The improved fast Gauss transform with applications to machine learning

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NIPS 2005 workshop
on
Large scale kernel machines
Whistler, December 9, 2005

Introduction

- Huge data sets containing
  - millions of training examples (*tall data*)
  - with large number of attributes (*fat data*)

  are relatively easy to gather.

- Nonparametric methods in machine leaning scale as either $\mathcal{O}(N^3)$ or $\mathcal{O}(N^2)$.

Supervised Learning

The key computational task is to compute a linear combination of local kernel functions centered on the training data, i.e.,

$$f(x) = \sum_{i=1}^{N} q_i k(x, x_i).$$

- Kernel machines (e.g. RLS, SVM) f is the regression/classification function. [Representer theorem]

- Gaussian processes f is the mean prediction.

- Density estimation f is the kernel density estimate.

Prediction

The computation complexity to predict at M points given N training examples scales as $\mathcal{O}(MN)$.

$$f(x) = \sum_{i=1}^{N} q_i k(x, x_i).$$

Training

Training these models scales as $\mathcal{O}(N^3)$ since most involve solving the linear system of equation

$$(\mathbf{K} + \sigma^2\mathbf{I})\xi = \mathbf{y}.$$

$\mathbf{K}$ is the $N \times N$ Gram matrix where $[\mathbf{K}]_{ij} = k(x_i, x_j)$.

- Direct inversion is $\mathcal{O}(N^3)$.
- Iterative methods like conjugate-gradient can bring it down to $\mathcal{O}(kN^2)$.
- The quadratic complexity is due to the matrix-vector product $\mathbf{K}q$ for some q.

Unsupervised Learning

Methods like kernel principal component analysis, spectral clustering, or Laplacian eigenmaps involve computing the eigen vectors of the Gram/Laplacian matrix.

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Gaussian kernel

The most commonly used kernel function is the *Gaussian kernel*

$$K(x, y) = e^{-\|x-y\|^2/h^2},$$

where h is called the *bandwidth* of the kernel.

Sum of multivariate Gaussian kernels is called the discrete Gauss transform – $\mathcal{O}(MN)$.

$$G(y_j) = \sum_{i=1}^{N} q_i e^{-\|y_j-x_i\|^2/h^2}.$$

Improved fast Gauss transform

Speed up of these tasks using rigorous ϵ-exact approximation algorithms to achieve

- $\mathcal{O}(N)$ training time.
- $\mathcal{O}(1)$ prediction/classification time.

One such algorithm was presented for the **Gaussian kernel** in NIPS2005*- the improved fast Gauss transform (IFGT).

*C. Yang, R. Duraiswami, and L. Davis. Efficient kernel machines using the improved fast Gauss transform. In Advances in Neural Information Processing Systems, pages 15611568, 2005.

ϵ can be arbitrarily small (e.g., machine precision) and speedup is maintained

Effectively we have an FFT like algorithm that is "drop-in," with no accuracy penalty.

Enables large scale kernel machines

Brief idea of the IFGT

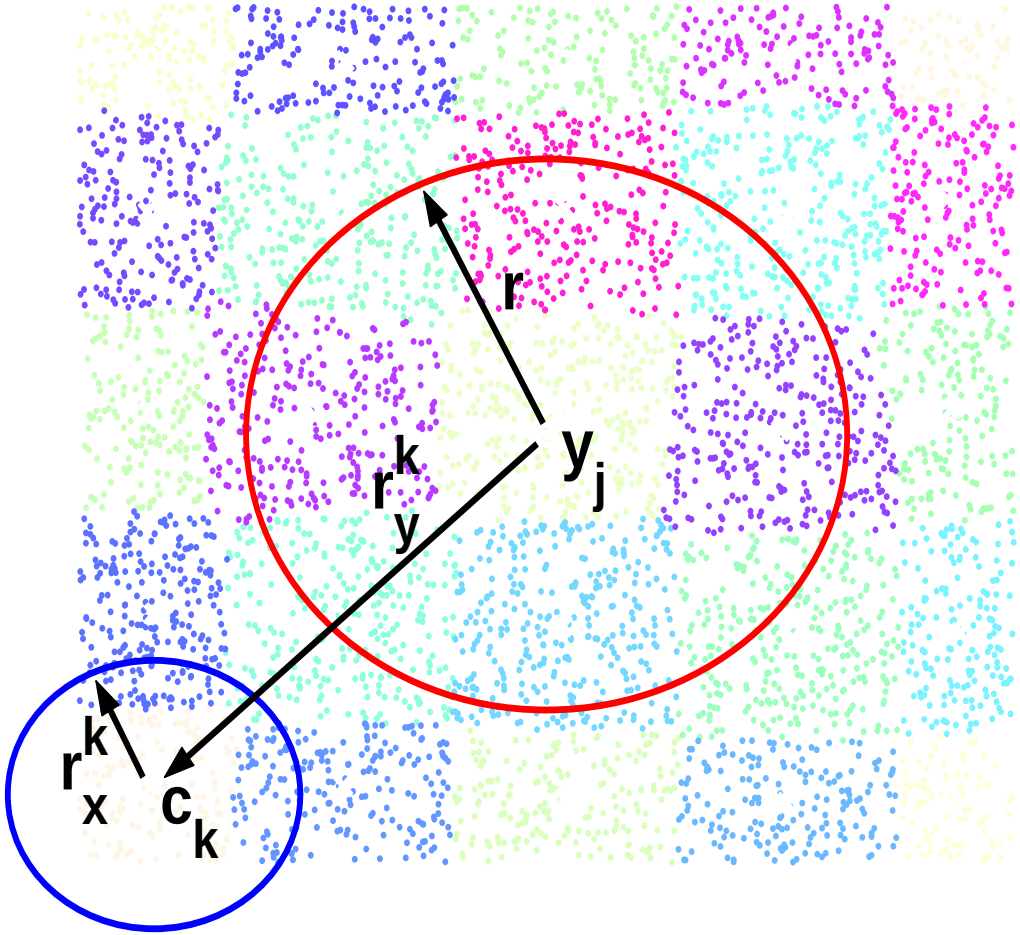
- **Step 1a** Determine parameters of algorithm based on specified error bound, kernel bandwidth, and data distribution

- **Step 1b** Subdivide the d-dimensional space using a k-center clustering based geometric data structure ($\mathcal{O}(N \log K)$).

- **Step 2** Build a p truncated representation of kernels inside each cluster using a set of decaying basis functions ($\mathcal{O}(Nd^p)$).

- **Step 3** Collect the influence of all the the data in a neighborhood using coefficients at cluster center and evaluate ($\mathcal{O}(Md^p)$).

The code was publicly made available for non-commercial use.



IFGT Illustration

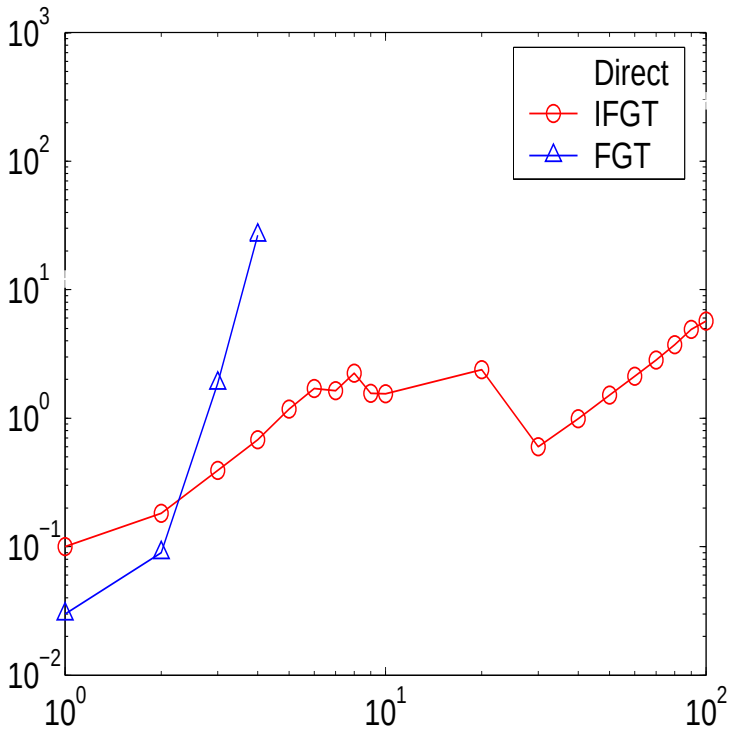
Sample results

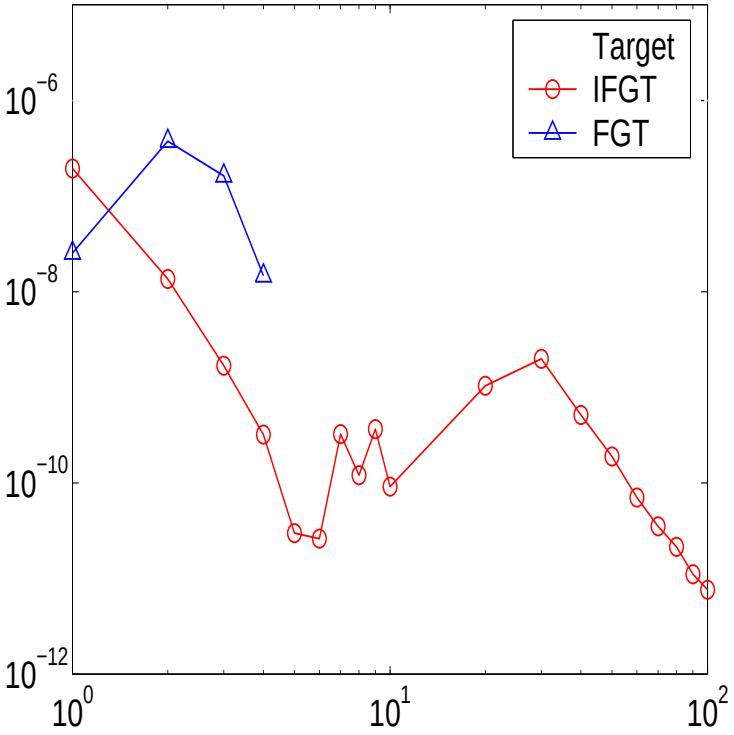
For example in three dimensions and 1 million training and test points [h=0.4]

- IFGT – 6 minutes.
- Direct – 34 hours.

with an error of 10^{-8}.

IFGT can handle large dimensions [$h = \sqrt{d}$]





Segmentation using adaptive mean-shift

1.34 hours vs 2.1 minutes

Gaussian process regression-Training times

- Abalone [4177 x 7] 7.41 secs
- comp-activ [8192 x 22] 5.92 secs
- pumadyn [8192 x 32] 6.01 secs
- census-house [11784 x 16] 109.81 secs

Issues with IFGT presented in Yang et.al. 2005

- The error bounds were tight but very pessimistic.
- Parameter selection was not automatic.
- Users*† found the selection of parameters hard. Incorrect choice of algorithm parameters by these authors sometimes lead to poor reported performance of IFGT.
- Method for IFGT parameter selection presented in Lang et.al. is not optimal‡.

*Lee, D., Gray, A., & Moore, A., Dual-tree fast Gauss transforms, NIPS 2006

†de Freitas, N., Wang, Y., Mahdaviani, M., and Lang, D., Fast Kylov Methods for N-body learning, NIPS 2006.

‡Lang, D., Klaas, M., and Freitas, N. 2005. Empirical testing of fast kernel density estimation algorithms. Tech. Rep. UBC TR-2005-03.

Improvements to IFGT since NIPS 2005*

- A tighter point-wise error bound.
- Choice of the algorithm parameters completely automatic.
- Truncation number for each source is different.

*V. C. Raykar, C. Yang, R. Duraiswami, and N. Gumerov, Fast computation of sums of Gaussians in high dimensions. CS-TR-4767, Department of Computer Science, University of Maryland, CollegePark, 2005. https://drum.umd.edu/dspace/bitstream/1903/3020/1/CS-TR-4767.pdf

Choice of parameters is crucial

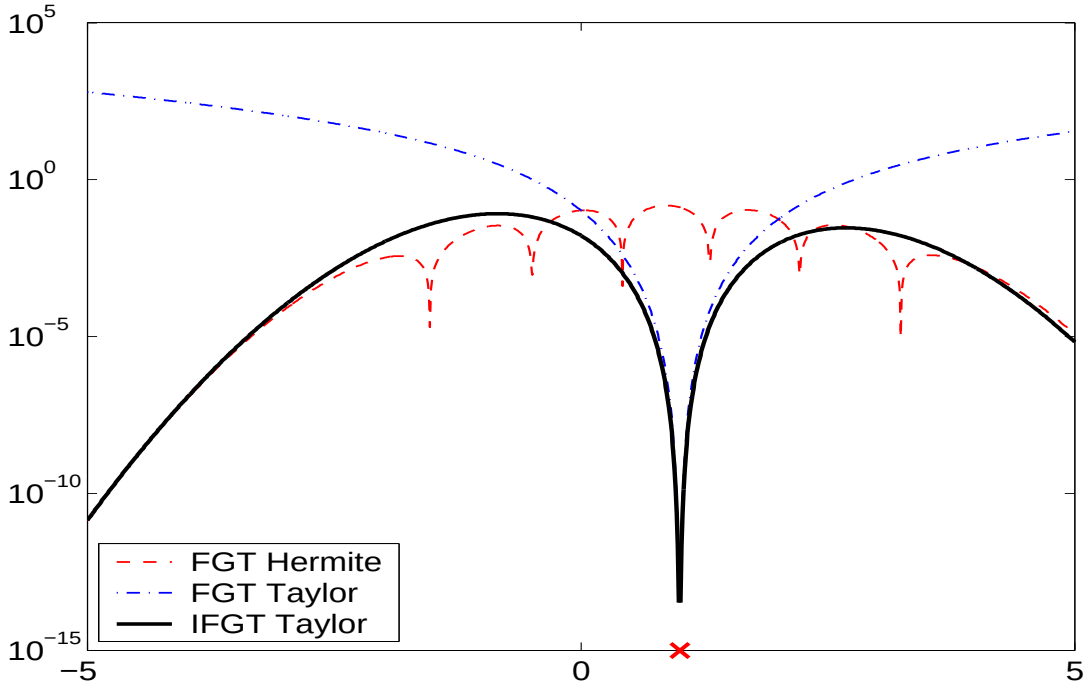
For 3 dimensions using $N = 50,000$ and $h = 0.76$

- Lee et.al.* report that IFGT takes greater than two times the direct time.

- With the parameters automatically chosen by the algorithm we take only 1.522 secs.

*Lee, D., Gray, A., & Moore, A.,Dual-tree fast Gauss transforms, NIPS 2006

IFGT expansion is both local as well as far-field!!



Hence we avoid the expensive translation operation that was required in the original FGT, and in some recently proposed algorithms.

Effect of bandwidth

- For small kernel bandwidth (h) where each training point only influences the immediate vicinity speedup is poor.

- Can use dual-tree methods*.

- In high dimensions the tails of the density contribute significantly to the total probability mass and is unlikely we have a dense sampling in tails.

*A. G. Gray and A. W. Moore. Nonparametric density estimation: Toward computational tractability. In SIAM International conference on Data Mining, 2003.

Some recent extensions

IFGT with variable source scales

$$G(y_j) = \sum_{i=1}^{N} q_i e^{-\|y_j - x_i\|^2 / h_i^2}.$$

Approach: Build a composite factorization that builds a Taylor series for h_i as well.

Resulting IFGT runs at about the same speed.

For example for N = M = 1,024,000 while the direct evaluation takes around 2.6 days the fast evaluation requires only 4.65 minutes with an error of around 10^{-5}.

Variable bandwidth density estimation

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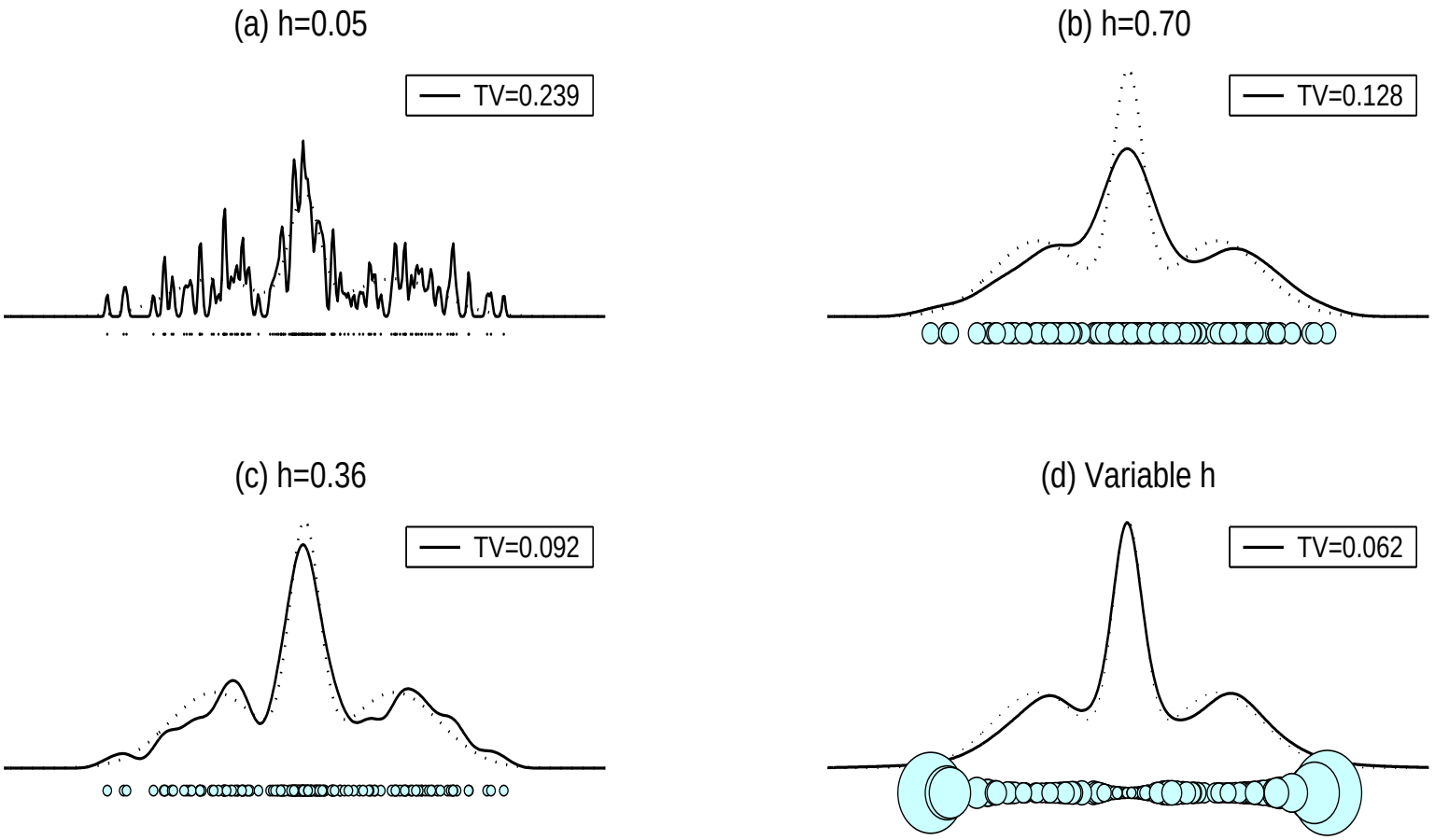
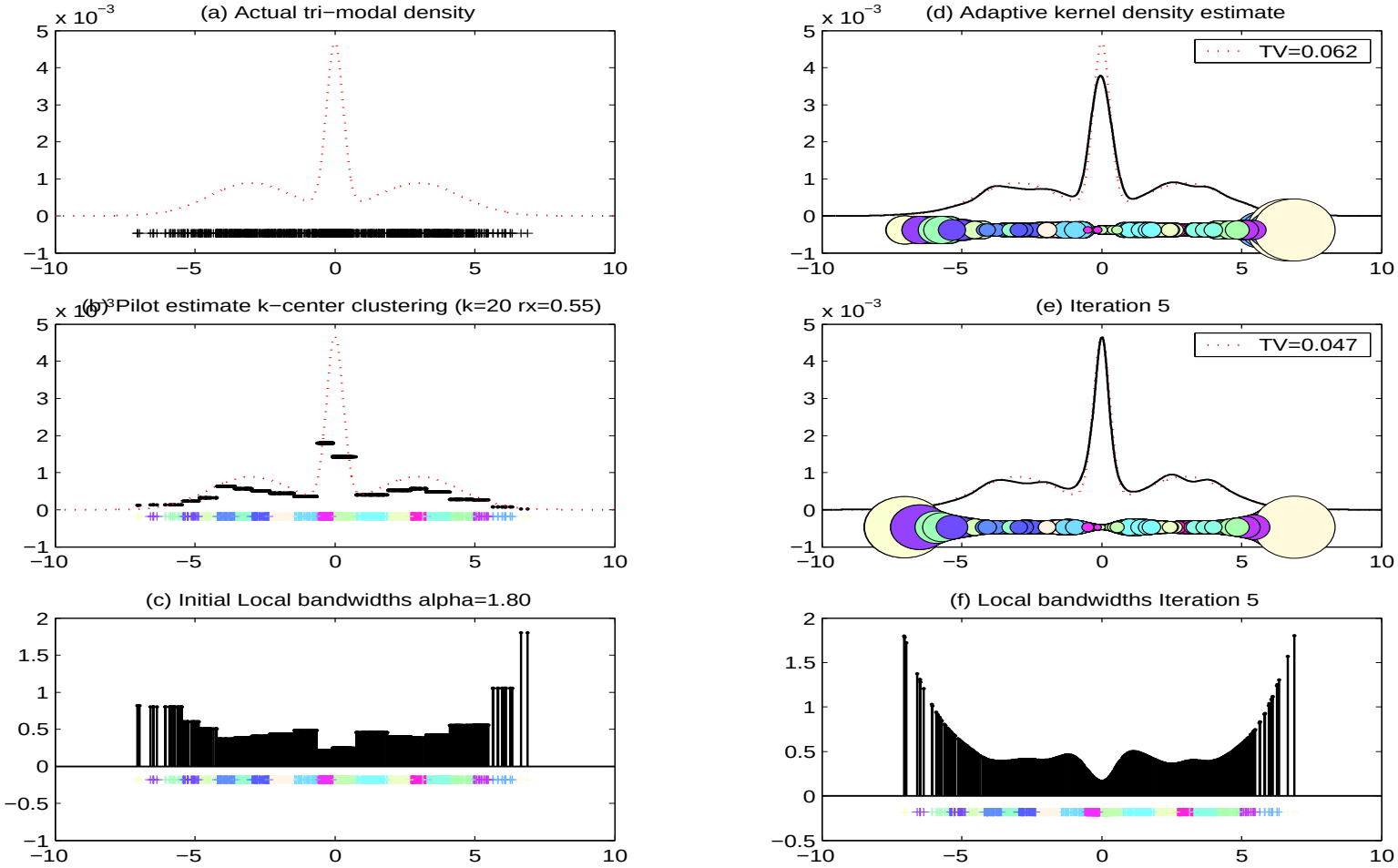


Data-structures imposed in the IFGT algorithm itself provide an easy way to locally adapt the bandwidth.



Derivative of kernel sums Many procedures (e.g., those involving optimal parameter estimation) involve taking the derivative of kernel sums.

- Automatic bandwidth selection for kernel density estimation.
- Selecting hyperparameters in Gaussian Process regression.

The derivatives of Gaussian sums involve sums of products of polynomials and Gaussians. IFGT algorithms have been developed for such kernels

$$G_r(y_j) = \sum_{i=1}^{N} q_i H_r\left(\frac{y_j - x_i}{h_1}\right) e^{-(y_j - x_i)^2/h_2^2}$$

Gaussian process regression

- Gaussian processes handle nonparametric regression in a Bayesian framework.

- The regression function is represented by an ensemble of functions, on which we place a Gaussian prior.

- This prior is updated in the light of the training data.

- As a result we obtain predictions together with valid estimates of uncertainty.

Speedup GP regression via IFGT

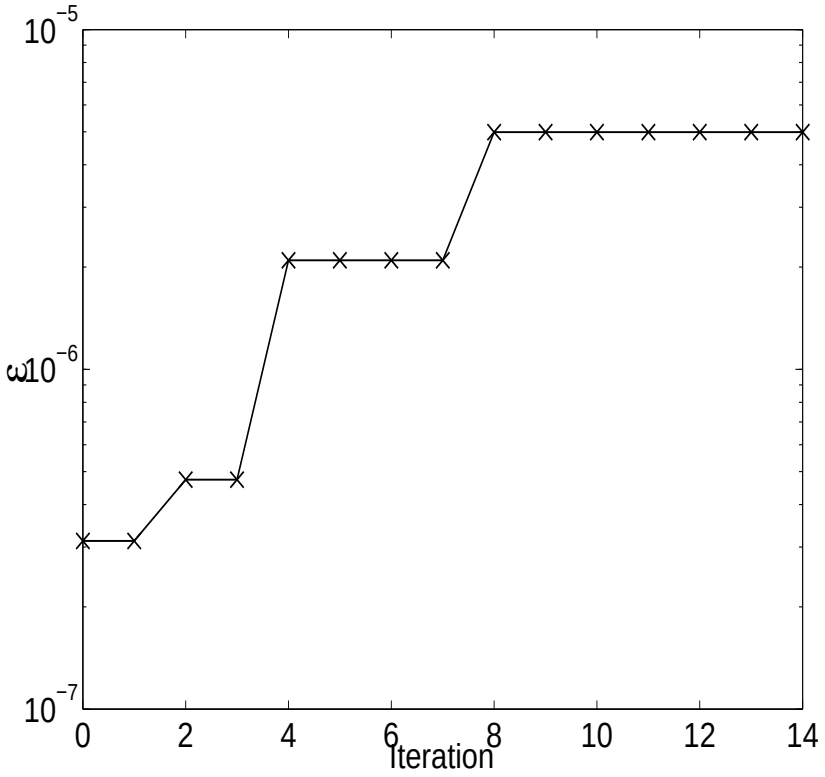
$\widetilde{\mathbf{K}} = \mathbf{K} + \sigma^2\mathbf{I}$	*Direct Inversion*		*Conjugate gradient*		*Conjugate gradient +IFGT*	
	Time	Space	Time	Space	Time	Space
Training phase $\xi = \widetilde{\mathbf{K}}^{-1}\mathbf{y}$	$\mathcal{O}(N^3)$	$\mathcal{O}(N^2)$	$\mathcal{O}(N^2)$	$\mathcal{O}(N)$	$\mathcal{O}(N)$	$\mathcal{O}(N)$
Mean prediction $y = \mathbf{k}(x)^T\xi$	$\mathcal{O}(N^2)$	$\mathcal{O}(N)$	$\mathcal{O}(N^2)$	$\mathcal{O}(N)$	$\mathcal{O}(N)$	$\mathcal{O}(N)$
Uncertainty $\mathbf{k}(x,x)$ $-\mathbf{k}(x)^T\widetilde{\mathbf{K}}^{-1}\mathbf{k}(x)$	$\mathcal{O}(N^3)$	$\mathcal{O}(N)$	$\mathcal{O}(N^3)$	$\mathcal{O}(N)$	$\mathcal{O}(N^2)$	$\mathcal{O}(N)$

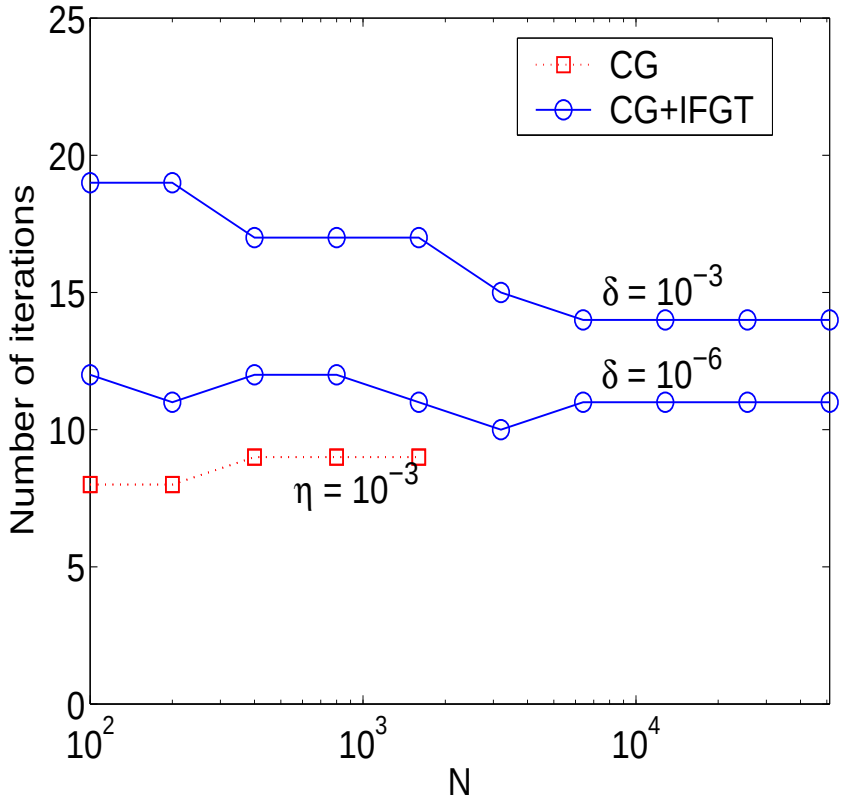
For example for N=25,600 training takes around 3 secs. (compare to 10 hours[direct] or 17 minutes[CG]).

The hyperparametrs can also be chosen in $\mathcal{O}(N)$.

How to choose ϵ

Matrix-vector product may be performed in an increasingly inexact manner as the iteration progresses and still allow convergence to the solution.





Conclusions

- The IFGT can reduce the computational complexity of numerous machine learning algorithms to linear time.
- Unlike methods which rely on choosing a subset of the dataset we use all the available points and still achieve $\mathcal{O}(N)$ complexity.
- The IFGT is now completely tweak free.
- Extensions to variable bandwidth, derivative estimation, and Gaussian processes.
- Good speedup for large bandwidths. For small bandwidths dual-tree methods can be used.