CMSC 858M/AMSC 698R

Fast Multipole Methods

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Lecture(s) 3(4)

Outline

- **Factorization – One of key parts of the FMM**
  - Extensions of our trick for fast summation
  - "Middleman" scheme
  - Singular and regular fields
  - Far field and near field
- **Local Expansions (or R-expansions)**
  - Local expansions of regular and singular potentials
  - Power series
  - Taylor series
- **Far Field Expansions (or S-expansions)**
  - Far field expansions of regular and singular potentials
  - Asymptotic series

Matrix-Vector Multiplication

Compute matrix vector product

$$\mathbf{v} = \mathbf{\Phi u}$$

or

$$v_j = \sum_{i=1}^{N} \Phi_{ji} u_i, \quad j = 1,\ldots,M,$$

where

$$\Phi_{ji} = \Phi(\mathbf{y}_j, \mathbf{x}_i), \quad j = 1,\ldots,M, \quad i = 1,\ldots,N,$$

or

$$\mathbf{\Phi} = \begin{pmatrix} \Phi_{11} & \Phi_{12} & \ldots & \Phi_{1N} \\ \Phi_{21} & \Phi_{22} & \ldots & \Phi_{2N} \\ \ldots & \ldots & \ldots & \ldots \\ \Phi_{M1} & \Phi_{M2} & \ldots & \Phi_{MN} \end{pmatrix} = \begin{pmatrix} \Phi(\mathbf{y}_1,\mathbf{x}_1) & \Phi(\mathbf{y}_1,\mathbf{x}_2) & \ldots & \Phi(\mathbf{y}_1,\mathbf{x}_N) \\ \Phi(\mathbf{y}_2,\mathbf{x}_1) & \Phi(\mathbf{y}_2,\mathbf{x}_2) & \ldots & \Phi(\mathbf{y}_2,\mathbf{x}_N) \\ \ldots & \ldots & \ldots & \ldots \\ \Phi(\mathbf{y}_M,\mathbf{x}_1) & \Phi(\mathbf{y}_M,\mathbf{x}_2) & \ldots & \Phi(\mathbf{y}_M,\mathbf{x}_N) \end{pmatrix}.$$

Generally we have two sets of points in d-dimensions:

$$\text{Sources}: \mathbb{X} = \{\mathbf{x}_1,\ldots,\mathbf{x}_N\}, \quad \mathbf{x}_i \in \mathbb{R}^d, \quad i = 1,\ldots,N,$$
$$\text{Receivers}: \mathbb{Y} = \{\mathbf{y}_1,\ldots,\mathbf{y}_M\}, \quad \mathbf{y}_j \in \mathbb{R}^d, \quad j = 1,\ldots,M,$$

The receivers also can be called “targets” or “evaluation points”.

Why $\mathbf{R}^d$?

- d = 1
  - Scalar functions, interpolation, etc.
- d = 2,3
  - Physical problems in 2 and 3 dimensional space
- d = 4
  - 3D Space + time, 3D grayscale images
- d = 5
  - Color 2D images, Motion of 3D grayscale images
- d = 6
  - Color 3D images
- d = 7
  - Motion of 3D color images
- d = arbitrary
  - d-parametric spaces, statistics, database search procedures

Fields (Potentials)

Field (Potential) of a single (ith) unit source

$$v(\mathbf{y}) = \sum_{i=1}^{M} u_i \Phi(\mathbf{y}, \mathbf{x}_i), \quad \mathbf{y} \in \mathbb{R}^d,$$

$$v_j = v(\mathbf{y}_j), \quad j = 1, \ldots, M$$

Field (Potential) of the set of sources of intensities $\{u_i\}$

Fields are continuous!
(Almost everywhere)

Examples of Fields

- There can be vector or scalar fields (we focus mostly on scalar fields)
- Fields can be *regular* or *singular*

Scalar Fields:

- Gravity

(singular at $\mathbf{y} = \mathbf{x}_i$)

$$\Phi(\mathbf{y}, \mathbf{x}_i) = \frac{1}{|\mathbf{y} - \mathbf{x}_i|}$$

- Monochromatic Wave (k is the wavenumber)

(singular at $\mathbf{y} = \mathbf{x}_i$)

$$\Phi(\mathbf{y}, \mathbf{x}_i) = \frac{\exp\{ik|\mathbf{y} - \mathbf{x}_i|\}}{|\mathbf{y} - \mathbf{x}_i|}$$

- Gaussian

(regular everywhere)

$$\Phi(\mathbf{y}, \mathbf{x}_i) = \exp\{-|\mathbf{y} - \mathbf{x}_i|^2/\sigma\}$$

Vector Field:

- 3D Velocity field:

(singular at $\mathbf{y} = \mathbf{x}_i$)

$$\Phi(\mathbf{y}, \mathbf{x}_i) = \nabla_y \frac{1}{|\mathbf{y} - \mathbf{x}_i|} = \mathbf{i}_1 \frac{\partial}{\partial y_1} \frac{1}{|\mathbf{y} - \mathbf{x}_i|} + \mathbf{i}_2 \frac{\partial}{\partial y_2} \frac{1}{|\mathbf{y} - \mathbf{x}_i|} + \mathbf{i}_3 \frac{\partial}{\partial y_3} \frac{1}{|\mathbf{y} - \mathbf{x}_i|},$$

$$\mathbf{y} = (y_1, y_2, y_3) \in \mathbb{R}^3.$$

Straightforward Computational Complexity:

$O(MN)$ Error: 0 (“machine” precision)

The Fast Multipole Methods look for computation of the same problem with complexity $o(MN)$ and error < prescribed error.

In the case when the error of the FMM does not exceed the machine precision error (for given number of bits) there is no difference between the “exact” and “approximate” solution.

Factorization
“Middleman Method”

Global Factorization

Expansion center

Truncation number

$$\forall \mathbf{x}_i, \mathbf{y}_j \in \Omega \subset \mathbb{R}^d :$$

$$\Phi\left(\mathbf{y}_j, \mathbf{x}_i\right) = \sum_{m=0}^{\infty} a_m(\mathbf{x}_i - \mathbf{x}_*) f_m\left(\mathbf{y}_j - \mathbf{x}_*\right) = \sum_{m=0}^{p-1} a_m(\mathbf{x}_i - \mathbf{x}_*) f_m\left(\mathbf{y}_j - \mathbf{x}_*\right) + Error(p, \mathbf{x}_i, \mathbf{y}_j)$$

Expansion coefficients

Basis functions

Factorization Trick

$$\begin{aligned} v_j &= \sum_{i=1}^{N} \Phi\left(\mathbf{y}_j, \mathbf{x}_i\right) u_i \\ &= \sum_{i=1}^{N} \left[\sum_{m=0}^{p-1} a_m(\mathbf{x}_i - \mathbf{x}_*) f_m\left(\mathbf{y}_j - \mathbf{x}_*\right) + Error(p, \mathbf{x}_i, \mathbf{y}_j) \right] u_i \\ &= \sum_{m=0}^{p-1} f_m\left(\mathbf{y}_j - \mathbf{x}_*\right) \sum_{i=1}^{N} a_m(\mathbf{x}_i - \mathbf{x}_*) u_i + \sum_{i=1}^{N} Error(p, \mathbf{x}_i, \mathbf{y}_j) u_i \\ &= \sum_{m=0}^{p-1} c_m f_m\left(\mathbf{y}_j - \mathbf{x}_*\right) + Error(N, p), \end{aligned}$$

where

$$c_m = \sum_{i=1}^{N} a_m(\mathbf{x}_i - \mathbf{x}_*) u_i.$$

Reduction of Complexity

Straightforward (nested loops):

for $j = 1,\ldots,M$
  $v_j = 0;$
  for $i = 1,\ldots,N$
    $v_j = v_j + \Phi(\mathbf{y}_j, \mathbf{x}_i) u_i;$
  end;
end;

Complexity: $O(MN)$

If $p \ll \min(M,N)$ then complexity reduces!

Factorized:

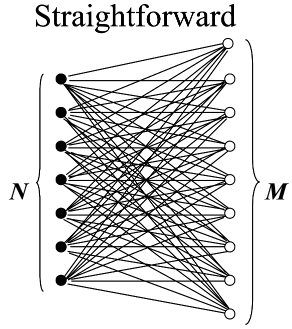
for $m = 0,\ldots,p-1$
  $c_m = 0;$
  for $i = 1,\ldots,N$
    $c_m = c_m + a_m(\mathbf{x}_i - \mathbf{x}_*) u_i;$
  end;
end;

for $j = 1,\ldots,M$
  $v_j = 0;$
  for $m = 0,\ldots,p-1$
    $v_j = v_j + c_m f_m(\mathbf{y}_j - \mathbf{x}_*);$
  end;
end;

Complexity: $O(pN+pM)$

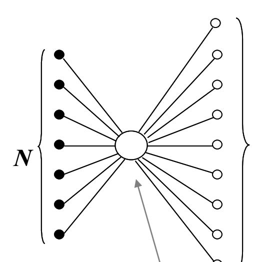
Middleman Scheme

Straightforward



Complexity: $O(pN+pM)$

Middleman

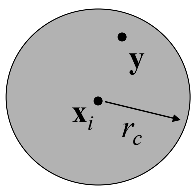


Set of coefficients $\{c_m\}$

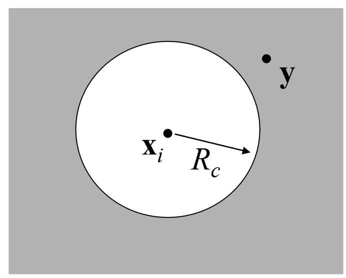
Far Field and Near Field

- Near Field of the ith source: $|\mathbf{y}-\mathbf{x}_i| < r_c.$
- Far Field of the ith source: $|\mathbf{y}-\mathbf{x}_i| > R_c.$

Near Field



Far Field



What are these r_c and R_c ?
depends on the potential + some conventions for the terminology

Local (Regular) Expansion

Do not confuse with the Near Field!

Let $\mathbf{x}_* \in \mathbb{R}^d.$

We call expansion

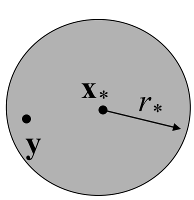
$$\Phi(\mathbf{y},\mathbf{x}_i) = \sum_{m=0}^{\infty} a_m(\mathbf{x}_i,\mathbf{x}_*)R_m(\mathbf{y}-\mathbf{x}_*)$$

Basis Functions

Expansion Coefficients

local (regular) inside a sphere $|\mathbf{y}-\mathbf{x}_*| < r_*,$

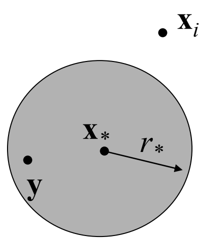
if the series converges for $\forall \mathbf{y},\ |\mathbf{y}-\mathbf{x}_*| < r_*.$



We also call this R-expansion,
since basis functions R_m should be *regular*

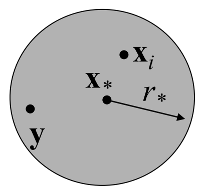
Local Expansion of a Regular Potential

Can be like this:



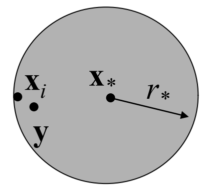
$|\mathbf{y} - \mathbf{x}_*| < r_* < |\mathbf{x}_i - \mathbf{x}_*|$

…or like this:



$r_* > |\mathbf{y} - \mathbf{x}_*| > |\mathbf{x}_i - \mathbf{x}_*|$

…or like this:



$r_* > |\mathbf{x}_i - \mathbf{x}_*| > |\mathbf{y} - \mathbf{x}_*|$

Local Expansion of a Regular Potential (Example)

Valid for any $r_* < \infty$, and x_i.

$x, y \in \mathbb{R}^1.$

$\Phi(y, x_i) = e^{-(y-x_i)^2}.$

Looking for factorization:

$$\Phi(y, x_i) = \sum_{m=0}^{\infty} a_m(x_i - x_*) R_m(y - x_*).$$

We have

$$e^{-(y-x_i)^2} = e^{-[y-x_*-(x_i-x_*)]^2} = e^{-(y-x_*)^2} e^{-(x_i-x_*)^2} e^{2(x_i-x_*)(y-x_*)}$$

$$= e^{-(y-x_*)^2} e^{-(x_i-x_*)^2} \sum_{m=0}^{\infty} \frac{2^m (x_i - x_*)^m (y - x_*)^m}{m!}.$$

Choose

$$a_m(x_i - x_*) = e^{-(x_i-x_*)^2} \sqrt{\frac{2^m}{m!}} (x_i - x_*)^m, \quad m = 0, 1, \ldots,$$

$$R_m(y - x_*) = e^{-(y-x_*)^2} \sqrt{\frac{2^m}{m!}} (y - x_*)^m, \quad m = 0, 1, \ldots$$

Local Expansion of a Regular Potential (The same kernel, Example 2)

$$e^{-(y-x_*)^2} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!}(y-x_*)^{2n}.$$

So

$$e^{-(y-x_i)^2} = e^{-(y-x_*)^2} e^{-(x_i-x_*)^2} \sum_{m=0}^{\infty} \frac{2^m (x_i-x_*)^m (y-x_*)^m}{m!} = e^{-(x_i-x_*)^2} \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{(-1)^n 2^m (x_i-x_*)^m (y-x_*)^{m+2n}}{m!n!}.$$

Rearrange summation:

$$m + 2n = l$$

$$m = l - 2n$$

$$e^{-(y-x_i)^2} = e^{-(x_i-x_*)^2} \sum_{l=0}^{\infty}\sum_{n=0}^{[l/2]} \frac{(-1)^n 2^{l-2n} (x_i-x_*)^{l-2n}}{(l-2n)!n!}(y-x_*)^l = \sum_{l=0}^{\infty} h_l(x_i-x_*)\frac{(y-x_*)^l}{l!}.$$

Hermit polynomials:

$$H_l(x) = l! \sum_{n=0}^{[l/2]} \frac{(-1)^n 2^{l-2n} (x)^{l-2n}}{(l-2n)!n!}.$$

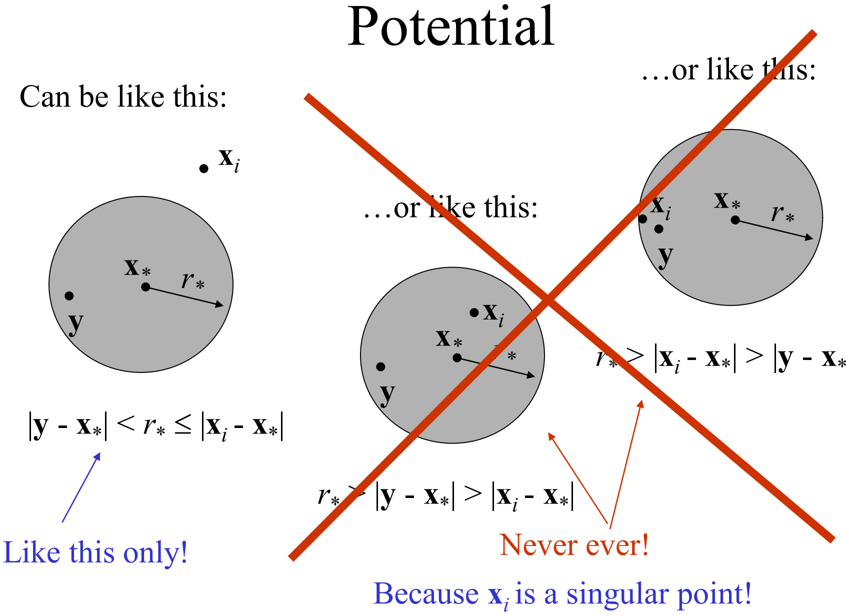
Hermit functions:

$$h_l(x) = e^{-x^2} H_l(x).$$

Choose

$$a_l(x_i - x_*) = h_l(x_i - x_*), \quad R_l(y - x_*) = \frac{1}{l!}(y-x_*)^l, \quad l = 0, 1, \ldots$$

Local Expansion of a Singular Potential



Local Expansion of a Singular Potential (Example)

Valid for any $|x_i - x_*| > |y - x_*|$

$$x, y \in \mathbb{R}^1.$$

$$\Phi(y, x_i) = \frac{1}{y - x_i}.$$

Looking for factorization:

$$\Phi(y, x_i) = \sum_{m=0}^{\infty} a_m(x_i - x_*) R_m(y - x_*).$$

We have

$$\frac{1}{y - x_i} = \frac{1}{y - x_* - (x_i - x_*)} = -\frac{1}{(x_i - x_*)[1 - \frac{y - x_*}{x_i - x_*}]} = -\frac{1}{(x_i - x_*)}\left[1 - \frac{y - x_*}{x_i - x_*}\right]^{-1}.$$

Geometric progression:

$$(1 - \alpha)^{-1} = 1 + \alpha + \alpha^2 + \ldots = \sum_{m=0}^{\infty} \alpha^m, \quad |\alpha| < 1.$$

$$\left[1 - \frac{y - x_*}{x_i - x_*}\right]^{-1} = \sum_{m=0}^{\infty} \frac{(y - x_*)^m}{(x_i - x_*)^m}, \quad |y - x_*| < |x_i - x_*|.$$

Choose

$$a_m(x_i - x_*) = -\frac{1}{(x_i - x_*)^{m+1}}, \quad m = 0, 1, \ldots,$$

$$R_m(y - x_*) = (y - x_*)^m, \quad m = 0, 1, \ldots$$

Power and Taylor Series

- Power and Taylor Series
  - Power Series in 1D
  - Taylor Series in 1D
- Multidimensional Taylor Series
- Factorization of Scalar Products in $\mathbf{R}^d$
- Compression of Factorized Series
- Factorization of Scalar Products in $\mathbf{R}^d$ (compression)
  - Factorization in 2D.
  - Factorization in 3D.
  - Factorization in *d*D.
  - Multinomial Coefficients.
  - Complexity of Fast Summation.
- General Forms of Factorization for Fast Summation

Power Series

Power series relative to real or complex variable y is a series of type

$$f(y - x_*) = \sum_{m=0}^{\infty} a_m (y - x_*)^m,$$

where a_m are real or complex numbers.

Properties of Power Series

1) For any power series there exists r_*,, such that the series converges absolutely at $|y - x_*| < r_*$, and diverges at $|y - x_*| > r_*$. The number r_*, is called *the convergence radius* of the series, $0 \leq r_* \leq \infty$.

For any number q, such that $0 < q < r_*$, the power series uniformly converges at $|y - x_*| < q$.

Properties of Power Series

2) Convergent power series can be summed, multiplied by a scalar, or multiplied according to the Cauchy rule.

For $|y-x_*|< r_*$, the sum of the series is a continuous and infinitely differentiable function of y.

The power series can be differentiated term by term at $|y-x_*|< r_*$ and integrated over any closed interval included in $|y-x_*|< r_*$.
Differentiated or integrated series (if integration is taken from x_* to $y-x_*$) have the same convergence radius r_* .

$$\sum_{m=0}^{\infty} a_m (y-x_*)^m + \sum_{m=0}^{\infty} b_m (y-x_*)^m = \sum_{m=0}^{\infty} (a_m + b_m)(y-x_*)^m,$$

$$a \sum_{m=0}^{\infty} a_m (y-x_*)^m = \sum_{m=0}^{\infty} a a_m (y-x_*)^m,$$

Cauchy's rule →

$$\left[\sum_{m=0}^{\infty} a_m (y-x_*)^m\right]\left[\sum_{m=0}^{\infty} b_m (y-x_*)^m\right] = \sum_{n=0}^{\infty}\left[\sum_{m=0}^{n} a_m b_{n-m}\right](y-x_*)^n.$$

Properties of Power Series

3) Uniqueness. If there exists such positive r that at any y satisfying $|y-x_*|< r$ two power series have the same sum, then the coefficients of these series are the same.

For those who love proofs

Prove the above properties!

(Not the course formal requirement, but a good exercise)

Taylor Series (Finite)

Let $f(y)$ be a real function, $f(y) \in D^n[x_*, x_* + r_*)$ (so the n-th derivative $f^{(n)}(y)$ exists for $x_* \leqslant y < x_* + r_*$). Then

$$f(y) = f(x_*) + f'(x_*)(y - x_*) + \frac{1}{2!}f''(x_*)(y - x_*)^2 + \ldots + \frac{1}{(n-1)!}f^{(n-1)}(x_*)(y - x_*)^{n-1} + \text{Residual}_n(y).$$

Cauchy's evaluation:

$$|\text{Residual}_n(y)| \leqslant \frac{|y - x_*|^n}{n!} \sup_{x_* \leqslant y < x_* + r_*} |f^{(n)}(y)|.$$

Lagrange evaluation:

$$\text{Residual}_n(y) = \int_{x_*}^{y} dx \int_{x_*}^{x} dx \ldots \int_{x_*}^{x} f^{(n)}(x)dx = \frac{1}{n!}f^{(n)}(X)(y - x_*)^n,$$
$$X \in (x_*, x_* + r_*).$$

We have similar formulae for $x_* - r_* \leqslant y < x_*$.

Taylor Series (Infinite)

Let $f(y) \in D^{\infty}(x_* - r_*, x_* + r_*)$ and let

$$\lim_{n\to\infty} \text{Residual}_n(y) = 0,$$

then

$$f(y) = \sum_{m=0}^{\infty} \frac{1}{m!} f^{(m)}(x_*)(y - x_*)^m, \quad |y - x_*| < r_*.$$

and the series uniformly converges to $f(y)$ for any $|y - x_*| \leqslant q$, where $0 \leqslant q \leqslant r$.

Local 1D Taylor Expansion

Looking for local expansion:

$$\Phi(y, x_i) = \sum_{m=0}^{\infty} a_m(x_i, x_*) R_m(y - x_*),$$

$$\Phi(y, x_i) = \sum_{m=0}^{\infty} \frac{1}{m!} \frac{\partial^m \Phi}{\partial y^m}(x_*, x_i)(y - x_*)^m.$$

$$a_m(x_i, x_*) = \frac{1}{m!} \frac{\partial^m \Phi}{\partial y^m}(x_*, x_i), \quad m = 0, 1, \ldots$$

$$R_m(y - x_*) = (y - x_*)^m, \quad m = 0, 1, \ldots$$

Local 1D Taylor Expansion (Example)

$$\Phi(y, x_i) = e^{x_i y}.$$

$$\frac{\partial^m \Phi}{\partial y^m}(y, x_i) = x_i^m e^{x_i y}, \quad \frac{\partial^m \Phi}{\partial y^m}(x_*, x_i) = x_i^m e^{x_i x_*},$$

$$a_m(x_i, x_*) = \frac{1}{m!}\frac{\partial^m \Phi}{\partial y^m}(x_*, x_i) = \frac{x_i^m}{m!} e^{x_i x_*},$$

$$\Phi(y, x_i) = e^{x_i x_*} \sum_{m=0}^{\infty} \frac{x_i^m}{m!}(y - x_*)^m.$$

Residual for $|y - x_*| < \alpha$ (assume $x_i > 0, x_* \geqslant 0$) :

$$|\text{Residual}_n(y)| \leqslant \frac{|y - x_*|^n}{n!} \sup_{x_* - \alpha \leq y \leq x_* + \alpha} \left| \frac{\partial^n \Phi}{\partial y^n}(y, x_i) \right| < \frac{\alpha^n}{n!} x_i^n e^{x_i(x_* + \alpha)}.$$

For $n = 5,\ \alpha = 0.5,\ x_i = 1, x_* = 0.5$ we have

$$|\text{Residual}_5(y)| < \frac{e}{2^5 5!} < \frac{3}{32 \cdot 120} = \frac{1}{1280} < 10^{-3}.$$

Multidimensional Taylor Series

Let $f(\mathbf{y})$ be a real function,

$$f(\mathbf{y}) \in D^\infty(\mathbf{U}_{\mathbf{x}_*}), \quad \mathbf{y} = (y_1, \ldots, y_d) \in \mathbf{U}_{\mathbf{x}_*} \subset \mathbb{R}^d, \quad \mathbf{x}_* = (x_{*1}, \ldots, x_{*d}) \subset \mathbb{R}^d$$

Then we can write

$$f(\mathbf{y}) = f(y_1, y_2, \ldots, y_d)$$

$$\begin{aligned}
f(y_1, y_2, \ldots, y_d) &= \sum_{m_1=0}^{\infty} \frac{1}{m_1!} \frac{\partial^{m_1} f}{\partial y_1^{m_1}}(x_{*1}, y_2, \ldots, y_d)(y_1 - x_{*1})^{m_1} \\
&= \sum_{m_1=0}^{\infty} \frac{1}{m_1!} \sum_{m_2=0}^{\infty} \frac{1}{m_2!} \frac{\partial^{m_1}}{\partial y_1^{m_1}} \frac{\partial^{m_2}}{\partial y_2^{m_2}} f(x_{*1}, x_{*2}, \ldots, y_d)(y_1 - x_{*1})^{m_1}(y_2 - x_{*2})^{m_2} \\
&= \ldots \\
&= \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \cdots \sum_{m_d=0}^{\infty} \frac{\partial^{m_1}}{\partial y_1^{m_1}} \frac{\partial^{m_2}}{\partial y_2^{m_2}} \cdots \frac{\partial^{m_d}}{\partial y_2^{m_d}} f(x_{*1}, x_{*2}, \ldots, x_{*d}) \prod_{i=1}^{d} \frac{1}{m_i!}(y_i - x_{*i})^{m_i}.
\end{aligned}$$

Multidimensional Taylor Series (using some vector algebra)

Operator ∇ :

$$\nabla = \mathbf{i}_1 \frac{\partial}{\partial y_1} + \ldots + \mathbf{i}_d \frac{\partial}{\partial y_d}.$$

Differential along direction $\mathbf{s}$:

$$\frac{d^n f(\mathbf{y})}{ds^n} = (\mathbf{s} \cdot \nabla)^n f(\mathbf{y}), \quad |\mathbf{s}| = 1.$$

Taylor series (let $\mathbf{s} = (\mathbf{y} - \mathbf{x}_*)/|\mathbf{y} - \mathbf{x}_*|$)

$$\begin{aligned} f(\mathbf{y}) &= f(\mathbf{x}_*) + \frac{df(\mathbf{x}_*)}{ds}|\mathbf{y} - \mathbf{x}_*| + \frac{1}{2!}\frac{d^2 f(\mathbf{x}_*)}{ds^2}|\mathbf{y} - \mathbf{x}_*|^2 + \ldots \\ &= f(\mathbf{x}_*) + [(\mathbf{y} - \mathbf{x}_*) \cdot \nabla] f(\mathbf{x}_*) + \frac{1}{2!}[(\mathbf{y} - \mathbf{x}_*) \cdot \nabla]^2 f(\mathbf{x}_*) + \ldots \\ &= \sum_{m=0}^{\infty} \frac{1}{m!}[(\mathbf{y} - \mathbf{x}_*) \cdot \nabla]^m f(\mathbf{x}_*). \end{aligned}$$

Example

$$\Phi(\mathbf{y}, \mathbf{x}_i) = e^{\mathbf{y} \cdot \mathbf{x}_i} = \sum_{m=0}^{\infty} \frac{1}{m!}[(\mathbf{y} - \mathbf{x}_*) \cdot \nabla_{\mathbf{x}_*}]^m \Phi(\mathbf{x}_*, \mathbf{x}_i),$$

Fix $(\mathbf{y} \quad \mathbf{x}_*)$:

$$\begin{aligned} \Phi(\mathbf{x}_*, \mathbf{x}_i) &= e^{\mathbf{x}_* \cdot \mathbf{x}_i}, \\ \nabla_{\mathbf{x}_*} \Phi(\mathbf{x}_*, \mathbf{x}_i) &= \mathbf{x}_i e^{\mathbf{x}_* \cdot \mathbf{x}_i} = \mathbf{x}_i \Phi(\mathbf{x}_*, \mathbf{x}_i), \\ [(\mathbf{y} - \mathbf{x}_*) \cdot \nabla_{\mathbf{x}_*}] \Phi(\mathbf{x}_*, \mathbf{x}_i) &= [(\mathbf{y} - \mathbf{x}_*) \cdot \mathbf{x}_i] \Phi(\mathbf{x}_*, \mathbf{x}_i), \\ [(\mathbf{y} - \mathbf{x}_*) \cdot \nabla_{\mathbf{x}_*}]^m \Phi(\mathbf{x}_*, \mathbf{x}_i) &= [(\mathbf{y} - \mathbf{x}_*) \cdot \mathbf{x}_i]^m \Phi(\mathbf{x}_*, \mathbf{x}_i), \end{aligned}$$

$$\Phi(\mathbf{y}, \mathbf{x}_i) = \sum_{m=0}^{\infty} \frac{1}{m!}[(\mathbf{y} - \mathbf{x}_*) \cdot \mathbf{x}_i]^m \Phi(\mathbf{x}_*, \mathbf{x}_i) = e^{\mathbf{x}_* \cdot \mathbf{x}_i} \sum_{m=0}^{\infty} \frac{1}{m!}[(\mathbf{y} - \mathbf{x}_*) \cdot \mathbf{x}_i]^m.$$

Check: $e^{\mathbf{y} \cdot \mathbf{x}_i} = e^{\mathbf{x}_* \cdot \mathbf{x}_i} e^{(\mathbf{y} - \mathbf{x}_*) \cdot \mathbf{x}_i} = e^{\mathbf{x}_* \cdot \mathbf{x}_i} \sum_{m=0}^{\infty} \frac{1}{m!}[(\mathbf{y} - \mathbf{x}_*) \cdot \mathbf{x}_i]^m.$

Is That a Factorization?

$$e^{\mathbf{y}\cdot\mathbf{x}_i} = e^{\mathbf{x}_*\cdot\mathbf{x}_i} \sum_{m=0}^{\infty} \frac{1}{m!} \left[(\mathbf{y} - \mathbf{x}_*) \cdot \mathbf{x}_i \right]^m$$

Scalar Product in d-Dimensional Space

Definition of scalar product:

$$\mathbf{a} = (a_1, \ldots, a_d), \quad \mathbf{b} = (b_1, \ldots, b_d),$$

$$\mathbf{a} \cdot \mathbf{b} = a_1 b_1 + \ldots + a_d b_d = \sum_{k=1}^{d} a_k b_k .$$

$$\mathbf{a} \cdot \mathbf{b} = |\mathbf{a}||\mathbf{b}| \cos\theta,$$

$$|\mathbf{a}| = \sqrt{\mathbf{a} \cdot \mathbf{a}} .$$

What if

$$a_1, \ldots, a_d, b_1, \ldots, b_d \in \mathbb{C} \quad ?$$

Definition:

complex conjugate

$$\mathbf{a} \cdot \mathbf{b} = \overline{a_1} b_1 + \ldots + \overline{a_d} b_d = \sum_{k=1}^{d} \overline{a_k} b_k .$$

Properties of Scalar Product

Commutativity:

$$\mathbf{a} \bullet \mathbf{b} = \mathbf{b} \bullet \mathbf{a}$$

Scaling:

$$(\lambda \mathbf{a}) \bullet \mathbf{b} = \mathbf{a} \bullet (\lambda \mathbf{b}) = \lambda(\mathbf{a} \bullet \mathbf{b}), \quad \lambda \in \mathbb{R}$$

Distributivity:

$$(\mathbf{a} + \mathbf{b}) \bullet \mathbf{c} = \mathbf{a} \bullet \mathbf{c} + \mathbf{b} \bullet \mathbf{c}$$

Factorization of Scalar Product Powers

$$(\mathbf{a} \bullet \mathbf{b})^n = \left(\sum_{k=1}^{d} a_k b_k \right)^n = \sum_{k_1=1}^{d} a_{k_1} b_{k_1} \sum_{k_2=1}^{d} a_{k_2} b_{k_2} \cdots \sum_{k_n=1}^{d} a_{k_n} b_{k_n}$$

$$= \sum_{k_1=1}^{d} \sum_{k_2=1}^{d} \cdots \sum_{k_n=1}^{d} a_{k_1} a_{k_2} \ldots a_{k_n} b_{k_1} b_{k_2} \ldots b_{k_n}$$

$$= [\mathbf{a} \otimes \mathbf{a} \otimes \ldots \otimes \mathbf{a}] \bullet [\mathbf{b} \otimes \mathbf{b} \otimes \ldots \otimes \mathbf{b}] = \mathbf{a}^n \bullet \mathbf{b}^n$$

$$\mathbf{a}^n \bullet \mathbf{b}^n = (\mathbf{a} \bullet \mathbf{b})^n = (\mathbf{b} \bullet \mathbf{a})^n = \mathbf{b}^n \bullet \mathbf{a}^n.$$

$$e^{\mathbf{y} \cdot \mathbf{x}_i} = e^{\mathbf{x}_* \cdot \mathbf{x}_i} \sum_{m}^{\infty} \frac{1}{m!} [(\mathbf{y} - \mathbf{x}_*) \bullet \mathbf{x}_i]^m = e^{\mathbf{x}_* \cdot \mathbf{x}_i} \sum_{m}^{\infty} \frac{1}{m!} \mathbf{x}_i^m \bullet (\mathbf{y} - \mathbf{x}_*)^m.$$

Is That a Factorization?

1) Truncation:

$$\Phi(\mathbf{y},\mathbf{x}_i) = e^{\mathbf{y}\cdot\mathbf{x}_i} = e^{\mathbf{x}_*\cdot\mathbf{x}_i}\left[\sum_{m=0}^{p-1}\frac{1}{m!}\mathbf{x}_i^m \bullet (\mathbf{y}-\mathbf{x}_*)^m + \text{Residual}_p\right]$$

2) Fast summation:

$$v_j = \sum_{i=1}^{N} u_i\Phi(\mathbf{y}_j,\mathbf{x}_i) = \sum_{i=1}^{N} u_i e^{\mathbf{x}_*\cdot\mathbf{x}_i}\left[\sum_{m=0}^{p-1}\frac{1}{m!}\mathbf{x}_i^m \bullet (\mathbf{y}_j-\mathbf{x}_*)^m + \text{Residual}_p\right]$$

$$= \sum_{i=1}^{N} u_i e^{\mathbf{x}_*\cdot\mathbf{x}_i}\sum_{m=0}^{p-1}\frac{1}{m!}\mathbf{x}_i^m \bullet (\mathbf{y}_j-\mathbf{x}_*)^m + N\max_i(u_i e^{\mathbf{x}_*\cdot\mathbf{x}_i})\text{Residual}_p$$

$$= \sum_{m=0}^{p-1}\frac{1}{m!}\left(\sum_{i=1}^{N} u_i e^{\mathbf{x}_*\cdot\mathbf{x}_i}\mathbf{x}_i^m\right)\bullet (\mathbf{y}_j-\mathbf{x}_*)^m + \text{Residual}$$

$$= \sum_{m=0}^{p-1}\mathbf{c}_m \bullet (\mathbf{y}_j-\mathbf{x}_*)^m + \text{Residual}, \qquad \mathbf{c}_m = \frac{1}{m!}\sum_{i=1}^{N} u_i e^{\mathbf{x}_*\cdot\mathbf{x}_i}\mathbf{x}_i^m.$$

Yes! It is!

Example (Let's Try To Get Explicit Forms in 2D)

$$\mathbf{a} = (a_1,a_2),$$

$$\mathbf{a}^2 = (a_1(a_1,a_2),a_2(a_1,a_2)) = (a_1^2,a_1a_2,a_2a_1,a_2^2),$$

$$\mathbf{a}^3 = (a_1^2(a_1,a_2),a_1a_2(a_1,a_2),a_2a_1(a_1,a_2),a_2^2(a_1,a_2))$$

$$= (a_1^3,a_1^2a_2,a_1a_2a_1,a_1a_2^2,a_2a_1^2,a_2a_1a_2,a_2^2a_1,a_2^3),\ldots$$

The length of $\mathbf{a}^n$ is 2^n! ← This is not factorial!

In d dimensions the length of $\mathbf{a}^n$ is even d^n

What to do in practical problems?

Use Compression!

Compression operator:

$$\mathbf{A}^n = \mathbf{Compress}(\mathbf{a}^n)$$

Required Property:

$$\mathbf{a}^n \bullet \mathbf{b}^n = \mathbf{Compress}(\mathbf{a}^n) \bullet \mathbf{Compress}(\mathbf{b}^n).$$

Consider $\mathbf{R}^2$:

$$\mathbf{a}^n \bullet \mathbf{b}^n = (\mathbf{a} \bullet \mathbf{b})^n = (a_1 b_1 + a_2 b_2)^n$$

$$= a_1^n b_1^n + \binom{n}{1} a_1^{n-1} b_1^{n-1} a_2 b_2 + \binom{n}{2} a_1^{n-2} b_1^{n-2} a_2^2 b_2^2 + \ldots + a_2^n b_2^n$$

The length is only $(n+1)$, not 2^n

Let us define:

$$\mathbf{A}^n = \mathbf{Compress}(\mathbf{a}^n) = \left(a_1^n, \sqrt{\binom{n}{1}} a_1^{n-1} a_2, \sqrt{\binom{n}{2}} a_1^{n-2} a_2^2, \ldots, a_2^n \right),$$

$$\mathbf{B}^n = \mathbf{Compress}(\mathbf{b}^n) = \left(b_1^n, \sqrt{\binom{n}{1}} b_1^{n-1} b_2, \sqrt{\binom{n}{2}} b_1^{n-2} b_2^2, \ldots, b_2^n \right)$$

Example of Fast Computation

$$v_j = \sum_{i=1}^{N} u_i \Phi(\mathbf{y}_j, \mathbf{x}_i) = \sum_{m=0}^{p-1} \mathbf{c}_m \bullet (\mathbf{y}_j - \mathbf{x}_*)^m + \text{Residual}, \qquad \mathbf{c}_m = \frac{1}{m!} \sum_{i=1}^{N} u_i e^{\mathbf{x}_* \bullet \mathbf{x}_i} \mathbf{x}_i^m.$$

Equivalent to:

$$v_j = \sum_{m=0}^{p-1} \mathbf{C}_m \bullet \mathbf{Compress}\left((\mathbf{y}_j - \mathbf{x}_*)^m\right) + \text{Residual}, \qquad \mathbf{C}_m = \frac{1}{m!} \sum_{i=1}^{N} u_i e^{\mathbf{x}_* \bullet \mathbf{x}_i} \mathbf{Compress}(\mathbf{x}_i^m).$$

Number of multiplications (complexity) to obtain v_j:

$$Complexity = 1 + 2 + \ldots + p = \frac{p(p+1)}{2}.$$

Compression Can be Performed for any Dimensionality (Example for 3D):

$$\mathbf{a}^n \bullet \mathbf{b}^n = (\mathbf{a} \bullet \mathbf{b})^n = (a_1b_1 + a_2b_2 + a_3b_3)^n$$

$$= [(a_1b_1 + a_2b_2) + a_3b_3]^n = \sum_{m=0}^{n} \binom{n}{m} (a_1b_1 + a_2b_2)^{n-m} a_3^m b_3^m$$

$$= \sum_{m=0}^{n} \sum_{l=0}^{n-m} \binom{n}{m} \binom{n-m}{l} a_1^{n-m-l} b_1^{n-m-l} a_2^l b_2^l a_3^m b_3^m$$

$$= a_1^n b_1^n + \binom{n}{1} a_1^{n-1} b_1^{n-1} a_2 b_2 + \binom{n}{2} a_1^{n-2} b_1^{n-2} a_2^2 b_2^2 + \ldots + a_2^n b_2^n$$

$$+ \binom{n}{1} a_1^{n-1} b_1^{n-1} a_3 b_3 + \binom{n}{1}\binom{n-1}{1} a_1^{n-2} b_1^{n-2} a_2 b_2 a_3 b_3 + \ldots + a_3^n b_3^n,$$

$$\mathbf{Compress}(\mathbf{a}^n) = \left(a_1^n, \sqrt{\binom{n}{1}} a_1^{n-1} a_2, \sqrt{\binom{n}{2}} a_1^{n-2} a_2^2, \ldots, a_2^n, \sqrt{\binom{n}{1}} a_1^{n-1} a_3, \ldots, a_3^n \right)$$

The length of $\mathbf{a}^n$ is $(n+1)+n+\ldots+1 = (n+1)(n+2)/2$

Compression Can be Performed for any Dimensionality (General Case):

$$(a_1 + a_2 + \ldots + a_d)^n = \sum_{n_1 + \ldots + n_d = n} (n, n_1, n_2, \ldots, n_d) a_1^{n_1} a_2^{n_2} \ldots a_d^{n_d}.$$

$$(n, n_1, n_2, \ldots, n_d) = \frac{n!}{n_1! n_2! \ldots n_d!}.$$

Multinomial coefficients

$$\mathbf{Compress}(\mathbf{a}^n) = \left(a_1^n, \sqrt{(n, n-1, 1, 0, \ldots, 0)} a_1^{n-1} a_2, \ldots, \sqrt{(n, n_1, n_2, \ldots, n_d)} a_1^{n_1} a_2^{n_2} \ldots a_d^{n_d}, \ldots, a_d^n \right)$$

So we have

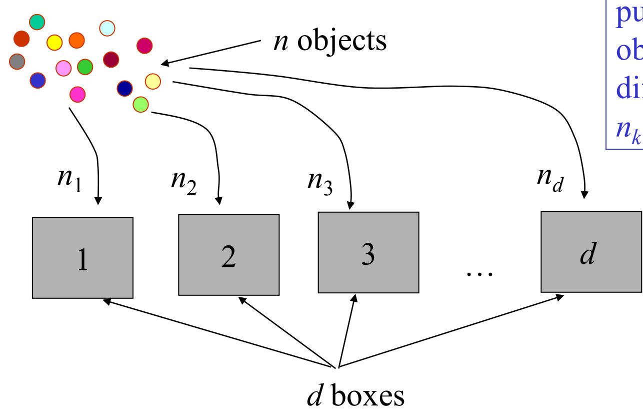
$$\mathbf{a}^n \cdot \mathbf{b}^n = \mathbf{Compress}(\mathbf{a}^n) \cdot \mathbf{Compress}(\mathbf{b}^n)$$

$$= \sum_{n_1 + \ldots + n_d = n} (n, n_1, n_2, \ldots, n_d) a_1^{n_1} a_2^{n_2} \ldots a_d^{n_d} b_1^{n_1} b_2^{n_2} \ldots b_d^{n_d}$$

$$= (a_1b_1 + a_2b_2 + \ldots + a_db_d)^n = (\mathbf{a} \cdot \mathbf{b})^n.$$

What are multinomial coefficients?

$(n\,; n_1, n_2, \ldots, n_d)$ is the number of ways of putting n different objects into d different boxes with n_k in the k-th box



$$n_1 + n_2 + \ldots + n_d = n$$

The length of the compressed vector

$$d = 1: \quad 1,$$
$$d = 2: \quad n - 1,$$
$$d = 3: \quad \frac{1}{2}(n-1)(n-2),$$

…

Theorem: If $\mathbf{a} \in \mathbb{R}^d$, then the length of compressed vector $\mathbf{Compress}(\mathbf{a}^n)$ is

$$\binom{n-d-1}{n} = \frac{(n-1)\ldots(n-d-1)}{(d-1)!}.$$

Proof: We have a basis for induction (see above). Let this holds for d dimensions. Consider $d+1$ dimensions:

$$((a_1 + \ldots + a_d) + a_{d+1})^n = \sum_{m=0}^{n} \binom{n}{m} (a_1 + \ldots + a_d)^m a_{d+1}^{n-m}$$

The number of terms is then

$$\sum_{m=0}^{n} \binom{m+d-1}{m} = \binom{d-1}{0} + \binom{d}{1} + \ldots + \binom{n+d-1}{n} = \binom{n+d}{n}$$

This proves the theorem.

Example of Fast Computation

$$v_j = \sum_{i=1}^{N} u_i \Phi(\mathbf{y}_j, \mathbf{x}_i) = \sum_{m=0}^{p-1} \mathbf{c}_m \bullet (\mathbf{y}_j - \mathbf{x}_*)^m + \text{Residual}, \qquad \mathbf{c}_m = \frac{1}{m!} \sum_{i=1}^{N} u_i e^{\mathbf{x}_* \cdot \mathbf{x}_i} \mathbf{x}_i^m.$$

Equivalent to:

$$v_j = \sum_{m=0}^{p-1} \mathbf{C}_m \bullet \mathbf{Compress}\left((\mathbf{y}_j - \mathbf{x}_*)^m\right) + \text{Residual}, \qquad \mathbf{C}_m = \frac{1}{m!} \sum_{i=1}^{N} u_i e^{\mathbf{x}_* \cdot \mathbf{x}_i} \mathbf{Compress}(\mathbf{x}_i^m).$$

Number of multiplications (complexity) to obtain v_j: (in 2D case!)

$$Complexity = 1 + 2 + \ldots + p = \frac{p(p+1)}{2}.$$

$$\mathbf{C}_0 = \sum_{i=1}^{N} u_i e^{\mathbf{x}_* \cdot \mathbf{x}_i},$$

$$\mathbf{C}_1 = (C_{11}, C_{12}) = \sum_{i=1}^{N} u_i e^{\mathbf{x}_* \cdot \mathbf{x}_i} (x_{i1}, x_{i2}),$$

$$\mathbf{C}_2 = (C_{21}, C_{22}, C_{23}) = \sum_{i=1}^{N} u_i e^{\mathbf{x}_* \cdot \mathbf{x}_i} \left(x_{i1}^2, \sqrt{2} x_{i1} x_{i2}, x_{i2}^2\right),$$

Complexity of Fast Summation

Let $\circ$ be a scalar product of vectors $\mathbf{A}_i$ and $\mathbf{F}_j$ of length $P(p)$ (p is the truncation number).
Complexity of summation over i is then $O(PN)$.
Complexity of scalar product operation is P.
Complexity of M scalar product operations is $O(PM)$ (for $j = 1,\ldots,M$).
Total complexity is $O(PM + PN)$.
Fast Method is more efficient than direct only if $O(PM + PN) < O(MN)$,
so we should have

$$P(p) \ll \min(M,N)$$