Outline

• Power and Taylor Series
  – Power Series in 1D
  – Taylor Series in 1D
• Multidimensional Taylor Series
• Factorization of Scalar Products in $\mathbb{R}^d$
• Compression of Factorized Series
• Factorization of Scalar Products in $\mathbb{R}^d$ (compression)
  – Factorization in 2D.
  – Factorization in 3D.
  – Factorization in $dD$. 
  – 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 $|y - x_*| < q$. 
2) Convergent power series can be summed, multiplied by a scalar, or multiplied according to the Cauchy rule.

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

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

\[
\sum_{m=0}^{\infty} a_m (y-x_\ast)^m + \sum_{m=0}^{\infty} b_m (y-x_\ast)^m = \sum_{m=0}^{\infty} (a_m + b_m) (y-x_\ast)^m,
\]

\[
a \sum_{m=0}^{\infty} a_m (y-x_\ast)^m = \sum_{m=0}^{\infty} a a_m (y-x_\ast)^m,
\]

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

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

Lagrange evaluation:

$$\text{Residual}_n(y) = \int_{x_*}^y dx \int_{x_*}^x dx_1 \int_{x_*}^{x_1} dx_2 \ldots \int_{x_*}^{x_{n-1}} dx_n f^{(n)}(x_1)dx_2 \ldots dx_n = \frac{1}{n!}f^{(n)}(X)(y - x_*)^n,$$

where $X \in (x_*, x_* + r_*).

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

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 $|y - x_*| \leq q$, where $0 \leq q \leq r$. 
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 \(x_i > 0, x_* \geq 0\)):

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

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

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

Let $f(y)$ be a real function,

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

Then we can write

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

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

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

$$= \ldots$$

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

Operator $\nabla$:

$$\nabla = i_1 \frac{\partial}{\partial y_1} + \ldots + i_d \frac{\partial}{\partial y_d}.$$ 

Differential along direction $s$:

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

Taylor series (let $s = (y - x_\ast)/|y - x_\ast|$)

$$f(y) = f(x_\ast) + \frac{df(x_\ast)}{ds} |y - x_\ast| + \frac{1}{2!} \frac{d^2f(x_\ast)}{ds^2} |y - x_\ast|^2 + \ldots$$

$$= f(x_\ast) + [(y - x_\ast) \cdot \nabla]f(x_\ast) + \frac{1}{2!} [(y - x_\ast) \cdot \nabla]^2 f(x_\ast) + \ldots$$

$$= \sum_{m=0}^{\infty} \frac{1}{m!} [(y - x_\ast) \cdot \nabla]^m f(x_\ast).$$
Example

\[ \Phi(y, x_i) = e^{y \cdot x_i} = \sum_{m=0}^{\infty} \frac{1}{m!} \left[ (y - x_*) \cdot \nabla_{x_*} \right]^m \Phi(x_*, x_i), \]

Fix \((y - x_*):\)

\[ \Phi(x_*, x_i) = e^{x_* \cdot x_i}, \]

\[ \nabla_{x_*} \Phi(x_*, x_i) = x_i e^{x_* \cdot x_i} = x_i \Phi(x_*, x_i), \]

\[ \left[ (y - x_*) \cdot \nabla_{x_*} \right] \Phi(x_*, x_i) = \left[ (y - x_*) \cdot x_i \right] \Phi(x_*, x_i), \]

\[ \left[ (y - x_*) \cdot \nabla_{x_*} \right]^m \Phi(x_*, x_i) = \left[ (y - x_*) \cdot x_i \right]^m \Phi(x_*, x_i), \]

\[ \Phi(y, x_i) = \sum_{m=0}^{\infty} \frac{1}{m!} \left[ (y - x_*) \cdot x_i \right]^m \Phi(x_*, x_i) = e^{x_* \cdot x_i} \sum_{m=0}^{\infty} \frac{1}{m!} \left[ (y - x_*) \cdot x_i \right]^m. \]

Check: \[ e^{y \cdot x_i} = e^{x_* \cdot x_i} e^{(y - x_*) \cdot x_i} = e^{x_* \cdot x_i} \sum_{m=0}^{\infty} \frac{1}{m!} \left[ (y - x_*) \cdot x_i \right]^m. \]
Is That a Factorization?

\[ e^{y \cdot x_i} = e^{x^* \cdot x_i} \sum_{m=0}^{\infty} \frac{1}{m!} [ (y - x^*) \cdot x_i ]^m \]
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:

\[ \mathbf{a} \cdot \mathbf{b} = \bar{a}_1 \bar{b}_1 + \ldots + \bar{a}_d \bar{b}_d = \sum_{k=1}^{d} \bar{a}_k \bar{b}_k. \]
Properties of Scalar Product

Commutativity:

\[ a \cdot b = b \cdot a \]

Scaling:

\[ (\lambda a) \cdot b = a \cdot (\lambda b) = \lambda (a \cdot b), \quad \lambda \in \mathbb{R} \]

Distributivity:

\[ (a + b) \cdot c = a \cdot c + b \cdot c \]
Factorization of Scalar Product Powers

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

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

\[= [a \otimes a \otimes \ldots \otimes a] \cdot [b \otimes b \otimes \ldots \otimes b] = a^n \cdot b^n \]

\[a^n \cdot b^n = (a \cdot b)^n = (b \cdot a)^n = b^n \cdot a^n.\]

\[e^{y \cdot x_i} = e^{x_i \cdot x_i} \sum_{m=0}^{\infty} \frac{1}{m!} [(y - x_*) \cdot x_i]_m = e^{x_i \cdot x_i} \sum_{m=0}^{\infty} \frac{1}{m!} x_i^m \cdot (y - x_*)^m.\]
Is That Factorization?

1) Truncation:

\[ \Phi(y, x_i) = e^{y \cdot x_i} = e^{x_i \cdot x_i} \left[ \sum_{m=0}^{p-1} \frac{1}{m!} x_i^m \cdot (y - x_*)^m + \text{Residual}_p \right] \]

2) Fast summation:

\[
\begin{align*}
\mathbf{v}_j &= \sum_{i=1}^{N} u_i \Phi(y_j, x_i) = \sum_{i=1}^{N} u_i e^{x_i \cdot x_i} \left[ \sum_{m=0}^{p-1} \frac{1}{m!} x_i^m \cdot (y_j - x_*)^m + \text{Residual}_p \right] \\
&= \sum_{i=1}^{N} u_i e^{x_i \cdot x_i} \sum_{m=0}^{p-1} \frac{1}{m!} x_i^m \cdot (y_j - x_*)^m + N \max_i (u_i e^{x_i \cdot x_i}) \text{Residual}_p \\
&= \sum_{m=0}^{p-1} \frac{1}{m!} \left( \sum_{i=1}^{N} u_i e^{x_i \cdot x_i} x_i^m \right) \cdot (y_j - x_*)^m + \text{Residual} \\
&= \sum_{m=0}^{p-1} c_m \cdot (y_j - x_*)^m + \text{Residual}, \quad c_m = \frac{1}{m!} \sum_{i=1}^{N} u_i e^{x_i \cdot x_i} x_i^m .
\end{align*}
\]

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

\[ f(x + h) = f(x) + h \cdot \nabla f + (h^2) \cdot \nabla^2 f + (hh) \cdot \nabla^3 f + \ldots \]

What are these things

\[ hh, \ hhh, \ \nabla \nabla f, \ \nabla \nabla \nabla f, \ \ldots \]

\[ h_i h_j \ h_i h_j h_k \quad \frac{\partial}{\partial x_i} \quad \frac{\partial f}{\partial x_j} \quad \frac{\partial}{\partial x_i} \quad \frac{\partial}{\partial x_j} \quad \frac{\partial}{\partial x_k} \quad \frac{\partial f}{\partial x_k} \]
Products of vectors & matrices

• Scalar multiplication. Multiply each element by a scalar. \( \alpha \) 
  \[ A = \alpha A_{ij} \]

• Dot product of two vectors with same dimension
  \[ x^t \cdot y = \sum_i x_i y_i = x_i y_i \]

• Dot product of Matrix with vector
  \[ A \cdot y = \sum_j A_{ij} y_j = x_i \]

• Contraction of two matrixes
  \[ c = A : B \quad c = \sum_i \sum_j A_{ij} B_{ij} \]

• Hadamard product: element by element product
  \[ C = A \odot B \quad C_{ij} = A_{ij} B_{ij} \]

• Tensor product or Dyadic product
  \[ C = A \otimes B \quad C_{ijkl} = A_{ij} B_{kl} \]
Products of vectors

- Higher order terms in Taylor series become contractions of Tensor products
  
  Arrange things in a matrix

\[
\begin{bmatrix}
h_1h_1 & h_1h_2 \\
h_2h_1 & h_2h_2
\end{bmatrix}
\begin{bmatrix}
\frac{\partial^2f}{\partial x_1^2} & \frac{\partial f}{\partial x_1} & \frac{\partial^2f}{\partial x_2^2} \\
\frac{\partial}{\partial x_2} & \frac{\partial f}{\partial x_1} & \frac{\partial^2f}{\partial x_2}
\end{bmatrix}
\]

Contraction

\[
\mathbf{hh} : \nabla \nabla \mathbf{f} = h_1^2 \frac{\partial^2f}{\partial x_1^2} + 2h_1h_2 \frac{\partial^2f}{\partial x_1 \partial x_2} + h_2^2 \frac{\partial^2f}{\partial x_2^2}
\]

- 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 $B$

\[
A = \begin{bmatrix}
a_{1,1} & \ldots & a_{1,m} \\
\vdots & \ddots & \vdots \\
a_{n,1} & \ldots & a_{n,m}
\end{bmatrix}_{n \times m} \quad B = \begin{bmatrix}
b_{1,1} & \ldots & b_{1,q} \\
\vdots & \ddots & \vdots \\
b_{p,1} & \ldots & b_{p,q}
\end{bmatrix}_{p \times q}
\]

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

\[
A \otimes B = \begin{bmatrix}
a_{1,1}B & \ldots & a_{1,m}B \\
\vdots & \ddots & \vdots \\
a_{n,1}B & \ldots & a_{n,m}B
\end{bmatrix}_{np \times mq}
\]
\[ A = \begin{bmatrix} 1 & 2 \\ 0 & -1 \end{bmatrix}_{2 \times 2} \quad B_{2 \times 3} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}_{2 \times 3} \]

\( A \otimes B \) 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
  
  \[ (A \otimes B) \otimes C = A \otimes (B \otimes C') \]
  \[ (A \otimes B) \neq (B \otimes A). \]

- NOT commutative
  
  \[ (A \otimes B)^T = A^T \otimes B^T. \]

- Transpose distributes
  
  \[ (A \otimes B)(C \otimes D) = (AC \otimes BD) \]
  \[ (A \otimes B)^{-1} = (A^{-1} \otimes B^{-1}). \]

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 …