e.g. kd-trees

[Bentley 1975], [Friedman, Bentley & Finkel 1977],[Moore & Lee 1995]



How can we compute these efficiently?

- **Generalized N-body algorithms (multiple trees) for distance/similarity-based computations** [2000, 2003, 2009]
- **Hierarchical series expansions for kernel summations** [2004, 2006, 2008]
- **Multi-scale Monte Carlo for linear algebra and summations** [2007, 2008]
- **Stochastic process approximations for time series** [2009]
- **Monte Carlo optimization: online, progressive** [2009]
- **Parallel computing** [1998, 2006, 2009]

Computational complexity using fast algorithms

- **Querying:** nearest-neighbor **O(logN),** spherical range-search **O(logN),** orthogonal range-search **O(logN),** contingency table
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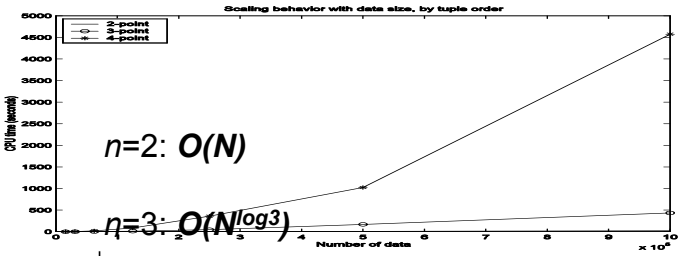
Ex: 3-point correlation runtime

(biggest previous: 20K)

VIRGO simulation data, N = **75,000,000**

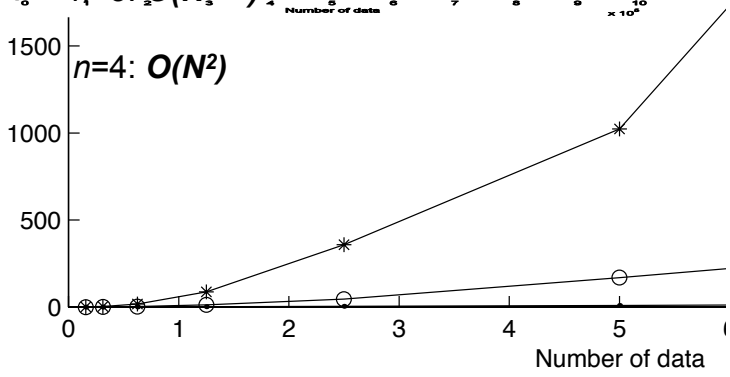
naïve: 5×10^9 sec. (~150 years)

multi-tree: **55 sec.** (exact)



n=2: ***O(N)***

n=3: ***O(N^{log3})***



n=4: ***O(N^2)***

Ex: support vector machine

Data: IJCNN1 [DP01a]
2 classes
49,990 training points
91,701 testing points
22 features

SMO: ***O(N^2-N^3)***

SFW: ***O(N/e + 1/e^2)***

SMO: 12,831 SV's, 84,360 iterations, 98.3% accuracy, 765 sec

SFW: 4,145 SV's, 4,500 iterations, 98.1% accuracy, **21 sec**

Software

- **MLPACK (C++)**
  - First scalable comprehensive ML library
- **MLPACK-db**
  - fast data analytics in relational databases (SQL Server)
- **MLPACK Pro**
  - Very-large-scale data

Issues

- **How to disseminate/integrate?**
- **In-database/centralized or not?**
- **Trust of complex algorithms?**
- **Other statistical/ML needs?**