Improved Fast Gauss Transform

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Fast Gauss Transform (FGT)

- Originally proposed by Greengard and Strain (1991) to efficiently evaluate the weighted sum of Gaussians:

\[ G(y_j) = \sum_{i=1}^{N} q_i e^{-\|y_j - x_i\|^2/h^2}, \quad j = 1, \ldots, M. \]

- FGT is an important variant of Fast Multipole Method (Greengard & Rolklin 1987, Greengard and Strain 1990).

- FGT similar to fast Fourier transform:
  - FFT is for the data on regular grid; FGT is for data on arbitrary position
  - FFT is arithmetic based; FGT is approximate analysis based

- Widely used in mathematical physics, computational chemistry, mechanics.
  - Recently applied in our group to RBF interpolation, acoustic scattering, EM scattering, non uniform FFT and computer vision.
Fast Gauss Transform (cont’d)

- The weighted sum of Gaussians

\[ G(y_j) = \sum_{i=1}^{N} q_i e^{-\|y_j-x_i\|^2/h^2}, \quad j = 1, \ldots, M. \]

is equivalent to the matrix-vector product:

\[
\begin{bmatrix}
G(y_1) \\
G(y_2) \\
\vdots \\
G(y_M)
\end{bmatrix} =
\begin{bmatrix}
e^{-\|x_1-y_1\|^2/h^2} & e^{-\|x_2-y_1\|^2/h^2} & \cdots & e^{-\|x_N-y_1\|^2/h^2} \\
e^{-\|x_1-y_2\|^2/h^2} & e^{-\|x_2-y_2\|^2/h^2} & \cdots & e^{-\|x_N-y_2\|^2/h^2} \\
\vdots & \vdots & \ddots & \vdots \\
e^{-\|x_1-y_M\|^2/h^2} & e^{-\|x_2-y_M\|^2/h^2} & \cdots & e^{-\|x_N-y_M\|^2/h^2}
\end{bmatrix}
\begin{bmatrix}
q_1 \\
q_2 \\
\vdots \\
q_N
\end{bmatrix}
\]

- Direct evaluation of the sum of Gaussians requires \(O(N^2)\) operations.
- Fast Gauss transform reduces the cost to \(O(N \log N)\) operations.
Fast Gauss Transform (cont’d)

- Three key components of the FGT:
  - The factorization or separation of variables
  - Space subdivision scheme
  - Error bound analysis
Factorization of Gaussian

- Factorization is one of the key parts of the FGT.
- Factorization breaks the entanglements between the sources and targets.
- The contributions of the sources are accumulated at the centers, then distributed to each target.
The Gaussian kernel is factorized into Hermite functions

\[
e^{-\frac{\|y-x_i\|^2}{h^2}} = \sum_{n=0}^{p-1} \frac{1}{n!} \left( \frac{x_i - x_\star}{h} \right)^n h_n \left( \frac{y - x_\star}{h} \right) + \epsilon(p),
\]

where Hermite function \( h_n(x) \) is defined by

\[
h_n(x) = (-1)^n \frac{d^n}{dx^n} \left( e^{-x^2} \right).
\]

Exchange the order of the summations

\[
G_{j,i} \equiv \sum_{i=1}^{N} q_i \sum_{n=0}^{p-1} \frac{1}{n!} \left( \frac{x_i - x_\star}{h} \right)^n h_n \left( \frac{y_j - x_\star}{h} \right) + \epsilon(p)
\]

a.k.a. Moment, \( A_n \)
The FGT Algorithm

- **Step 0**: Subdivide the space into uniform boxes.
- **Step 1**: Assign sources and targets into boxes.
- **Step 2**: For each pair of source and target boxes, compute the interactions using one of the four possible ways:
  - $N_B \leq N_F, M_C \leq M_L$: Direct evaluation
  - $N_B \leq N_F, M_C > M_L$: Taylor expansion
  - $N_B > N_F, M_C \leq M_L$: Hermite expansion
  - $N_B > N_F, M_C > M_L$: Hermite expansion --> Taylor expansion
- **Step 3**: Loop through boxes evaluating Taylor series for boxes with more than $M_L$ targets.

$N_B$: # of sources in Box B  
$M_C$: # of targets in Box C  
$N_F$: cutoff of Box B  
$M_L$: cutoff of Box C
The higher dimensional Hermite expansion is the Kronecker product of \( d \) univariate Hermite expansions. Total number of terms is \( \Theta(p^d) \), \( p \) is the number of truncation terms. The number of operations in one factorization is \( \Theta(p^d) \).
Too Many Boxes in Higher Dimensions

- The FGT subdivides the space into uniform boxes and assigns the source points and target points into boxes.
- For each box the FGT maintain a neighbor list.
- The number of the boxes increases exponentially with the dimensionality.
The FGT was originally designed to solve the problems in mathematical physics (heat equation, vortex methods, etc), where the dimension is up to 3.

The higher dimensional Hermite expansion is the product of univariate Hermite expansion along each dimension. Total number of terms is $O(p^d)$.

The space subdivision scheme in the original FGT is uniform boxes. The number of boxes grows exponentially with dimension. Most boxes are empty.

The exponential dependence on the dimension makes the FGT extremely inefficient in higher dimensions.
The Decay of Gaussian Functions

- The decay of the Gaussian kernel function is very fast.
- The effect of Gaussian kernel outside of certain range can be safely ignored.
- The time consuming translation operators in original FGT can be safely removed.

<table>
<thead>
<tr>
<th>$r_x/h$</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f(r_x/h)$</td>
<td>1</td>
<td>0.367879</td>
<td>0.018316</td>
<td>0.000123</td>
<td>1.13E-07</td>
<td>1.39E-11</td>
<td>2.32E-16</td>
<td>5.24E-22</td>
<td>1.6E-28</td>
<td>6.64E-36</td>
<td>3.72E-44</td>
</tr>
</tbody>
</table>
Improved Fast Gauss Transform

- Multivariate Taylor expansion
- Multivariate Horner’s Rule
- Space subdivision based on $k$-center algorithm
- Error bound analysis
The Taylor expansion of the Gaussian function:

\[ e^{-\|y_j-x_i\|^2/h^2} = e^{-\|y_j-x_*\|^2/h^2} e^{-\|x_i-x_*\|^2/h^2} e^{2(y_j-x_*) \cdot (x_i-x_*)/h^2}, \]

The first two terms can be computed independently.

The Taylor expansion of the last term is:

\[ e^{2(y_j-x_*) \cdot (x_i-x_*)/h^2} = \sum_{\alpha \geq 0} \frac{2^{|\alpha|}}{\alpha!} \left( \frac{x_i - x_*}{h} \right)^\alpha \left( \frac{y_j - x_*}{h} \right)^\alpha. \]

where \( \alpha = (\alpha_1, \ldots, \alpha_d) \) is multi-index.

The multivariate Taylor expansion about center \( x_* \):

\[ G(y_j) = \sum_{\alpha \geq 0} C_\alpha e^{-\|y_j-x_*\|^2/h^2} \left( \frac{y_j - x_*}{h} \right)^\alpha, \]

where coefficients \( C_\alpha \) are given by

\[ C_\alpha = \frac{2^{|\alpha|}}{\alpha!} \sum_{i=1}^{N} q_i e^{-\|x_i-x_*\|^2/h^2} \left( \frac{x_i - x_*}{h} \right)^\alpha. \]
Reduction from Taylor Expansions

- The idea of Taylor expansion of Gaussian kernel is first introduced in the course CMSC878R by Ramani and Nail.
- The number of terms in multivariate Hermite expansion is $O(p^d)$.
- The number of terms in multivariate Taylor expansion is $\binom{p+d-1}{d}$, asymptotically $O(d^p)$, a big reduction for large $d$. 

![Graphs showing the number of terms in Hermite and Taylor expansions for varying dimensions and truncation orders.](image)
Improved Fast Gauss Transform

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Monomial Orders

Let \( \alpha = (\alpha_1, \ldots, \alpha_n) \), \( \beta = (\beta_1, \ldots, \beta_n) \), then three standard monomial orders:

- **Lexicographic order**, or “dictionary” order:
  \( \alpha \prec_{\text{lex}} \beta \iff \) the leftmost nonzero entry in \( \alpha - \beta \) is negative.

- **Graded lexicographic order** (Veronese map, a.k.a, polynomial embedding):
  \( \alpha \prec_{\text{grlex}} \beta \iff \sum_{1 \leq i \leq n} \alpha_i < \sum_{1 \leq i \leq n} \beta_i \) or \( \sum_{1 \leq i \leq n} \alpha_i = \sum_{1 \leq i \leq n} \beta_i \) and \( \alpha \prec_{\text{lex}} \beta \).

- **Graded reverse lexicographic order**.
  \( \alpha \prec_{\text{grevlex}} \beta \iff \sum_{1 \leq i \leq n} \alpha_i < \sum_{1 \leq i \leq n} \beta_i \) or \( \sum_{1 \leq i \leq n} \alpha_i = \sum_{1 \leq i \leq n} \beta_i \) and the rightmost nonzero entry in \( \alpha - \beta \) is positive.

**Example**:
- Let \( f(x,y,z) = xy^5z^2 + x^2y^3z^3 + x^3 \), then
- w.r.t. **lex** \( f \) is: \( f(x,y,z) = x^3 + x^2y^3z^3 + xy^5z^2 \);
- w.r.t. **grlex** \( f \) is: \( f(x,y,z) = x^2y^3z^3 + xy^5z^2 + x^3 \);
- w.r.t. **grevlex** \( f \) is: \( f(x,y,z) = xy^5z^2 + x^2y^3z^3 + x^3 \).
The Horner’s Rule

- The Horner’s rule (W.G.Horner 1819) is to *recursively* evaluate the polynomial \( p(x) = a_n x^n + \cdots + a_1 x + a_0 \) as:
  \[ p(x) = (((\cdots(a_n x + a_{n-1})x+\cdots)x + a_0. \]
  It costs \( n \) multiplications and \( n \) additions, no extra storage.

- We evaluate the multivariate polynomial *iteratively* using the graded lexicographic order. It costs \( n \) multiplications and \( n \) additions, and \( n \) storage.

![Figure 1: Efficient expansion of the multivariate polynomials. The arrows point to the leading terms.](image)
Suppose $x = (x_1, x_2, x_3)$ and $y = (y_1, y_2, y_3)$, then

$$e^{x \cdot y} \approx \sum_{\alpha \geq 0} x^\alpha y^\alpha$$

**Constant**
- 19 ops
- Direct: 29 ops

**Direct:**
- 29 ops

**$x_1$**
- 19 ops
- Direct: 29 ops

**$y_1$**
- 19 ops
- Direct: 29 ops

**$x_2$**
- 19 ops
- Direct: 29 ops

**$y_2$**
- 19 ops
- Direct: 29 ops

**$x_3$**
- 19 ops
- Direct: 29 ops

**$y_3$**
- 19 ops
- Direct: 29 ops

**$x_1^2$**
- 19 ops
- Direct: 29 ops

**$y_1^2$**
- 19 ops
- Direct: 29 ops

**$x_1 x_2$**
- 19 ops
- Direct: 29 ops

**$y_1 y_2$**
- 19 ops
- Direct: 29 ops

**$x_1 x_3$**
- 19 ops
- Direct: 29 ops

**$y_1 y_3$**
- 19 ops
- Direct: 29 ops

**$x_2^2$**
- 19 ops
- Direct: 29 ops

**$y_2^2$**
- 19 ops
- Direct: 29 ops

**$x_2 x_3$**
- 19 ops
- Direct: 29 ops

**$y_2 y_3$**
- 19 ops
- Direct: 29 ops

**$x_1^2 x_2$**
- 19 ops
- Direct: 29 ops

**$y_1^2 y_2$**
- 19 ops
- Direct: 29 ops

**$x_1^2 x_3$**
- 19 ops
- Direct: 29 ops

**$y_1^2 y_3$**
- 19 ops
- Direct: 29 ops

**$x_1 x_2 x_3$**
- 19 ops
- Direct: 29 ops

**$y_1 y_2 y_3$**
- 19 ops
- Direct: 29 ops

**$x_1 x_2^2$**
- 19 ops
- Direct: 29 ops

**$y_1 y_2^2$**
- 19 ops
- Direct: 29 ops

**$x_1 x_3^2$**
- 19 ops
- Direct: 29 ops

**$y_1 y_3^2$**
- 19 ops
- Direct: 29 ops

**$x_2 x_3^2$**
- 19 ops
- Direct: 29 ops

**$y_2 y_3^2$**
- 19 ops
- Direct: 29 ops

**$x_3^2$**
- 19 ops
- Direct: 29 ops

**$y_3^2$**
- 19 ops
- Direct: 29 ops

**$x_3^3$**
- 19 ops
- Direct: 29 ops

**$y_3^3$**
- 19 ops
- Direct: 29 ops
An Example of Taylor Expansion (Cont’d)

\[ \sum_{i} q_i e^{-\|x_i - y\|^2} \sum_{i} q_i e^{-\|x_i\|^2} e^{-\|y\|^2} \sum_{\alpha \geq 0} \alpha! x_\alpha y^\alpha \]

\[ e^{-\|y\|^2} \sum_{\alpha \geq 0} \alpha! y^\alpha \sum_{i} q_i e^{-\|x_i\|^2} x_\alpha^i \]

\[ e^{-\|y\|^2} \sum_{\alpha \geq 0} \alpha! y^\alpha \sum_{i} q_i e^{-\|x_i\|^2} x_\alpha^i \approx \]

\[ \begin{array}{cccccc}
1 & 2 & 2 & 2 & \approx & 4/3
2 & 4 & 4 & 2 & 4 & 2
4/3 & 4 & 4 & 4 & 8 & 4
\end{array} \]

\[ 21N \text{ ops} \quad \text{Direct: 31Nops} \]

\[ N \sum_{i} q_i e^{-\|x_i\|^2} e^{-\|y\|^2} \]

\[ \begin{array}{cccccc}
1 & x_1 & x_2 & x_3 & \times & \times
x_1^2 & x_1 x_2 & x_1 x_3 & x_2^2 & x_2 x_3 & x_3^2
x_1^3 & x_1^2 x_2 & x_1^2 x_3 & x_1 x_2^2 & x_1 x_2 x_3 & x_1 x_3^2
\end{array} \]

\[ 20 \text{ ops} \quad \text{Direct: 30ops} \]

\[ e^{-\|y\|^2} \sum_{\alpha \geq 0} \alpha! y^\alpha \sum_{\alpha \geq 0} \alpha! y^\alpha \]

\[ \begin{array}{cccccc}
1 & y_1 & y_2 & y_3 & \times & \times
y_1^2 & y_1 y_2 & y_1 y_3 & y_2^2 & y_2 y_3 & y_3^2
y_1^3 & y_1^2 y_2 & y_1^2 y_3 & y_1 y_2^2 & y_1 y_2 y_3 & y_1 y_3^2
\end{array} \]

\[ \text{Constant 19 ops} \quad \text{Direct: 29ops} \]
Improved Fast Gauss Transform

- Multivariate Taylor expansion
- Multivariate Horner’s Rule
- Space subdivision based on $k$-center algorithm
- Error bound analysis
Space Subdivision Scheme

- The space subdivision scheme in the original FGT is uniform boxes. The number of boxes grows exponentially with the dimensionality.
- The desirable space subdivision should adaptively fit the density of the points.
- The cell should be as compact as possible.
- The algorithm is better to be a progressive one, that is the current space subdivision is from the previous one.
- Based on the above considerations, we model the task as $k$-center problem.
The $k$-center problem is defined to seek the “best” partition of a set of points into clusters (Gonzalez 1985, Hochbaum and Shmoys 1985, Feder and Greene 1988). Given a set of points and a predefined number $k$, $k$-center clustering is to find a partition $S = S_1 \cup S_2 \cup \ldots \cup S_k$ that minimizes $\max_{1 \leq i \leq k} \text{radius}(S_i)$, where $\text{radius}(S_i)$ is the radius of the smallest disk that covers all points in $S_i$.

The $k$-center problem is NP-hard but there exists a simple 2-approximation algorithm.
Farthest-Point Algorithm

- The farthest-point algorithm (a.k.a. $k$-center algorithm) is a 2-approximation of the optimal solution (Gonzales 1985).

- The total running time is $O(kn)$, $n$ is the number of points. It can be reduced to $O(n \log k)$ using a slightly more complicated algorithm (Feder and Greene 1988).

1. Initially randomly pick a point $v_0$ as the first center and add it to the center set $C$.

2. For $i = 1$ to $k - 1$ do

   - For every point $v \in V$, compute the distance from $v$ to the current center set $C = \{v_0, v_1, \ldots, v_{i-1}\}$: $d_i(v, C) = \min_{c \in C} \|v - c\|$.
   - From the points $V - C$ find a point $v_i$ that is farthest away from the current center set $C$, i.e. $d_i(v_i, C) = \max_v \min_{c \in C} \|v - c\|$.
   - Add $v_i$ to the center set $C$.

3. Return the center set $C = \{v_0, v_1, \ldots, v_{k-1}\}$ as the solution to $k$-center problem.
A Demo of \( k \)-center Algorithm

\[ k = 4 \]
The results of k-center algorithm. 40,000 points are divided into 64 clusters in 0.48 sec on a 900MHZ PIII PC.
More Results of k-center Algorithm

- The 40,000 points are on the manifolds.
Results of k-center Algorithm

- The computational complexity of k-center algorithm is $O(n \log k)$. Points are generated using uniform distribution. (Left) Number of points varies from 1000 to 40000 for 64 clusters; (Right) The number of clusters $k$ varies from 10 to 500 for 40000 points.
Improved Fast Gauss Transform Algorithm

**Step 1** Assign the $N$ sources into $K$ clusters using the farthest-point clustering algorithm such that the radius is less than $r_x$.

**Step 2** Choose $p$ sufficiently large such that the error estimate is less than the desired precision $\epsilon$.

**Step 3** For each cluster $S_k$ with center $c_k$, compute the coefficients:

$$ C^k_{\alpha} = \frac{2^{\lvert \alpha \rvert}}{\alpha!} \sum_{x_i \in S_k} q_i e^{-\|x_i - c_k\|^2/h^2} \left( \frac{x_i - c_k}{h} \right)^{\alpha}. $$

**Step 4** Repeat for each target $y_j$, find its neighbor clusters whose centers lie within the range $r_y$. Then the sum of Gaussians can be evaluated by the expression:

$$ G(y_j) = \sum_{\|y_j - c_k\| < h\rho_y} \sum_{\lvert \alpha \rvert < p} C^k_{\alpha} e^{-\|y_j - c_k\|^2/h^2} \left( \frac{y_j - c_k}{h} \right)^{\alpha}. $$
Improved Fast Gauss Transform

- Multivariate Taylor expansion
- Multivariate Horner’s Rule
- Space subdivision based on $k$-center algorithm
- Error bound analysis
The total error from the series truncation and the cutoff outside of the neighborhood of targets is bounded by

$$|E(y)| \leq \sum |q_i| \left( \frac{2^p}{p!} \left( \frac{r_x}{h} \right)^p \left( \frac{r_y}{h} \right)^p + e^{-\frac{(r_y/h)^2}{2}} \right).$$

**Error Bound of IFGT**

- **Sources**
- **Targets**
- **Truncation error**
- **Cutoff error**
Error Bound Analysis

- Increase the number of truncation terms $p$, the error bound will decrease.
- With the progress of k-center algorithm, the radius of the source points $r_x$ will decrease, until the error bound is less than a given precision.
- The error bound first decreases, then increases with respect to the cutoff radius $r_y$.

![Graphs showing error bound analysis](image)
The speedup of the fast Gauss transform in 4, 6, 8, 10 dimensions ($h=1.0$).
Programming Issues

- Streaming SIMD Extensions (SSE) and SSE2 (Intel)
Example of SSE/SSE2 Codes

```asm

mov  eax, DWORD PTR [ebp+8]  ; h
mov  edi, DWORD PTR [ebp+12] ; w
mov  ebx, DWORD PTR [ebp+20] ; img
mov  ecx, DWORD PTR [ebp+24] ; ii
xor  edx, edx

nextcol1: movdqa xmm0, XMMWORD PTR [ebx]
movdqa XMMWORD PTR [ecx], xmm0
mov  esi, 1
add  ebx, 16

nextrow1: paddd xmm0, XMMWORD PTR [ebx]
add  ecx, 16
movdqa XMMWORD PTR [ecx], xmm0
add  ebx, 16
inc  esi
cmp  esi, eax
jl   nextrow1
add  ecx, 16
inc  edx
cmp  edx, edi
jl   nextcol1

}
```
Some Applications

- Kernel density estimation
- Mean-shift based segmentation
- Object tracking
- Robot navigation
Kernel density estimation (a.k.a. Parzen method, Rosenblatt 1956, Parzen 1962) is an important nonparametric technique.

KDE is the keystone of many algorithms:
- Radial basis function networks
- Support vector machines
- Mean shift algorithm
- Regularized particle filter

The main drawback is the quadratic computational complexity. Very slow for large dataset.
Kernel Density Estimation

- Given a set of observations \( \{x_1, \ldots, x_n\} \), an estimate of density function is

\[
\hat{f}_n(x) = \frac{1}{nh^d} \sum_{i=1}^{n} K\left(\frac{\|x - x_i\|}{h}\right)
\]

- Some commonly used kernel functions

- The computational requirement for large datasets is \( O(N^2) \), for \( N \) points.
Efficient KDE and FGT

In practice, the most widely used kernel is the Gaussian

\[ K_N(x) = (2\pi)^{-d/2} e^{-\frac{1}{2} \|x\|^2}. \]

The density estimate using the Gaussian kernel:

\[ \hat{p}_n(x) = c_N \sum_{i=1}^{N} e^{-\|x-x_i\|^2 / h^2} \]

Fast Gauss transform can reduce the cost to \( O(N \log M) \) in low-dimensional spaces.

Improved fast Gauss transform accelerates the KDE in both lower and higher dimensions.
Experimental Result

- Image segmentation results of the mean-shift algorithm with the Gaussian kernel.

  - Size: 432X294
  - Time: 7.984 s
  - Direct evaluation: more than 2 hours

  - Size: 481X321
  - Time: 12.359 s
  - Direct evaluation: more than 2 hours
Some Applications

- Kernel density estimation
- Mean-shift based segmentation
- Object tracking
- Robot Navigation
Object Tracking

- Goal of object tracking: find the moving objects between consecutive frames.
- A model image or template is given for tracking.
- Usually a feature space is used, such as pixel intensity, colors, edges, etc.
- Usually a similarity measure is used to measure the difference between the model image and current image.
- Temporal correlation assumption: the change between two consecutive frames is small.

![Model image](image1.png) ![Target image](image2.png)

Similarity function
Proposed Similarity Measures

Our similarity measure

\[ J(I_x, I_y) = \frac{1}{MN} \sum_{i=1}^{N} \sum_{j=1}^{M} w(\|x_i - y_j\| \sigma^2) k(\|u_i - v_j\| \eta^2). \]

- Directly computed from the data points.
- Well scaled into higher dimensions.
- Ready to be speeded up by fast Gauss transform, if Gaussian kernels are employed.
- Interpreted as the expectation of the density estimations over the model and target images.
Experimental results

- Pure translation
  - Feature space: $RGB + 2D$ spatial space
  - Average processing time per frame: $0.0169s$.  

Our method: 

Histogram tracking using Bhattacharyya distance
Experimental results

- Pure translation
  - Feature space: $RGB + 2D$ gradient + $2D$ spatial space
  - Average processing time per frame: 0.0044 s.
Experimental results

- Pure translation
  - Feature space: *RGB* + 2D spatial space
  - The similarity measure is robust and accurate to the small target, compared with the other methods, such as histogram.
Experimental Results

- Translation + Scaling
  - Feature space: RGB + 2D spatial space
Conclusions

- Improved fast Gauss transform is presented for higher dimensional spaces.
- Kernel density estimation is accelerated by the IFGT.
- A similarity measure in joint feature-spatial space is proposed for robust object tracking.
- With different motion models, we derived several tracking algorithms.
- The improved fast Gauss transform is applied to speed up the tracking algorithms to real-time performance.