Automatic online tuning for fast Gaussian summation

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Problem

$$G(\mathbf{y}_j) = \sum_{i=1}^{N} q_i \exp\left(-\frac{||\mathbf{x}_i - \mathbf{y}_j||^2}{h^2}\right), \quad j = 1, \ldots, M$$

- Direct computation is quadratic, O(MN)
- Slows down kernel machines
- Algorithms such as FGT [1] and IFGT [2] obtain speedup by approximating to specified error ε, but do not perform well across all bandwidths *h*, point distributions, and error ε and need tuning

Our solution

- Uses the IFGT and a tree data structure
- Four methods, each optimal in different situations
- **Black box approach:** Automatically predicts fastest method and tunes its parameters for the given dataset
- Compares favorably to Dual-Tree methods [3]

Improved Fast Gauss Transform

- Reduces cost of Gauss Transform to O(*N*+*M*) [2]
- Uses truncated Taylor expansion of exponential term

$$e^{-\|y_j - x_i\|^2/h^2} = e^{-\|x_i - x_*\|^2/h^2} e^{-\|y_j - x_*\|^2/h^2} \left[\sum_{|\alpha| \le p-1} \frac{2^\alpha}{\alpha!} \left(\frac{y_j - x_*}{h}\right)^\alpha \left(\frac{x_i - x_*}{h}\right)^\alpha\right] + \Delta_{ij}$$

- The error of truncating series starting at p^{th} term is bounded by

$$\Delta_{ij} \le \frac{2^p}{p!} \left(\frac{||x_i - x_*||}{h}\right)^p \left(\frac{||y_j - x_*||}{h}\right)^p e^{-(||x_i - x_*|| - ||y_j - x_*||)^2/h^2}$$

- Truncation number is chosen for each source point by assuming worst possible placement of a target point and choosing p s.t.

  $\Delta_{ij} \le \epsilon$ which guarantees that $|\hat{g}(y_j) - g(y_j)|/Q \le \epsilon$

  where Q is the sum of all q_i

Summary of approach:

1) Choose number of centers *K* and max truncation p_{max}
2) Cluster source points using *K*-center algorithm
3) Pre-compute contributions from sources

$$C_\alpha^k = \frac{2^\alpha}{\alpha!} \sum_{x_i \in S_k} q_i e^{-\frac{||x_i - c_k||^2}{h^2}} \left(\frac{x_i - c_k}{h}\right)^\alpha \mathbf{1}_{|\alpha| \le p_i - 1}$$

4) For each target y_j evaluate by collecting contributions from clusters within cut-off radius

$$\hat{g}(y_j) = \sum_{||y_i - c_k|| \le r_k^y} \sum_{|\alpha| \le p_{\max}-1} C_\alpha^k e^{-\frac{||y_j - c_k||^2}{h^2}} \left(\frac{y_j - c_k}{h}\right)^\alpha$$

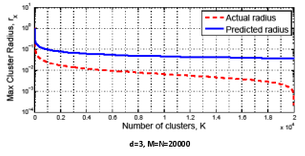
Problems:

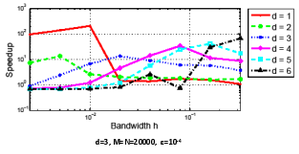
- Parameters are optimized for uniform distributions
- IFGT performs poorly for low bandwidths where kernels are local

Automatic IFGT parameter tuning

Choosing number of clusters without assuming a uniform distribution

- Instead of estimating cluster radius as $k^{-1/d}$, use incremental clustering to evaluate actual cluster radius, thus choosing optimal K based on *actual* distribution





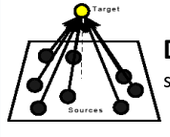
Choosing cluster-wise truncation numbers

- Allow some points to have higher error as long as other points in the same cluster have low enough error to compensate
- Ensure that for each cluster S_k

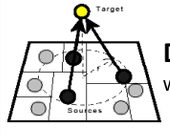
$$\sum_{x_i \in S_k} |q_i| \Delta_{ij} \le \sum_{x_i \in S_k} |q_i| \epsilon = Q_k \epsilon$$

Tree data structure

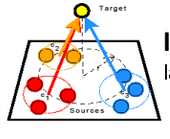
- Using a tree data structure, we can compute Gauss Transform efficiently across bandwidths
- Must choose one of four evaluation methods



Direct: evaluate equation directly; works well for small N and M, and does not have high overhead cost



Direct+Tree: build tree directly on sources; works well for small bandwidths



IFGT: works well for large N and M, and medium to large bandwidths

IFGT+Tree: build tree on cluster centers, works well for case where number of clusters K is large

Comparison of methods

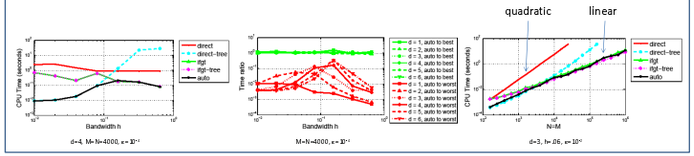
$Cost_{\text{direct}}(d, N, M)$	$O(dMN)$
$Cost_{\text{direct+tree}}(d, N, M, n_s)$	$O(d(N + Mn_s)\log N)$
$Cost_{\text{ifgt}}(d, N, M, K, n_c, p_{\max})$	$O(dN \log K + (N + Mn_c)r_{(p_{\max}-1)d} + dMK)$
$Cost_{\text{ifgt+tree}}(d, N, M, K, n_c, p_{\max})$	$O((N + Mn_c)(d \log K + r_{(p_{\max}-1)d}))$

Automatic method selection

- n_s and n_c are the average number of sources and cluster centers, respectively, that are within the cut-off radius of a query target
- n_s and n_c can be approximated from sub-sampled dataset
- Given *d, N, M, K,* n_c, and n_s, we can estimate cost of each method

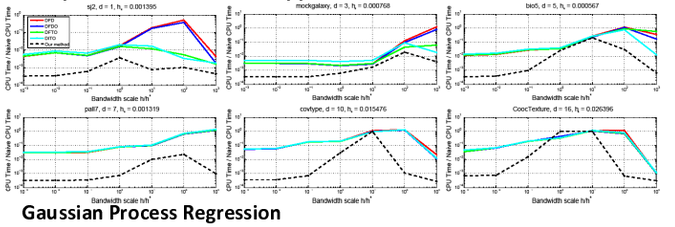
Summary of method selection approach:

1) Estimate n_s
2) Calculate $\text{Cost}_{\text{direct}}(d,N,M)$ and $\text{Cost}_{\text{direct+tree}}(d,N,M,n_s)$
3) Estimate highest K_{limit} for which *ifgt* and *ifgt+tree* could be faster
4) If $K_{limit} > 0$
   a) Compute IFGT parameters K and p_{max}
   b) Estimate n_c ; estimate $\text{Cost}_{\text{ifgt}}$ and $\text{Cost}_{\text{ifgt+tree}}$
5) Return arg $\min_i \text{Cost}_i$



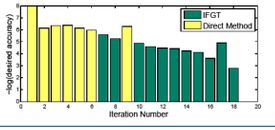
Results

Comparison with Dual-Tree approach



Gaussian Process Regression

	Robotarm	Abalone	Housing	Elevator
Dims	2	7	12	18
Size	1000	4177	506	8752
direct	0.578s	**16.1s**	**0.313s**	132s
ifgt	**0.0781s**	52.3s	1317s	133s
direct-tree	5.45s	328s	2.27s	**0.516s**
ifgt-tree	**0.0781s**	35.2s	549s	101s
auto	**0.0938s**	**14.5s**	**0.547s**	**0.797s**



References

[1] L. Greengard and J. Strain. The fast Gauss transform. SIAM J. Sci. Stat. Comput., 1991

[2] V. Raykar, C. Yang, R. Duraiswami, and N. Gumerov. Fast computation of sums of Gaussians in high dimensions. UMD-CS-TR-4767, 2005

[3] D. Lee and A. G. Gray. Faster Gaussian summation: Theory and experiment. In UAI, 2006

Open source C/C++ and MATLAB bindings

http://sourceforge.net/projects/figtree