FMM CMSC 878R/AMSC 698R

Lecture 3

Outline

- 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 continous 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_*.

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

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

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 $x_i > 0, x_* \geqslant 0$) :

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

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

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

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

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

$$f(y_1, y_2, \ldots, y_d) = \sum_{m_1=0}^{\infty} \frac{1}{m_1!} \frac{\partial^{m_1} f}{\partial y_1^{m_1}}(x_{*1}, y_2, \ldots, y_d)(y_1 - x_{*1})^{m_1}$$

$$= \sum_{m_1=0}^{\infty} \frac{1}{m_1!} \sum_{m_2=0}^{\infty} \frac{1}{m_2!} \frac{\partial^{m_1}}{\partial y_1^{m_1}} \frac{\partial^{m_2}}{\partial y_2^{m_2}} f(x_{*1}, x_{*2}, \ldots, y_d)(y_1 - x_{*1})^{m_1}(y_2 - x_{*2})^{m_2}$$

$$= \ldots$$

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

Multidimensional Taylor Series (using some vector algebra)

Operator ∇ :

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

Differential along direction $\mathbf{s}$:

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

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

$$f(\mathbf{y}) = f(\mathbf{x}_*) + \frac{df(\mathbf{x}_*)}{ds}|\mathbf{y} - \mathbf{x}_*| + \frac{1}{2!}\frac{d^2 f(\mathbf{x}_*)}{ds^2}|\mathbf{y} - \mathbf{x}_*|^2 + \ldots$$

$$= f(\mathbf{x}_*) + [(\mathbf{y} - \mathbf{x}_*) \cdot \boldsymbol{\nabla}] f(\mathbf{x}_*) + \frac{1}{2!}[(\mathbf{y} - \mathbf{x}_*) \cdot \boldsymbol{\nabla}]^2 f(\mathbf{x}_*) + \ldots$$

$$= \sum_{m=0}^{\infty} \frac{1}{m!}[(\mathbf{y} - \mathbf{x}_*) \cdot \boldsymbol{\nabla}]^m f(\mathbf{x}_*).$$

Example

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

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

$$\Phi(\mathbf{x}_*,\mathbf{x}_i) = e^{\mathbf{x}_*\cdot\mathbf{x}_i},$$

$$\nabla_{\mathbf{x}_*}\Phi(\mathbf{x}_*,\mathbf{x}_i) = \mathbf{x}_i e^{\mathbf{x}_*\cdot\mathbf{x}_i} = \mathbf{x}_i\Phi(\mathbf{x}_*,\mathbf{x}_i),$$

$$\left[(\mathbf{y}-\mathbf{x}_*)\cdot\nabla_{\mathbf{x}_*}\right]\Phi(\mathbf{x}_*,\mathbf{x}_i) = \left[(\mathbf{y}-\mathbf{x}_*)\cdot\mathbf{x}_i\right]\Phi(\mathbf{x}_*,\mathbf{x}_i),$$

$$\left[(\mathbf{y}-\mathbf{x}_*)\cdot\nabla_{\mathbf{x}_*}\right]^m\Phi(\mathbf{x}_*,\mathbf{x}_i) = \left[(\mathbf{y}-\mathbf{x}_*)\cdot\mathbf{x}_i\right]^m\Phi(\mathbf{x}_*,\mathbf{x}_i),$$

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

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

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:

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

Distributivity:

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

Factorization of Scalar Product Powers

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

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

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

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

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

Is That Factorization?

1) Truncation:

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

2) Fast summation:

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

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

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

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

Yes! It is!

Multidimensional Taylor series

- Taylor series

$$f(x+h) = f(x) + h\frac{df}{dx} + \frac{h^2}{2!}\frac{d^2f}{dx^2} + \ldots.$$

In multiple dimensions

$$f(\mathbf{x}+\mathbf{h}) = f(\mathbf{x}) + \mathbf{h} \bullet \nabla f + (\mathbf{hh}) : \nabla\nabla f + (\mathbf{hhh}) : \nabla\nabla\nabla f + \ldots$$

What are these things

$$\mathbf{hh}, \quad \mathbf{hhh}, \quad \nabla\nabla f, \quad \nabla\nabla\nabla f, \quad \ldots$$

$$h_i h_j \quad h_i h_j h_k \quad \frac{\partial}{\partial x_i}\frac{\partial f}{\partial x_j} \quad \frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j}\frac{\partial f}{\partial x_k}\bigg|$$

Products of vectors & matrices

- Scalar multiplication. Multiply each element by a scalar. $\alpha \mathbf{A} = \alpha A_{ij}$
- Dot product of two vectors with same dimension

$$\mathbf{x}^{t}\,\mathbf{y} = \mathbf{x} \cdot \mathbf{y} = \sum_{\mathrm{i}} x_i\, y_i = x_i\, y_i$$

- Dot product of Matrix with vector

$$\mathbf{A}\,\mathbf{y} = \mathbf{A} \cdot \mathbf{y} = \sum_{\mathrm{j}} A_{ij}\, y_j = x_i$$

- Contraction of two matrixes

$$c\mathbf{=A:B} \qquad c=\sum_{\mathrm{i}}\sum_{\mathrm{j}} A_{ij}B_{ij}$$

- Hadamard product: element by element product

$$\mathbf{C=A}\odot\mathbf{B} \qquad C_{ij}=A_{ij}B_{ij}$$

- Tensor product or Dyadic product

$$\mathbf{C=A\ B} \qquad C_{ijkl}=A_{ij}B_{kl}$$

Products of vectors

- Higher order terms in Taylor series become contractions of Tensor products

Arrange things in a matrix

$$\begin{bmatrix} h_1 h_1 & h_1 h_2 \\ h_2 h_1 & h_2 h_2 \end{bmatrix} \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial}{\partial x_1}\frac{\partial f}{\partial x_2} \\ \frac{\partial}{\partial x_2}\frac{\partial f}{\partial x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix}$$

Contraction

$$\mathbf{hh} : \nabla\nabla\mathbf{f} = h_1^2 \frac{\partial^2 f}{\partial x_1^2} + 2h_1 h_2 \frac{\partial^2 f}{\partial x_1 \partial x_2} + h_2^2 \frac{\partial^2 f}{\partial x_2^2}$$

- However TPs involve higher dimensional things
- Not convenient to treat using matrices and vectors
- Need another kind of product to achieve same result with regular 2-D matrices and vectors

Kronecker Product

- A way to represent products of vectors and matrices that create higher dimensional objects
- KP of $n \times m$ matrix A and $p \times q$ matrix B

$$A = \begin{bmatrix} a_{1,1} & \cdots & a_{1,m} \\ \vdots & \ddots & \vdots \\ a_{n,1} & \cdots & a_{n,m} \end{bmatrix}_{n \times m} \qquad B = \begin{bmatrix} b_{1,1} & \cdots & b_{1,q} \\ \vdots & \ddots & \vdots \\ b_{p,1} & \cdots & b_{p,q} \end{bmatrix}_{p \times q}$$

Kronecker product, denoted $A \otimes B$, is the $np \times mq$ matrix with the block structur

$$A \otimes B = \begin{bmatrix} a_{1,1}B & \cdots & a_{1,m}B \\ \vdots & \ddots & \vdots \\ a_{n,1}B & \cdots & a_{n,m}B \end{bmatrix}_{np \times mq} .$$

$$A = \begin{bmatrix} 1 & 2 \\ 0 & -1 \end{bmatrix}_{2\times 2} \qquad B_{2\times 3} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}_{2\times 3}$$

$A \otimes B$ is

$$A \otimes B = \begin{bmatrix} 1 & 2 & 3 & 2 & 4 & 6 \\ 4 & 5 & 6 & 8 & 10 & 12 \\ 0 & 0 & 0 & -1 & -2 & -3 \\ 0 & 0 & 0 & -4 & -5 & -6 \end{bmatrix}_{4\times 6} .$$

Properties of the Kronecker Product

- Bilinear
  $$A \otimes (\alpha B) = \alpha (A \otimes B)$$
  $$(\alpha A) \otimes B = \alpha (A \otimes B).$$
- Distributes over addition
  $$(A + B) \otimes C = (A \otimes C) + (B \otimes C)$$
  $$A \otimes (B + C) = (A \otimes B) + (A \otimes C).$$
- Associative
  $$(A \otimes B) \otimes C = A \otimes (B \otimes C)$$
- NOT commutative
  $$(A \otimes B) \neq (B \otimes A).$$
- Transpose distributes
  $$(A \otimes B)^T = A^T \otimes B^T.$$
- Matrix multiplication
  $$(A \otimes B)(C \otimes D) = (AC \otimes BD).$$
- Inverse
  $$(A \otimes B)^{-1} = (A^{-1} \otimes B^{-1}).$$

From http://robotics.me.jhu.edu/~llw/courses/me530647/kron_1.pdf

- If you recognize the Kronecker product structure then it can result in great savings
  - Inverse: If a matrix is a KP of two $N \times N$ matrices (I.e., is $N^2 \times N^2$), then can construct inverse via KP in $O(N^3)$ operations. Need $O(N^6)$ operations otherwise
- In the case of Taylor series we use KP notation to perform factorization

- Advantage
- Use regular data structures
- More importantly can do things efficiently
- FMM factorization can be viewed as approximation by a sum of Kronecker products

$$\sum_{i=1}^{N} \Phi(x_i, y_j) u_i = v_j$$

$$\sum_{i=1}^{N} \Phi(x_i, y_j) u_i = \sum_{i=1}^{N} u_i \sum_{l=0}^{p} a_l(x_i, x_*) b_l(x_*, y_j)$$

$$v_j = \sum_{l=0}^{p} b_l(x_*, y_j) \sum_{i=1}^{N} u_i a_l(x_i, x_*)$$

- More later …