discrete Fourier transform : DFT

given $v = (v_0, v_1, \ldots, v_{N-1})^T \in \mathbb{C}^N$, define $\widehat{v} = (\widehat{v}_0, \widehat{v}_1, \ldots, \widehat{v}_{N-1})^T \in \mathbb{C}^N$

$$\widehat{v}_n = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} v_j e^{-2\pi i n j/N} \ , \ n = 0 : N-1$$

note : given $v(t)$ for $0 \le t \le 1$

define $\widetilde{v}_n = \int_0^1 v(t) e^{-2\pi i n t} dt$ for $n = 0, \pm 1, \ldots$: Fourier coefficients

set $\Delta t = 1/N$, $t_j = j/N$, $j = 0 : N-1$, $v_j = v(t_j)$

then $\widetilde{v}_n \approx \sum_{j=0}^{N-1} v_j e^{-2\pi i n t_j} \Delta t = \frac{1}{N} \sum_{j=0}^{N-1} v_j e^{-2\pi i n j/N} = \frac{1}{\sqrt{N}} \widehat{v}_n$

matrix form of DFT

$$\widehat{v}_n = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} v_j \omega^{nj} = \sum_{j=0}^{N-1} F_{nj} v_j = (Fv)_n \Rightarrow \widehat{v} = Fv$$

$\omega = e^{-2\pi i/N} \Rightarrow \omega^N = 1$

$F_{nj} = \frac{1}{\sqrt{N}} \omega^{nj}$, where $j = 0 : N-1$, $n = 0 : N-1$

$$F = \frac{1}{\sqrt{N}} \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega & \omega^2 & \cdots & \omega^{N-1} \\ 1 & \omega^2 & \omega^4 & \cdots & \omega^{2(N-1)} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & \omega^{N-1} & \omega^{2(N-1)} & \cdots & \omega^{(N-1)^2} \end{pmatrix} = F_N \in \mathbb{C}^{N \times N}$$

ex

$N = 2$, $\omega = -1$, $F_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & \omega \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$

$N = 4$, $\omega = -i$, $F_4 = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega & \omega^2 & \omega^3 \\ 1 & \omega^2 & \omega^4 & \omega^6 \\ 1 & \omega^3 & \omega^6 & \omega^9 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -i & -1 & i \\ 1 & -1 & 1 & -1 \\ 1 & i & -1 & -i \end{pmatrix}$

<u>claim</u>

1. F is symmetric, i.e. $F^T = F$, but F is not hermitian, i.e. $F^* \neq F$.

2. F is unitary, i.e. $F^*F = I$ and $F^{-1} = F^*$

<u>pf</u>

1. <u>ok</u>

2. $(F^*F)_{nj} = \sum_{k=0}^{N-1} F^*_{nk} F_{kj} = \frac{1}{N}\sum_{k=0}^{N-1} \overline{\omega}^{kn}\,\omega^{kj} = \frac{1}{N}\sum_{k=0}^{N-1} \omega^{(j-n)k}$, $\overline{\omega} = \omega^{-1}$

$$= \begin{cases} \frac{1}{N}\cdot\frac{\omega^{(j-n)N}-1}{\omega^{(j-n)}-1} & \text{if} \quad n \neq j \\ 1 & \text{if} \quad n = j \end{cases} = \begin{cases} 0 & \text{if} \quad n \neq j \\ 1 & \text{if} \quad n = j \end{cases}$$ <u>ok</u>

<u>note</u>

1. $\widehat{v} = Fv \;\Rightarrow\; v = F^*\widehat{v}$: inverse DFT , $v_j = \frac{1}{\sqrt{N}}\sum_{n=0}^{N-1} \widehat{v}_n e^{2\pi i n j/N}$

2. The columns of F^* form an orthonormal basis for $\mathbb{C}^N$. (<u>discrete Fourier basis</u>)

<u>ex</u>

$v(t) = \sin 2\pi k t$

assume $0 \leq k \leq N/2$

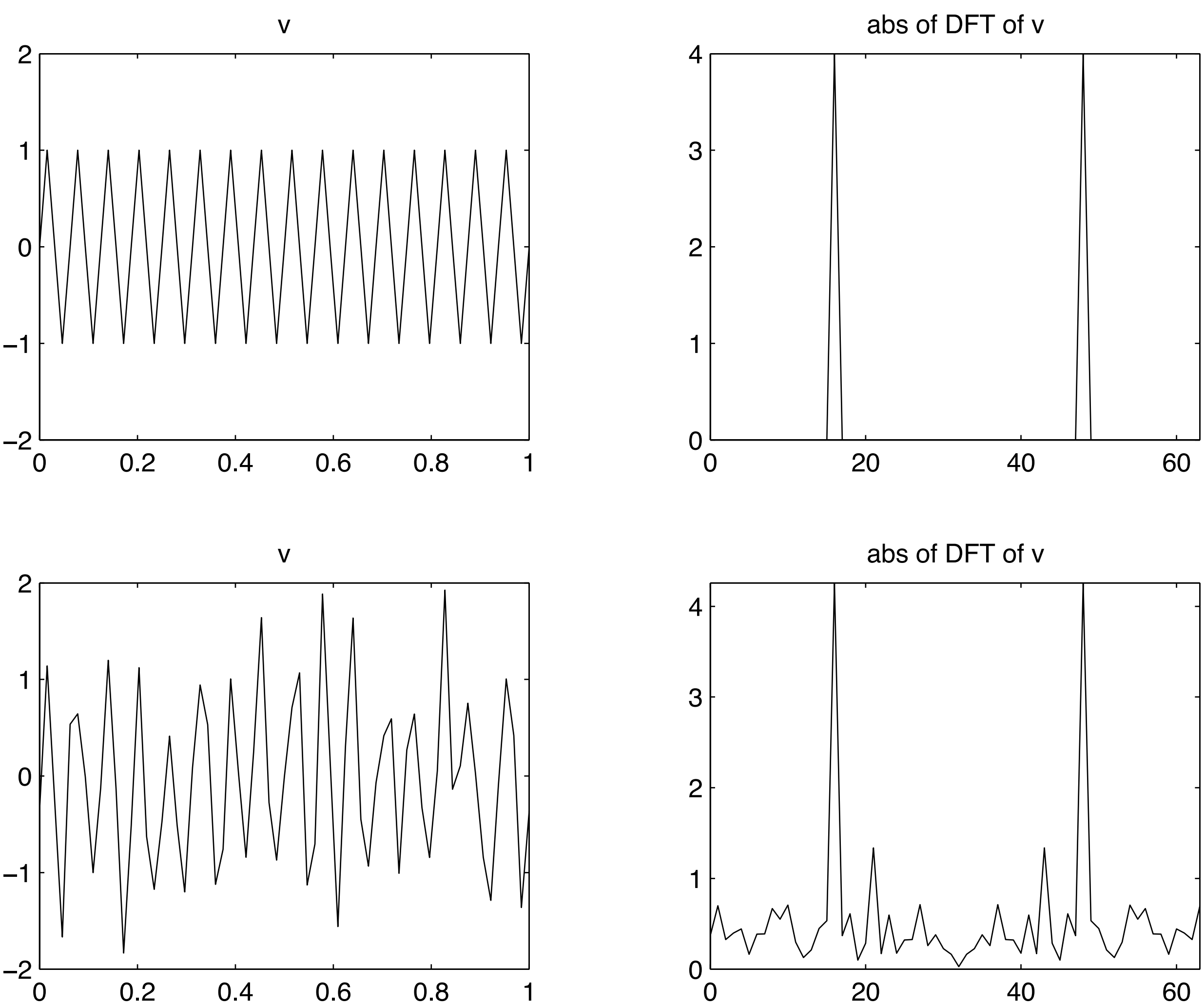
$$v_j = \sin 2\pi k t_j = \frac{e^{2\pi i k j/N} - e^{-2\pi i k j/N}}{2i} = \frac{e^{2\pi i k j/N} - e^{2\pi i (N-k) j/N}}{2i}$$

$$\Rightarrow \quad \widehat{v}_n = \begin{cases} \sqrt{N}/2i & \text{if} \;\; n = k \\ -\sqrt{N}/2i & \text{if} \;\; n = N-k \\ 0 & \text{otherwise} \end{cases}$$

for example : $N = 64\,,\; k = 16 \;\Rightarrow\; v_j = \sin 2\pi\cdot 16\cdot j/64 = \sin j\pi/2$

$\Rightarrow |\widehat{v}_{16}| = |\widehat{v}_{48}| = 4$, all other $\widehat{v}_n = 0$

```
% Matlab code for demonstrating DFT
N = 64;
dt = 1/N;
t = 0:dt:1;
k=16;
frame = 1;
for icase = 1:2
  v = sin(2*pi*k*t);
  if icase==2; v = v + 0.5*randn(1,N+1); frame = 3; end
  subplot(2,2,frame); plot(t,v); axis([0 1 -2 2]); title('v');
  vhat = fft(v,N)/sqrt(N); n = 0:N-1;
  subplot(2,2,frame+1); plot(n,abs(vhat));
  axis([0 N-1 0 max(abs(vhat))]); title('abs of DFT of v');
end
```



<u>note</u>

Computing $\widehat{v} = Fv$ by direct matrix-vector multiplication requires $O(N^2)$ operations, but F is a structured matrix with only N distinct entries and there is a fast algorithm (FFT) that requires only $O(N \log N)$ operations.

<u>idea</u> : $N = 8$, $\widehat{v} = F_8 v$

$$\widehat{v}_n = \frac{1}{\sqrt{8}}(v_0 + v_1\omega^n + v_2\omega^{2n} + v_3\omega^{3n} + v_4\omega^{4n} + v_5\omega^{5n} + v_6\omega^{6n} + v_7\omega^{7n})$$

$$= \frac{1}{\sqrt{8}}(v_0 + v_2(\omega^2)^n + v_4(\omega^2)^{2n} + v_6(\omega^2)^{3n} + \omega^n(v_1 + v_3(\omega^2)^n + v_5(\omega^2)^{2n} + v_7(\omega^2)^{3n}))$$

$\Rightarrow$ 1 DFT of length $N \approx 2$ DFTs of length $N/2$

<u>lemma</u> (Danielson-Lanczos)

$$F_{2M} = \frac{1}{\sqrt{2}} B_{2M}(F_M \oplus F_M)P_{2M} \ : \ \text{matrix factorization}$$

$$B_{2M} = \begin{pmatrix} I_M & \Omega_M \\ I_M & -\Omega_M \end{pmatrix} \ , \ \Omega_M = \text{diag}(\underset{\substack{\uparrow \\ e^{-2\pi i n/2M} = \omega^n \ , \text{ where } \omega = e^{-2\pi i/N}}}{e^{-\pi i n/M}}) \ , \ n = 0 : M-1 \ : \ \underline{\text{butterfly}}$$

$$F_M \oplus F_M = \begin{pmatrix} F_M & 0 \\ 0 & F_M \end{pmatrix}$$

$$P_{2M} = \begin{pmatrix} P_M^e \\ P_M^o \end{pmatrix} \ , \ \left.\begin{array}{l} (P_M^e)_{mn} = \delta_{2m,n} \\ (P_M^o)_{mn} = \delta_{2m+1,n} \end{array}\right\} \text{ for } m = 0 : M-1 \ , \ n = 0 : 2M-1$$

<u>ex</u> : $M = 4$, $2M = 8$

$$P_8 = \begin{pmatrix} P_4^e \\ \\ P_4^o \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \ , \ v = \begin{pmatrix} v_0 \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \end{pmatrix} \Rightarrow P_8 v = \begin{pmatrix} v_0 \\ v_2 \\ v_4 \\ v_6 \\ v_1 \\ v_3 \\ v_5 \\ v_7 \end{pmatrix}$$

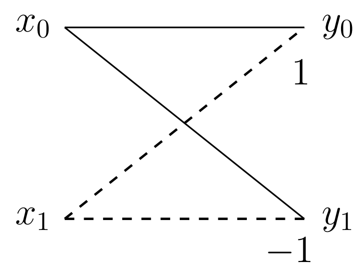
in general, if $v \in \mathbb{C}^{2M}$, then $\left.\begin{array}{l} (P_M^e v)_m = v_{2m} \\ (P_M^o v)_m = v_{2m+1} \end{array}\right\}$ for $m = 0 : M-1$

P_{2M} is a permutation matrix : <u>unshuffle</u>

why butterfly?

$$N = 2 \ , \ \omega = -1 \ , \ B_2 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

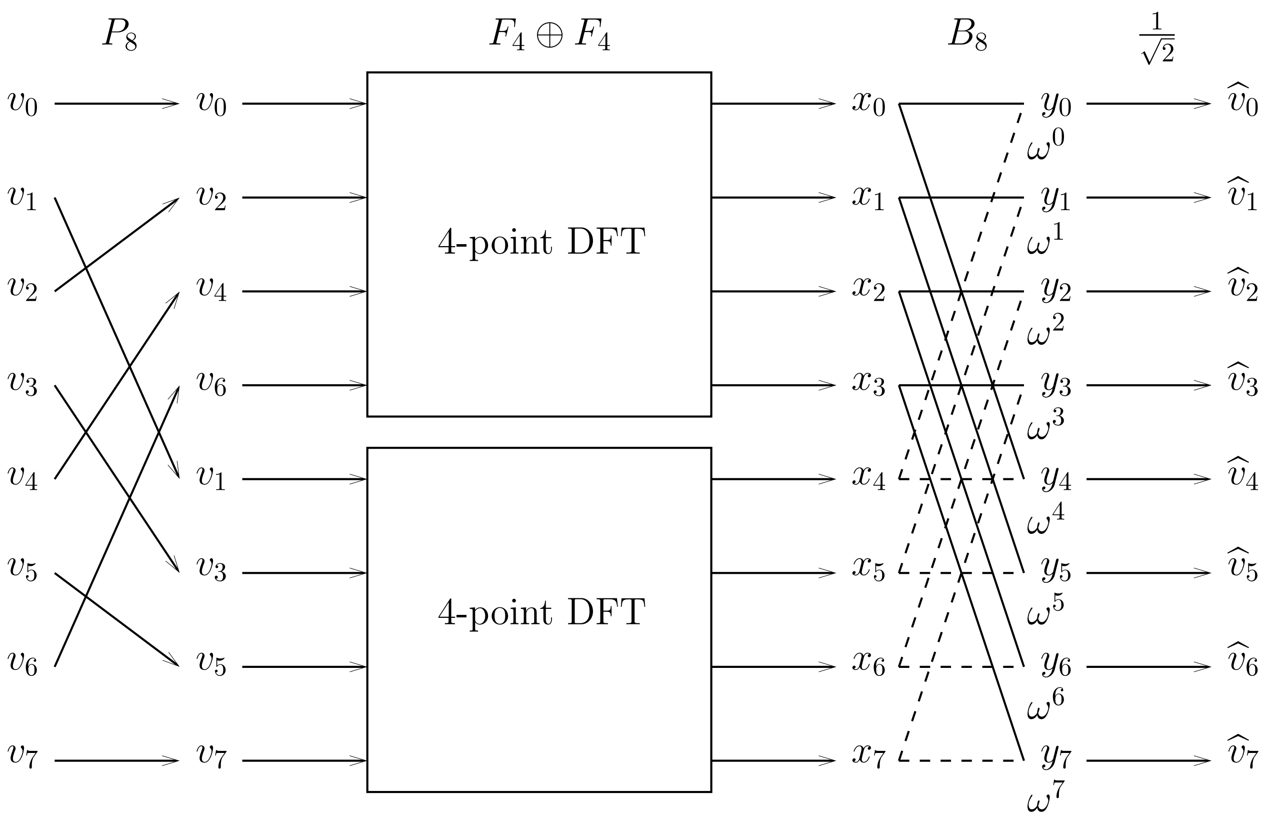
$$B_2 \begin{pmatrix} x_0 \\ x_1 \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \end{pmatrix} \ \Rightarrow \ \begin{matrix} x_0 + x_1 = y_0 \\ x_0 - x_1 = y_1 \end{matrix} \ \Rightarrow$$



$$N = 8 \ , \ B_8 = \left(\begin{array}{cccc:cccc} 1 & 0 & 0 & 0 & \omega^0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & \omega & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & \omega^2 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & \omega^3 \\ \hdashline 1 & 0 & 0 & 0 & -\omega^0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -\omega^1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -\omega^2 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & -\omega^3 \end{array}\right) , \ \omega = e^{-2\pi i/8} = e^{-\pi i/4}$$

note : $(-\omega^0, -\omega^1, -\omega^2, -\omega^3) = (\omega^4, \omega^5, \omega^6, \omega^7)$

8-point DFT : $F_8 v \ = \ \frac{1}{\sqrt{2}} \, B_8 \, (F_4 \oplus F_4) \, P_8 v \ = \ \widehat{v}$



<u>pf</u>

$$(F_{2M}v)_n = \frac{1}{\sqrt{2M}} \sum_{j=0}^{2M-1} v_j e^{-2\pi inj/2M}$$

$$= \frac{1}{\sqrt{2M}} \Big(\sum_{j=0}^{M-1} v_{2j} e^{-2\pi in(2j)/2M} + \sum_{j=0}^{M-1} v_{2j+1} e^{-2\pi in(2j+1)/2M} \Big)$$

$$= \frac{1}{\sqrt{2M}} \Big(\sum_{j=0}^{M-1} (P_M^e v)_j e^{-2\pi inj/M} + e^{-\pi in/M} \sum_{j=0}^{M-1} (P_M^o v)_j e^{-2\pi inj/M} \Big)$$

$$\frac{1}{\sqrt{2}} B_{2M}(F_M \oplus F_M) P_{2M}$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} I_M & \Omega_M \\ I_M & -\Omega_M \end{pmatrix} \begin{pmatrix} F_M & 0 \\ 0 & F_M \end{pmatrix} \begin{pmatrix} P_M^e \\ P_M^o \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} F_M & \Omega_M F_M \\ F_M & -\Omega_M F_M \end{pmatrix} \begin{pmatrix} P_M^e \\ P_M^o \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} F_M P_M^e + \Omega_M F_M P_M^o \\ F_M P_M^e - \Omega_M F_M P_M^o \end{pmatrix}$$

<u>case 1</u> : $n = 0 : M-1$

$$(F_{2M}v)_n = \frac{1}{\sqrt{2}}((F_M P_M^e v)_n + (\Omega_M F_M P_M^o v)_n)$$

<u>case 2</u> : $n = M : 2M-1$

for an M-point DFT , we need to replace n by $n - M$

$e^{-2\pi inj/M} = e^{-2\pi i(n-M)j/M}$, $e^{-\pi in/M} = -e^{-\pi i(n-M)/M}$

$$(F_{2M}v)_n = \frac{1}{\sqrt{2}}((F_M P_M^e v)_{n-M} - (\Omega_M F_M P_M^o v)_{n-M}) \qquad \underline{\text{ok}}$$

<u>thm</u> (FFT)

Let $N = 2^q$, $q \geq 1$.

Then $F_N = \dfrac{1}{\sqrt{N}} A_0^N A_1^N \cdots A_{q-1}^N P^N$, where P^N is a permutation matrix ,

$A_0^N = B_N$: 1 term,

$A_1^N = B_{N/2} \oplus B_{N/2}$: 2 terms,

$A_2^N = B_{N/4} \oplus B_{N/4} \oplus B_{N/4} \oplus B_{N/4}$: 4 terms,

$\cdots$

$A_{q-1}^N = B_{N/2^{q-1}} \oplus \cdots \oplus B_{N/2^{q-1}} = B_2 \oplus \cdots \oplus B_2$: $2^{q-1} = N/2$ terms,

and superscript N is the matrix dimension, not an N-fold product.

<u>pf</u> : induction on q

If $q = 1$, then $N = 2$, $A_0^2 = B_2 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$, and let $P^2 = I_2$.

Then $F_2 = \dfrac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \dfrac{1}{\sqrt{2}} A_0^2 P^2$ as required.

Assume true for $M = 2^{q-1}$, must show true for $N = 2^q = 2M$.

preliminaries

1. $A_k^N = B_{N/2^k} \oplus \cdots \oplus B_{N/2^k}$: 2^k terms

$\quad = B_{M/2^{k-1}} \oplus \cdots \oplus B_{M/2^{k-1}}$: $2 \cdot 2^{k-1}$ terms

$\quad = A_{k-1}^M \oplus A_{k-1}^M$

2. $(A \oplus B)(C \oplus D) = AC \oplus BD$, ...

$$
\begin{aligned}
F_N &= \frac{1}{\sqrt{2}} B_N (F_M \oplus F_M) P_N \\
&= \frac{1}{\sqrt{2}} A_0^N \Big(\frac{1}{\sqrt{M}} A_0^M A_1^M \cdots A_{q-2}^M P^M \oplus \frac{1}{\sqrt{M}} A_0^M A_1^M \cdots A_{q-2}^M P^M \Big) P_N \\
&= \frac{1}{\sqrt{2M}} A_0^N (A_0^M \oplus A_0^M)(A_1^M \oplus A_1^M) \cdots (A_{q-2}^M \oplus A_{q-2}^M)(P^M \oplus P^M) P_N \\
&= \frac{1}{\sqrt{N}} A_0^N A_1^N A_2^N \cdots A_{q-1}^N P^N \text{ , where } P^N = (P^M \oplus P^M) P_N \qquad \underline{\text{ok}}
\end{aligned}
$$

<u>operation count</u> for computing $F_N v = \dfrac{1}{\sqrt{N}} A_0^N A_1^N \cdots A_{q-1}^N P^N v$

applying P^N : N ops (more soon)

A_k^N has 2 nonzero entries in each row : $2N$ ops

multiplication by $\dfrac{1}{\sqrt{N}}$: N ops

total : $N + 2N \cdot q + N$ ops , $q = \log_2 N \Rightarrow O(N \log_2 N)$ ops

<u>interpretation of P^N</u>

Let $N = 2^q$. Then any n st $0 \leq n \leq N-1$ can be written as

$n = b_0 + b_1 \cdot 2 + b_2 \cdot 4 + \cdots + b_{q-1} \cdot 2^{q-1}$, where $b_j \in \{0, 1\}$.

$n = (b_{q-1}\, b_{q-2} \cdots b_1\, b_0)_2$

$n' = (b_{q-2} \cdots b_1\, b_0\, b_{q-1})_2$: <u>N-point periodic shift</u>

$n'' = (b_0\, b_1 \cdots b_{q-2}\, b_{q-1})_2$: <u>N-point bit-reversal</u>

<u>ex</u> : $q = 3$, $N = 8$

n	n'	n''
000	000	000
001	010	100
010	100	010
011	110	110
100	001	001
101	011	101
110	101	011
111	111	111

n	n'	n''
0	0	0
1	2	4
2	4	2
3	6	6
4	1	1
5	3	5
6	5	3
7	7	7

<u>claim</u> : $(P_N v)_n = v_{n'}$, $(P^N v)_n = v_{n''}$

<u>pf</u> : $N = 2^q = 2M$, $0 \leq n \leq N-1$

define $m = (b_{q-2} \cdots b_1\, b_0)_2$, so $0 \leq m \leq M-1$

then $n = b_{q-1} \cdot 2^{q-1} + m$, $n' = 2m + b_{q-1}$

1. $(P_N v)_n = \begin{cases} (P_M^e v)_m & \text{if } b_{q-1} = 0 \\ (P_M^o v)_m & \text{if } b_{q-1} = 1 \end{cases} = \begin{cases} v_{2m} & \text{if } b_{q-1} = 0 \\ v_{2m+1} & \text{if } b_{q-1} = 1 \end{cases} = v_{2m+b_{q-1}} = v_{n'}$

2. induction on q

$q = 1 \Rightarrow N = 2$, $P^2 = I_2$, $0 \le n \le 1$, $n = (b_0)_2 = n''$

now assume P^M is M-point bit reversal

must show $P^N = (P^M \oplus P^M)P_N$ is N-point bit reversal

$n'' = (b_0\, b_1\, \cdots\, b_{q-2}\, b_{q-1})_2 \;=\; 2m'' + b_{q-1}$

$$P^N = (P^M \oplus P^M)\begin{pmatrix} P_M^e \\ P_M^o \end{pmatrix} = \begin{pmatrix} P^M P_M^e \\ P^M P_M^o \end{pmatrix}$$

$$(P^N v)_n \;=\; \begin{cases} (P^M P_M^e v)_m & \text{if } \ b_{q-1} = 0 \\ (P^M P_M^o v)_m & \text{if } \ b_{q-1} = 1 \end{cases} \;=\; \begin{cases} (P_M^e v)_{m''} & \text{if } \ b_{q-1} = 0 \\ (P_M^o v)_{m''} & \text{if } \ b_{q-1} = 1 \end{cases}$$

$$= \begin{cases} v_{2m''} & \text{if } \ b_{q-1} = 0 \\ v_{2m''+1} & \text{if } \ b_{q-1} = 1 \end{cases} \;=\; v_{2m''+b_{q-1}} \;=\; v_{n''} \qquad \underline{\text{ok}}$$

<u>note</u>

1. FFT is based on divide-and-conquer, recursion, sparse factorization

2. $O(N \log N)$ ops, but this neglects the cost of memory access/communication

3. inverse FFT : $F_N^{-1} = F_N^* = \overline{F_N} = \dfrac{1}{\sqrt{N}}\, \overline{A_0^N}\ \overline{A_1^N} \cdots \overline{A_{q-1}^N}\ P^N$

4. variants

DST : $\widehat{v}_n = \sqrt{\dfrac{2}{N}}\, \displaystyle\sum_{j=1}^{N-1} v_j \sin\frac{\pi n j}{N}$, $n = 1 : N-1$

5. multi-dimensional versions

6. FFTW : code adapts to the machine it's running on , auto-tuning

<u>application</u> : trigonometric interpolation

Let $v(x)$ be given for $0 \le x \le 1$ and assume $v(0) = v(1)$.

$$v(x) = \sum_{n=-\infty}^{\infty} \widetilde{v}_n \, e^{2\pi i n x} \ , \ \widetilde{v}_n = \int_0^1 v(x) e^{-2\pi i n x} dx \ : \ \text{Fourier series}$$

set $v_j = v(x_j)$, $x_j = j/N$, $j = 0 : N-1$: uniform mesh

$$v_j = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \widehat{v}_n e^{2\pi i n x_j} \ , \ \widehat{v}_n = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} v_j e^{-2\pi i n x_j} \ , \ \text{pf} : \ v = F_N^* F_N v = F_N^* \widehat{v}$$

set $I_1(x) = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \widehat{v}_n e^{2\pi i n x}$: trigonometric polynomial

then $I_1(x) \approx v(x)$, two sources of error : finite N , $\widetilde{v}_n \neq \widehat{v}_n$

In fact, $I_1(x_j) = v_j$ for $j = 0 : N-1$, i.e. $I_1(x)$ <u>interpolates</u> $v(x)$ at $x = x_j$.

However, $I_1(x)$ is a poor approximation to $v(x)$ in between the mesh points; consider instead a balanced set of wavenumbers.

$$\text{set} \ \ I_2(x) = \frac{1}{\sqrt{N}} \sum_{n=-N/2}^{N/2-1} \widehat{v}_{n \bmod N} \, e^{2\pi i n x} \ , \ n \bmod N = \begin{cases} n & \text{if } n = 0 : N/2-1 \\ n+N & \text{if } n = -N/2 : -1 \end{cases}$$

1. e.g. $7 \bmod 16 = 7$, $-7 \bmod 16 = 9$

2. this assumes N is even; a similar formula is used if N is odd

$$\text{note} : \ \ I_2(x_j) = \frac{1}{\sqrt{N}} \sum_{n=-N/2}^{N/2-1} \widehat{v}_{n \bmod N} \, e^{2\pi i n x_j}$$

$$= \frac{1}{\sqrt{N}} \left(\sum_{n=0}^{N/2-1} \widehat{v}_n \, e^{2\pi i n j/N} + \sum_{n=-N/2}^{-1} \widehat{v}_{n+N} \, e^{2\pi i n j/N} \right)$$

$$= \frac{1}{\sqrt{N}} \left(\sum_{n=0}^{N/2-1} \widehat{v}_n \, e^{2\pi i n j/N} + \sum_{n=N/2}^{N-1} \widehat{v}_n \, e^{2\pi i (n-N) j/N} \right)$$

$$= \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \widehat{v}_n \, e^{2\pi i n j/N} = v_j$$

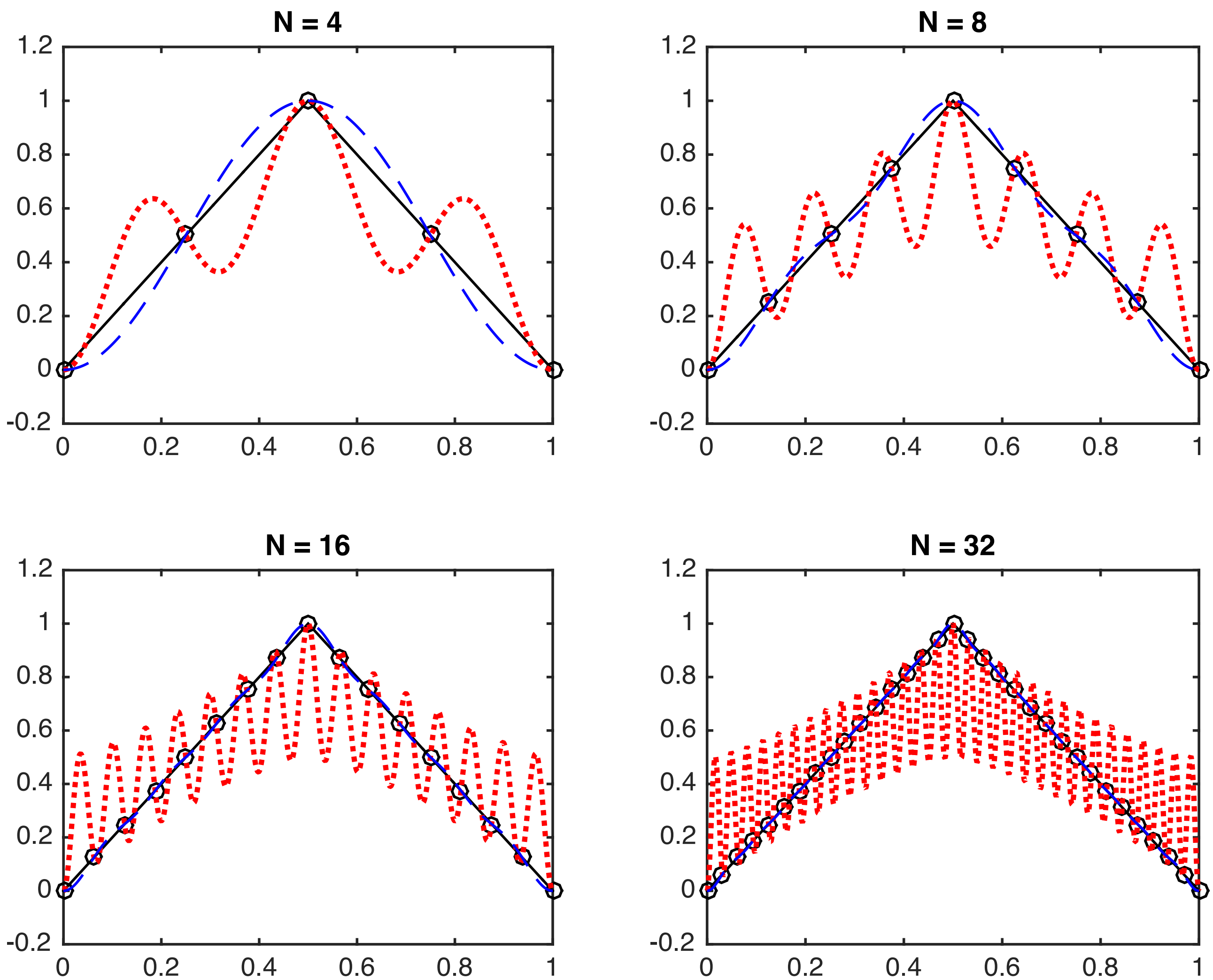
So $I_2(x)$ also interpolates $v(x)$ at $x = x_j$, but it gives a better approximation in between the mesh points.

<u>trigonometric interpolation</u>

$v(x) = 1 - 2|x - \frac{1}{2}|$

$$I_1(x) = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \widehat{v}_n e^{2\pi i n x} \;:\; \text{unbalanced}$$

$$I_2(x) = \frac{1}{\sqrt{N}} \sum_{n=-N/2}^{N/2-1} \widehat{v}_{n \bmod N}\, e^{2\pi i n x} \;:\; \text{balanced}$$



1. The balanced interpolant <u>converges uniformly</u> to the given function as $N \to \infty$, i.e. $\lim_{N\to\infty} \max_{0\le x\le 1} |v(x) - I_2(x)| = 0$.

2. The unbalanced interpolant does not converge uniformly to the given function.

application : BVP

given $f(x)$ for $0 \le x \le 1$ and $\sigma > 0$

find $\phi(x)$ st $-\phi'' + \sigma^2\phi = f$, $\phi(0) = \phi(1)$, $\phi'(0) = \phi'(1)$: PBC

We will consider 3 solution methods: finite-differences, pseudospectral, Green's function.

finite-difference scheme

set $h = 1/N$, $x_j = jh = j/N$ for $j = 0 : N-1$, $\phi_j = \phi(x_j)$, $f_j = f(x_j)$

$\phi_j'' = D_+D_-\phi_j + O(h^2)$, where $D_+D_-\phi_j = \dfrac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{h^2}$

u_j : numerical solution , $u_j \approx \phi_j$

$$-D_+D_-u_j + \sigma^2 u_j = f_j \;\Rightarrow\; \frac{-u_{j+1} + (2+\sigma^2h^2)u_j - u_{j-1}}{h^2} = f_j$$

$$j = 0 \quad\Rightarrow\quad \frac{-u_1 + (2+\sigma^2h^2)u_0 - u_{-1}}{h^2} = f_0 \quad , \quad u_{-1} = ?$$

$$j = N-1 \quad\Rightarrow\quad \frac{-u_N + (2+\sigma^2h^2)u_{N-1} - u_{N-2}}{h^2} = f_{N-1} \quad , \quad u_N = ?$$

PBC $\Rightarrow$ $\phi(x+1) = \phi(x)$, so we set $u_{-1} = u_{N-1}$, $u_N = u_0$

$$\frac{1}{h^2}\begin{pmatrix} 2+\sigma^2h^2 & -1 & & & & -1 \\ -1 & 2+\sigma^2h^2 & -1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots \\ & & & -1 & 2+\sigma^2h^2 & -1 \\ -1 & & & & -1 & 2+\sigma^2h^2 \end{pmatrix}\begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ \vdots \\ \vdots \\ u_{N-2} \\ u_{N-1} \end{pmatrix} = \begin{pmatrix} f_0 \\ f_1 \\ \vdots \\ \vdots \\ \vdots \\ f_{N-2} \\ f_{N-1} \end{pmatrix}$$

$Au = f$, A : symmetric, positive definite, almost tridiagonal, ...

solution methods : Cholesky, SOR, conjugate gradient, multigrid, FFT, ...

claim

The e-vectors of A are the columns of F_N^*.

pf

Let q be the nth column of F_N^* for some $n = 0 : N-1$.

$$q = \frac{1}{\sqrt{N}}(1, \omega^{-n}, \omega^{-2n}, \ldots, \omega^{-(N-1)n})^T \;\;,\;\; \omega = e^{-2\pi i/N}$$

$$Aq = \lambda q \;\Leftrightarrow\; (Aq)_j = \lambda q_j \;\text{ for }\; j = 0 : N-1$$

$$(Aq)_j \;=\; \frac{-q_{j+1} + (2+\sigma^2 h^2)q_j - q_{j-1}}{h^2} \;\;,\;\; \text{set } q_{-1} = q_{N-1}\,,\, q_N = q_0$$

$$\Rightarrow\; \frac{1}{\sqrt{N}} \frac{-\omega^{-(j+1)n} + (2+\sigma^2 h^2)\omega^{-jn} - \omega^{-(j-1)n}}{h^2} \;=\; \lambda \frac{1}{\sqrt{N}}\,\omega^{-jn}$$

$$\Rightarrow\; \lambda \;=\; \frac{-\omega^{-n} + (2+\sigma^2 h^2) - \omega^n}{h^2} \;=\; \frac{2+\sigma^2 h^2 - (e^{2\pi i n/N} + e^{-2\pi i n/N})}{h^2}$$

$$= \;\frac{2(1-\cos(2\pi n/N)) + \sigma^2 h^2}{h^2} \;=\; \frac{4\sin^2(\pi n h)}{h^2} + \sigma^2 \;=\; \lambda_n \quad \underline{\text{ok}}$$

note

$$\Rightarrow\; AF_N^* = F_N^* D \;\;,\;\; D = \text{diag}(\lambda_0, \ldots, \lambda_{N-1})$$

$$\Rightarrow\; A = F_N^* D F_N \;\;:\;\; \text{spectral factorization}$$

$$\Rightarrow\; u = A^{-1}f = F_N^* D^{-1} F_N f \;\;:\;\; O(N\log N) \text{ ops}$$

Next we'll show that this is a general fact.

def

Given $(c_0, \ldots, c_{N-1})^T \in \mathbb{C}^N$, define $C = (C_{nj}) = c_{(n-j)\text{mod}N}$: circulant matrix.

ex : $N = 6$

$$C = \begin{pmatrix} c_0 & c_5 & c_4 & c_3 & c_2 & c_1 \\ c_1 & c_0 & c_5 & c_4 & c_3 & c_2 \\ c_2 & c_1 & c_0 & c_5 & c_4 & c_3 \\ c_3 & c_2 & c_1 & c_0 & c_5 & c_4 \\ c_4 & c_3 & c_2 & c_1 & c_0 & c_5 \\ c_5 & c_4 & c_3 & c_2 & c_1 & c_0 \end{pmatrix}$$

note

1. A circulant matrix has constant diagonals, and each column is a periodic shift of the previous column.

2. The finite-difference matrix A is circulant.

<u>def</u>

$c * v \;=\; Cv$: <u>convolution</u>

$$(c*v)_n \;=\; (Cv)_n \;=\sum_{j=0}^{N-1} C_{nj}v_j \;=\sum_{j=0}^{N-1} c_{(n-j)\mathrm{mod}N}v_j$$

$$=\; c_{n\mathrm{mod}N}v_0 \;+\; c_{(n-1)\mathrm{mod}N}v_1 \;+\;\cdots\;+\; c_{(n-(N-1))\mathrm{mod}N}v_{N-1}$$

<u>ex</u> : $N=6\,,\; n=3 \;\Rightarrow\; (c*v)_3 \;=\; c_3v_0 \;+\; c_2v_1 \;+\; c_1v_2 \;+\; c_0v_3 \;+\; c_5v_4 \;+\; c_4v_5$

<u>claim</u>

1. $\widehat{(c*v)} = \sqrt{N}\,\widehat{c}\,\widehat{v}$: component-wise product

2. $\langle c\,,v\rangle = \langle \widehat{c}\,,\widehat{v}\rangle$, where $\langle c\,,v\rangle = \sum_{j=0}^{N-1} c_j\overline{v_j}$: inner product

3. $C = F_N^*DF_N$, where $D = \mathrm{diag}(\sqrt{N}\,\widehat{c}_n)$

<u>pf</u>

1. $\widehat{(c*v)}_n = (F_N(c*v))_n \;=\dfrac{1}{\sqrt{N}}\sum_{j=0}^{N-1}\omega^{nj}(c*v)_j$, $\omega = e^{-2\pi i/N}$, $\omega^N = 1$

$$=\frac{1}{\sqrt{N}}\sum_{j=0}^{N-1}\omega^{nj}\sum_{k=0}^{N-1}c_{(j-k)\mathrm{mod}N}v_k$$

$$=\frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}\;\sum_{j=0}^{N-1}\omega^{n(j-k)}c_{(j-k)\mathrm{mod}N}\cdot\omega^{nk}v_k \quad , \text{ set } l = j-k$$

$$=\frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}\;\sum_{l=-k}^{N-1-k}\omega^{nl}c_{l\mathrm{mod}N}\cdot\omega^{nk}v_k \;=\; \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}\;\sum_{l=0}^{N-1}\omega^{nl}c_l\cdot\omega^{nk}v_k$$

$$=\frac{1}{\sqrt{N}}\sum_{l=0}^{N-1}\omega^{nl}c_l\;\cdot\sum_{k=0}^{N-1}\omega^{nk}v_k = \sqrt{N}\,\widehat{c}_n\widehat{v}_n$$

2. $\langle \widehat{c}\,,\widehat{v}\rangle = \langle F_Nc\,,F_Nv\rangle = \langle c\,,F_N^*F_Nv\rangle = \langle c\,,v\rangle$

3. Let p and q be the mth and nth columns of F_N^*.

$F_N^*e_m = p$, $F_N^*e_n = q \;\Rightarrow\; e_m = F_Np = \widehat{p}$, $e_n = F_Nq = \widehat{q}$

$$\langle Cp\,,q\rangle = \langle c*p\,,q\rangle = \langle \widehat{(c*p)},\widehat{q}\,\rangle = \langle \sqrt{N}\,\widehat{c}\,\widehat{p}\,,\widehat{q}\,\rangle = \langle \sqrt{N}\,\widehat{c}\,e_m\,,\widehat{q}\,\rangle$$

$$= \langle \sqrt{N}\,\widehat{c}_m\,e_m\,,\widehat{q}\,\rangle = \langle De_m\,,\widehat{q}\,\rangle = \langle DF_Np\,,F_Nq\rangle = \langle F_N^*DF_Np\,,q\rangle$$ <u>ok</u>

<u>note</u> : The general expression for D agrees with the result derived for the e-values of the finite-difference matrix A. (hw2)

pseudospectral method

given u_j , $j = 0 : N-1$

set $I(x) = \dfrac{1}{\sqrt{N}} \displaystyle\sum_{n=-N/2}^{N/2-1} \widehat{u}_{n\text{mod}N}\, e^{2\pi i n x}$, so $I(x_j) = u_j$, $x_j = j/N$

set $u_j' = I'(x_j) = \dfrac{1}{\sqrt{N}} \displaystyle\sum_{n=-N/2}^{N/2-1} \widehat{u}_{n\text{mod}N}\, 2\pi i n\, e^{2\pi i n j/N}$

$$= \frac{1}{\sqrt{N}} \left(\sum_{n=0}^{N/2-1} \widehat{u}_n\, 2\pi i n\, e^{2\pi i n j/N} + \sum_{n=-N/2}^{-1} \widehat{u}_{n+N}\, 2\pi i n\, e^{2\pi i n j/N} \right)$$

$$\downarrow$$

$$\sum_{n=N/2}^{N-1} \widehat{u}_n\, 2\pi i (n-N) e^{2\pi i (n-N) j/N}$$

$$= \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \widehat{u}_n d_n e^{2\pi i n j/N} \ , \ \ d_n = \begin{cases} 2\pi i n & \text{if } n = 0 : N/2-1 \\ 2\pi i (n-N) & \text{if } n = N/2 : N-1 \end{cases}$$

$\Rightarrow$ $u' = F_N^* D F_N u$, $D = \text{diag}(d_n)$

$-\phi'' + \sigma^2 \phi = f \ \rightarrow \ -F_N^* D^2 F_N u + \sigma^2 u = f$

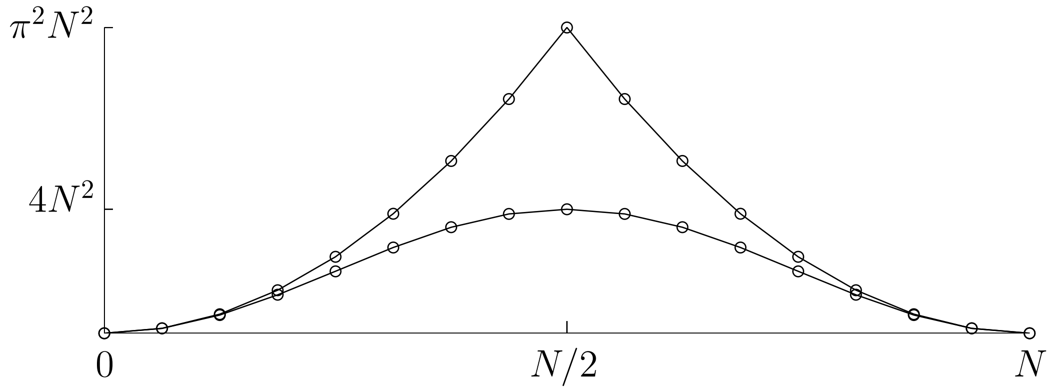
$\Rightarrow$ $F_N^*(-D^2 + \sigma^2 I) F_N u = f \Rightarrow u = F_N^*(-D^2 + \sigma^2 I)^{-1} F_N f$: $O(N \log N)$ ops

note

1. PBC are enforced by the choice of $I(x)$.

2. The pseudospectral scheme resembles the finite-difference/FFT scheme, but the diagonal matrix representing $-\phi''$ is different.

$$-d_{n,fd}^2 = \frac{4 \sin^2 \pi n h}{h^2} \ , \ -d_{n,ps}^2 = \begin{cases} 4\pi^2 n^2 & \text{if } n = 0 : N/2-1 \\ 4\pi^2 (n-N)^2 & \text{if } n = N/2 : N-1 \end{cases}$$



Green's function

$$-\phi'' + \sigma^2\phi = f \ , \ \phi(0) = \phi(1) \ , \ \phi'(0) = \phi'(1)$$

$$g(x,y) = \frac{\cosh\sigma(|x-y| - \frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} \quad , \quad 0 \le x \, , \, y \le 1$$

claim

1. $-g_{xx}(x,y) + \sigma^2 g(x,y) = 0$ for $x \neq y$

2. $g(y^+,y) = g(y^-,y)$, $g_x(y^+,y) - g_x(y^-,y) = -1$

note : properties 1 and 2 $\Leftrightarrow$ $-g_{xx}(x,y) + \sigma^2 g(x,y) = \delta(x-y)$

3. $g(0,y) = g(1,y)$, $g_x(0,y) = g_x(1,y)$ for $0 < y < 1$

4. $\phi(x) = \displaystyle\int_0^1 g(x,y) f(y)\, dy$

pf

$$g(x,y) = \begin{cases} \dfrac{\cosh\sigma(x-y-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} & \text{if } \ 0 \le y \le x \le 1 \\[2ex] \dfrac{\cosh\sigma(y-x-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} & \text{if } \ 0 \le x \le y \le 1 \end{cases}$$

$$g_x(x,y) = \begin{cases} \dfrac{\sigma\sinh\sigma(x-y-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} & \text{if } \ 0 \le y \le x \le 1 \\[2ex] \dfrac{-\sigma\sinh\sigma(y-x-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} & \text{if } \ 0 \le x \le y \le 1 \end{cases}$$

1. ok

2. $g(y^+,y) = \dfrac{\cosh(-\frac{1}{2}\sigma)}{2\sigma\sinh\frac{1}{2}\sigma} = g(y^-,y)$

$$g_x(y^+,y) - g_x(y^-,y) = -\frac{1}{2} - \frac{1}{2} = -1 \qquad \text{ok}$$

3. $g(0,y) = \dfrac{\cosh\sigma(y-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} = \dfrac{\cosh\sigma(\frac{1}{2}-y)}{2\sigma\sinh\frac{1}{2}\sigma} = g(1,x)$

$$g_x(0,y) = \frac{-\sigma\sinh\sigma(y-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} = \frac{\sigma\sinh\sigma(\frac{1}{2}-y)}{2\sigma\sinh\frac{1}{2}\sigma} = g_x(1,y) \qquad \text{ok}$$

4. define $\phi(x) = \displaystyle\int_0^1 g(x,y)f(y)\,dy$

$$\phi(0) = \int_0^1 g(0,y)f(y)\,dy = \int_0^1 g(1,y)f(y)\,dy = \phi(1)$$

$$\phi(x) = \int_0^x g(x,y)f(y)\,dy \, + \int_x^1 g(x,y)f(y)\,dy$$

$$\phi'(x) = \int_0^x g_x(x,y)f(y)\,dy \, + \int_x^1 g_x(x,y)f(y)\,dy \, + \, \cancelto{0}{(g(x,x^-) - g(x,x^+))}f(x)$$

$$\phi'(0) = \int_0^1 g_x(0,y)f(y)\,dy = \int_0^1 g_x(1,y)f(y)\,dy = \phi'(1)$$

$$\phi''(x) = \int_0^x g_{xx}(x,y)f(y)\,dy \, + \int_x^1 g_{xx}(x,y)f(y)\,dy + \cancelto{-1}{(g_x(x,x^-) - g_x(x,x^+))}f(x)$$

note : $g_x(x,x^-) - g_x(x,x^+) = g_x(x^+,x) - g_x(x^-,x) = -1$

$$\phi''(x) = \int_0^x \sigma^2 g(x,y)f(y)\,dy \, + \int_x^1 \sigma^2 g(x,y)f(y)\,dy \, - \, f(x)$$

$$= \sigma^2 \int_0^1 g(x,y)f(y)\,dy - f(x) = \sigma^2\phi(x) - f(x) \quad \underline{\text{ok}}$$

<u>discretization</u>

$$\phi(x) = \int_0^1 g(x,y)f(y)\,dy \, , \; g(x,y) = \frac{\cosh\sigma(|x-y| - \frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma}$$

$$u_j = \sum_{k=0}^{N-1} g(x_j,x_k)f_k h \, , \; x_j = jh \, , \; h = 1/N \, , \; j = 0 : N-1 \; : \; \text{Riemann sum}$$

$u = Gf$, $G_{jk} = g(x_j,x_k)h$: $O(N^2)$ ops

<u>note</u>

$g(x,y) \neq 0$, $g(x,y) = g(y,x)$, $g(x,y) = g(|x-y|,0)$

$\Rightarrow$ G : dense , symmetric , constant on diagonals

<u>claim</u> : G is a circulant matrix

<u>pf</u>

$0 \leq x \, , \, y \leq 1 \; \Rightarrow \; -1 \leq x - y \leq 1$

then $g(x,y) = \begin{cases} g(x-y,0) & \text{if} \quad 0 \le x-y \le 1 \\ g(x-y+1,0) & \text{if} \ -1 \le x-y \le 0 \end{cases}$

the case $0 \le x-y \le 1$ is clear , check the case $-1 \le x-y \le 0$

$$g(x-y+1,0) \;=\; \frac{\cosh\sigma(|x-y+1|-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} \;=\; \frac{\cosh\sigma(x-y+1-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma}$$

$$= \frac{\cosh\sigma(x-y+\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} \;=\; \frac{\cosh\sigma(y-x-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} \;=\; \frac{\cosh\sigma(|x-y|-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} \;=\; g(x,y)$$

now set $c_j = g(x_j,0)h$, $j = 0:N-1$, $0 \le x_j \le 1-h$

$$G_{jk} \;=\; g(x_j,x_k)h \;=\; \begin{cases} g(x_j-x_k,0)h & \text{if} \qquad 0 \le x_j-x_k \le 1-h \\ g(x_j-x_k+1,0)h & \text{if} \ -1+h \le x_j-x_k \le 0 \end{cases}$$

$$= \begin{cases} c_{j-k} & \text{if} \ \ j-k = 0:N-1 \\ c_{j-k+N} & \text{if} \ \ j-k = -N+1:-1 \end{cases} = \ c_{(j-k)\mathrm{mod}N} \qquad \underline{\text{ok}}$$

---

ex : $N = 4$

$$G = \begin{pmatrix} g(x_0,x_0) & g(x_0,x_1) & g(x_0,x_2) & g(x_0,x_3) \\ g(x_1,x_0) & g(x_1,x_1) & g(x_1,x_2) & g(x_1,x_3) \\ g(x_2,x_0) & g(x_2,x_1) & g(x_2,x_2) & g(x_2,x_3) \\ g(x_3,x_0) & g(x_3,x_1) & g(x_3,x_2) & g(x_3,x_3) \end{pmatrix} h$$

$$= \begin{pmatrix} g(x_0,0) & g(x_1,0) & g(x_2,0) & g(x_3,0) \\ g(x_1,0) & g(x_0,0) & g(x_1,0) & g(x_2,0) \\ g(x_2,0) & g(x_1,0) & g(x_0,0) & g(x_1,0) \\ g(x_3,0) & g(x_2,0) & g(x_1,0) & g(x_0,0) \end{pmatrix} h$$

$$= \begin{pmatrix} c_0 & c_1 & c_2 & c_3 \\ c_1 & c_0 & c_1 & c_2 \\ c_2 & c_1 & c_0 & c_1 \\ c_3 & c_2 & c_1 & c_0 \end{pmatrix} = \begin{pmatrix} c_0 & c_1 & c_2 & c_1 \\ c_1 & c_0 & c_1 & c_2 \\ c_2 & c_1 & c_0 & c_1 \\ c_1 & c_2 & c_1 & c_0 \end{pmatrix} \ : \ \text{circulant}$$

$c_3 = g(x_3,0)h = g(0,x_3)h = g(1,x_3)h = g(1-x_3,0)h = g(x_1,0)h = c_1$

$\Rightarrow G = F_N^* D F_N$, $D = \mathrm{diag}(\sqrt{N}\,\widehat{c}_n)$

$\Rightarrow u = Gf = F_N^* D F_N f \ : \ O(N\log N)$ ops particle systems

ex : charged particles in 3D

position : $x_j(t)$, $j = 1, \ldots, N$

charge : q_j , mass : m_j

configuration : $x(t) = (x_1(t), \ldots, x_N(t))^T$: molecule , beam , . . .

Coulomb potential : $\phi(x) = \dfrac{1}{|x|}$

electric field : $E(x) = -\nabla\phi(x) = \dfrac{x}{|x|^3}$

dynamics : $m_i x_i'' = \displaystyle\sum_{\substack{j=1 \\ j\neq i}}^{N} q_i q_j \frac{x_i - x_j}{|x_i - x_j|^3}$

1. Using direct summation, the cost is $O(N^2)$ ops/timestep; we will investigate faster methods.

2. These methods can also be applied to energy minimization.

$V(x_1, \ldots, x_N) = \dfrac{1}{2} \displaystyle\sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{q_i q_j}{|x_i - x_j|}$: electrostatic potential energy

problem : find x^* such that $V(x^*) = \min\limits_x V(x)$

deterministic/Monte Carlo methods

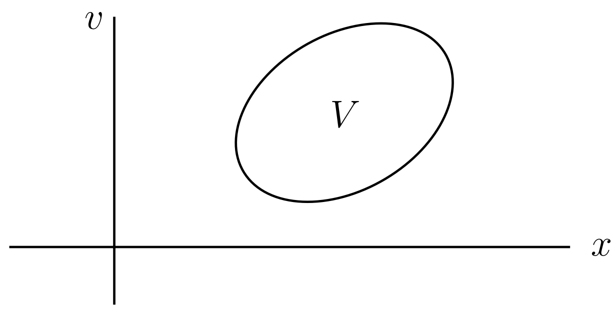
<u>kinetic model</u>

Consider a set of interacting particles that carry charge or mass.

$(x,v) \in \mathbb{R}^{2d}$, $d = 1,2,3$: <u>phase space</u> coordinates

$f(x,v,t)$: <u>number density</u> of particles in phase space

$N_V(t) = \int_V f(x,v,t)\,dx\,dv$: number of particles in a fixed volume V in phase space



In the absence of collisions and sources, particles can enter or leave the volume V only by crossing the boundary ∂V.

velocity of the <u>phase fluid</u> : $U = (v,a)$

v : velocity in the x-direction

$a = a(x,v,t)$: acceleration = velocity in the v-direction

$fU(x,v,t)$: particle flux in phase space

$$\begin{aligned}\frac{dN_V}{dt} &= \frac{d}{dt}\int_V f(x,v,t)\,dx\,dv = \int_V f_t(x,v,t)\,dx\,dv \\ &= -\int_{\partial V} fU(x,v,t)\cdot dS = -\int_V \nabla\cdot fU(x,v,t)\,dx\,dv\end{aligned}$$

$\nabla = (\nabla_x, \nabla_v)$: gradient operator in phase space

$$\Rightarrow \quad \int_V (f_t + \nabla\cdot fU)(x,v,t)\,dx\,dv = 0$$

$$\Rightarrow \quad f_t + \nabla\cdot fU = 0 \quad\Rightarrow\quad f_t + \nabla_x\cdot(fv) + \nabla_v\cdot(fa) = 0$$

We consider <u>conservative forces</u>, i.e. $a = -\nabla\Phi(x,t)$, and hence $a = a(x,t)$.

$\Rightarrow \quad f_t + v\cdot\nabla_x f + a\cdot\nabla_v f = 0$: <u>Vlasov equation</u>

note : Under these assumptions, the phase space flow is incompressible.

pf : $\nabla \cdot U \;=\; (\nabla_x\,,\nabla_v)\cdot(v,a) \;=\; \nabla_x v + \nabla_v a \;=\; 0$ ok

ex : electrons (one-species plasma)

q : charge , m : mass

$$f_t + v\cdot\nabla_x f + \frac{F}{m}\cdot\nabla_v f = 0$$

$F = q\,E(x,t)$: electrostatic force

$E(x,t) = -\nabla_x\phi(x,t)$: electric field

$-\nabla^2\phi = \rho$: Poisson equation

$\rho \;=\; \rho(x,t) \;=\; q\,n(x,t) + \overline{\rho}$: macroscopic charge density in physical space

$n(x,t) = \displaystyle\int_{\mathbb{R}^d} f(x,v,t)\,dv$: number density of electrons in physical space

$\overline{\rho}$: uniform background charge density (e.g. immobile heavy ions)

Vlasov-Poisson system in 1d : $0\le x\le 1$, PBC, $-\infty < v < \infty$

$$f_t + v f_x + \frac{F}{m} f_v = 0\ ,\ f(0,v,t) = f(1,v,t)\ ,\ \lim_{v\to\pm\infty} f(x,v,t) = 0$$

$$F = q\,E(x,t)\ ,\ E(x,t) = -\phi_x(x,t)$$

$$-\phi_{xx} = \rho\ ,\ \phi(0,t) = \phi(1,t)\ ,\ \phi_x(0,t) = \phi_x(1,t)$$

$$\rho \;=\; \rho(x,t) \;=\; q\,n(x,t) \;+\; \overline{\rho}$$

$$n(x,t) = \int_{-\infty}^{\infty} f(x,v,t)\,dv$$

note : solution of Poisson equation with PBC

$\displaystyle\int_0^1 \rho(x,t)\,dx \;=\; \int_0^1 -\phi_{xx}(x,t)\,dx \;=\; \phi_x(0,t) - \phi_x(1,t) = 0$: charge neutrality

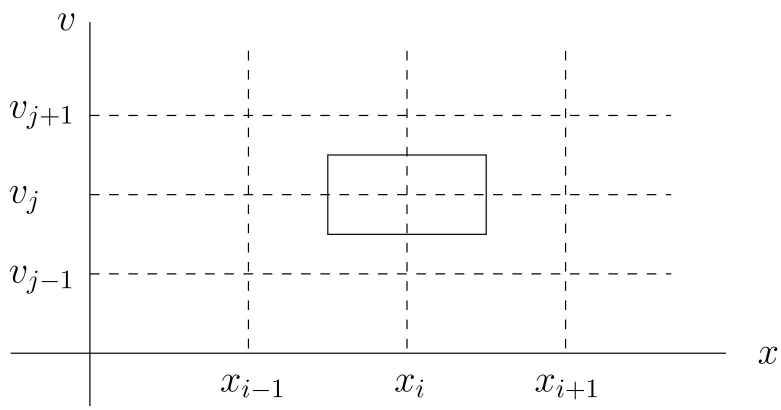
1. This condition is necessary and sufficient for existence of a solution $\phi(x,t)$; the background charge density $\overline{\rho}$ ensures it is satisfied.

2. If $\phi(x,t)$ is a solution, then so is $\phi(x,t)+c$ for any constant c, so the potential function is not unique, but the induced force is unique.

<u>numerical methods for Vlasov-Poisson in 1d</u>

<u>Vlasov-Poisson method 1</u> : finite-difference scheme

$x_i = i\Delta x\ ,\ v_j = j\Delta v$: mesh in phase space



$C_{ij} = \{(x,v) : x_{i-1/2} \le x < x_{i+1/2}\ ,\ v_{j-1/2} \le v < v_{j+1/2}\}$: cell

$f^n_{ij}\,\Delta x\,\Delta v$ = number of particles in cell C_{ij} at time $t^n = n\Delta t$

<u>Lax-Friedrichs</u>

$$f_t + vf_x + \frac{F}{m}f_v = 0$$

$$\frac{f^{n+1}_{ij} - \frac{1}{4}(f^n_{i+1,j} + f^n_{i-1,j} + f^n_{i,j+1} + f^n_{i,j-1})}{\Delta t} + v_j D^x_0 f^n_{ij} + \frac{F^n_i}{m} D^v_0 f^n_{ij} = 0$$

$$D^x_0 f^n_{ij} = \frac{f^n_{i+1,j} - f^n_{i-1,j}}{2\Delta x}\ ,\ D^v_0 f^n_{ij} = \frac{f^n_{i,j+1} - f^n_{i,j-1}}{2\Delta v}$$

$$F^n_i = qE^n_i\ ,\ E^n_i = -D^x_0\phi^n_i$$

$-D^x_+ D^x_- \phi^n_i = \rho^n_i$ + PBC : comment soon

$$\rho^n_i = q\sum_{j=-J}^{J} f^n_{ij}\,\Delta v + \overline{\rho}\ ,\ \text{where } f^n_{ij} \le \epsilon \text{ for } |j| \ge J$$

1. In practice, we may take $v_{\min} \le v \le v_{\max}$ or $J_1 \le j \le J_2$.
2. CFL condition : $\Delta t \le \min\left\{\dfrac{\Delta x}{\max|v_j|}\ ,\ \dfrac{\Delta v}{\max|F^n_i|/m}\right\}$
3. artificial diffusion/collisions

<u>discrete Poisson equation in 1d with PBC</u>

$$\frac{-\phi_{i+1}+2\phi_i-\phi_{i-1}}{\Delta x^2}=\rho_i\ ,\ i=0:N-1\ ,\ \Delta x=1/N\ ,\ \phi_{-1}=\phi_{N-1}\ ,\ \phi_N=\phi_0$$

$$\frac{1}{\Delta x^2}\begin{pmatrix} 2 & -1 & \cdots & \cdots & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & \cdots & \cdots & -1 & 2 \end{pmatrix}\begin{pmatrix}\phi_0\\ \phi_1\\ \vdots \\ \phi_{N-2}\\ \phi_{N-1}\end{pmatrix}=\begin{pmatrix}\rho_0\\ \rho_1\\ \vdots \\ \rho_{N-2}\\ \rho_{N-1}\end{pmatrix}$$

1. adding all eqs $\Rightarrow \sum_{i=0}^{N-1}\rho_i=0$: discrete charge neutrality

2. if $\{\phi_i\}_{i=0}^{N-1}$ is a solution, then so is $\{\phi_i+c\}_{i=0}^{N-1}$ for any constant c

This is analogous to the continuous case.

<u>method 1a</u> : spectral

$A\phi=\rho\ ,\ A=F_N^*DF_N\ ,\ D=\mathrm{diag}(\lambda_0,\ldots,\lambda_{N-1})$

e-values : $\lambda_n=\dfrac{4\sin^2(\pi n/N)}{\Delta x^2}\ ,\ n=0:N-1$

e-vectors : $q_n=F_N^*e_n=\dfrac{1}{\sqrt{N}}(1,\omega^{-n},\omega^{-2n},\ldots,\omega^{-(N-1)n})^T\ ,\ \omega=e^{-2\pi i/N}$

note : $\lambda_0=0\Rightarrow A$ is not invertible , $\mathrm{null}A=\mathrm{span}(q_0)$, $q_0=\dfrac{1}{\sqrt{N}}(1,\ldots,1)^T$

A necessary and sufficient condition for a solution ϕ to exist is that the RHS ρ should be orthogonal to the null space of A^*.

$$\Rightarrow\ \langle\rho,q_0\rangle=\frac{1}{\sqrt{N}}\sum_{i=0}^{N-1}\rho_i=0\ :\ \text{discrete charge neutrality}$$

Moreover, if ϕ is a solution, then so is $\phi+cq_0$ for any constant c.

<u>claim</u>: $\phi=F_N^*D^{-1}F_N\rho$, where $D^{-1}=\mathrm{diag}(0,\lambda_1^{-1},\ldots,\lambda_{N-1}^{-1})$: $O(N\log N)$ ops

<u>pf</u>

$$\begin{aligned} A\phi &= F_N^*DF_NF_N^*D^{-1}F_N\rho = F_N^*\,\mathrm{diag}(0,1,\ldots,1)F_N\rho \\ &= F_N^*\,\mathrm{diag}(1,1,\ldots,1)F_N\rho=\rho \end{aligned}$$

$(F_N\rho)_0=\langle F_N\rho,e_0\rangle=\langle\rho,F_N^*e_0\rangle=\langle\rho,q_0\rangle=0$ <u>ok</u>

method 1b : elimination

set $\phi_0 = 0$, write down eqs for $i = 1 : N-1$, then eq for $i = 0$

$$
\begin{aligned}
2\phi_1 - \phi_2 \qquad\qquad\qquad\qquad\qquad\qquad &= \rho_1 \Delta x^2 \\
-\phi_1 + 2\phi_2 - \phi_3 \qquad\qquad\qquad\qquad &= \rho_2 \Delta x^2 \\
-\phi_2 + 2\phi_3 - \phi_4 \qquad\qquad\qquad &= \rho_3 \Delta x^2 \\
&\ \vdots \\
-\phi_{N-3} + 2\phi_{N-2} - \phi_{N-1} &= \rho_{N-2} \Delta x^2 \\
-\phi_{N-2} + 2\phi_{N-1} &= \rho_{N-1} \Delta x^2 \\
-\phi_1 \qquad\qquad\qquad\qquad - \phi_{N-1} &= \rho_N \Delta x^2 \ , \ \text{set } \rho_N = \rho_0
\end{aligned}
$$

multiply 1st eq by 1, 2nd eq by 2, ..., Nth eq by N, then add

$$\Rightarrow \ -N\phi_1 = \Delta x^2 \sum_{i=1}^{N} i\rho_i$$

check : for $i = 2 : N-1$, coeff of ϕ_i is $-(i-1) + 2i - (i+1) = 0$ <u>ok</u>

solve for ϕ_1, then ϕ_2, then ϕ_3, ..., then ϕ_{N-1}

to show Nth eq is satisfied : add all eqs, ok by discrete charge neutrality

<u>note</u> : $O(N)$ ops

<u>Vlasov-Poisson method 2</u> : particle-in-cell (PIC)

idea : convect particles in phase space, solve Poisson equation on a mesh

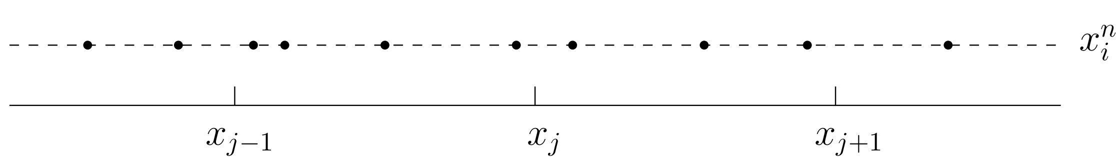
particles : $x_i(t)$, $v_i(t)$, $i = 1 : N_p$, charge q , mass $m = 1$

Newton's equation : $x_i' = v_i$, $v_i' = F(x_i)$

leap-frog method : $\dfrac{x_i^{n+1} - x_i^n}{\Delta t} = v_i^{n+1/2}$, $\dfrac{v_i^{n+1/2} - v_i^{n-1/2}}{\Delta t} = F_i^n$

$t^n = n\Delta t$, $t^{n+1/2} = (n + \frac{1}{2})\Delta t$

mesh : $x_j = j\Delta x$, $\Delta x = 1/N_m$, $j = 0 : N_m$



$-D_+^x D_-^x \phi_j^n = \rho_j^n$ + PBC , $E_j^n = -D_0^x \phi_j^n$, $F_j^n = qE_j^n$

<u>one timestep</u>

input : x_i^n , $v_i^{n-1/2}$ $\rightarrow$ output : x_i^{n+1} , $v_i^{n+1/2}$, $i = 1 : N_p$

1. <u>assign charge</u> from particles to mesh : $x_i^n \rightarrow \rho_j^n$
2. solve Poisson equation for potential on mesh : $\rho_j^n \rightarrow \phi_j^n$
3. compute forces on mesh : $\phi_j^n \rightarrow F_j^n$
4. <u>interpolate forces</u> from mesh to particles : $F_j^n \rightarrow F_i^n$
5. convect particles in phase space : $F_i^n \rightarrow v_i^{n+1/2},\ x_i^{n+1}$

<u>nearest mesh point scheme</u> : NMP

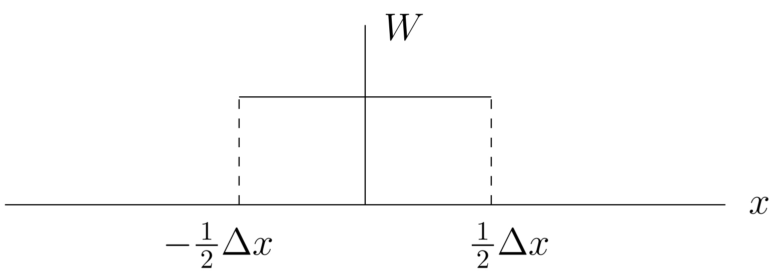
cell j : $x_{j-1/2} \leq x < x_{j+1/2}$

charge assignment : $\rho_j^n = \dfrac{q\, n_j^n}{\Delta x} + \overline{\rho}$, n_j^n : number of particles in cell j at time t^n

force interpolation : $F_i^n = F_j^n$, if particle x_i^n is in cell j

NMP has low accuracy, but there is an alternative viewpoint that can be used to derive more accurate assignment/interpolation schemes.

define : $W(x) = \begin{cases} 1 & \text{if } -\frac{1}{2}\Delta x \leq x < \frac{1}{2}\Delta x \\ 0 & \text{otherwise} \end{cases}$: weight function



$$\rho_j^n = \frac{q\, n_j^n}{\Delta x} + \overline{\rho}\ ,\ n_j^n = \sum_{i=1}^{N_p} W(x_i^n - x_j)\ ,\ F_i^n = \sum_{j=0}^{N_m-1} W(x_i^n - x_j) F_j^n$$

<u>coding details</u> : assume $-\frac{1}{2}\Delta x \leq x_i^n < 1 - \frac{1}{2}\Delta x$ by PBC

<u>code 1</u> : $O(N_m N_p)$ ops

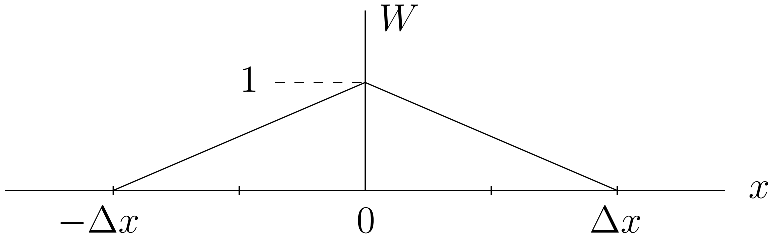
```
for j = 0 : N_m - 1
   n_j^n = 0
   for i = 1 : N_p
      n_j^n = n_j^n + W(x_i^n - x_j)
   end
end
```

<u>code 2</u> : $O(N_m + N_p)$ ops

```
for j = 0 : N_m - 1
   n_j^n = 0
end
for i = 1 : N_p
   j = integer_part((x_i^n + 1/2 Δx)/Δx)
   n_j^n = n_j^n + 1
end
```

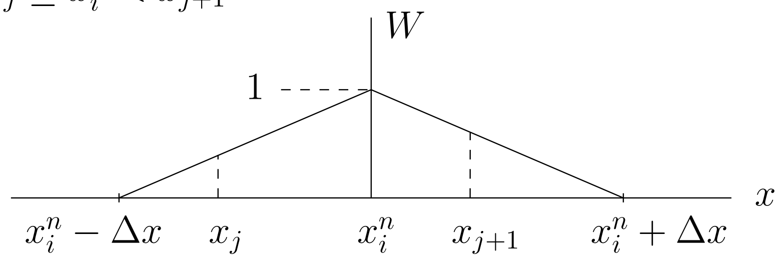
<u>cloud-in-cell scheme</u> : CIC

$$W(x) = \begin{cases} 1 - |x|/\Delta x & \text{if } -\Delta x \le x < \Delta x \\ 0 & \text{otherwise} \end{cases}$$



<u>force interpolation</u> : $F_i^n = \sum_{j=0}^{N_m-1} W(x_i^n - x_j)F_j^n$

assume $x_j \le x_i^n < x_{j+1}$



$$\Rightarrow\ F_i^n = W(x_i^n - x_j)F_j^n + W(x_i^n - x_{j+1})F_{j+1}^n = c_1 F_j^n + c_2 F_{j+1}^n$$

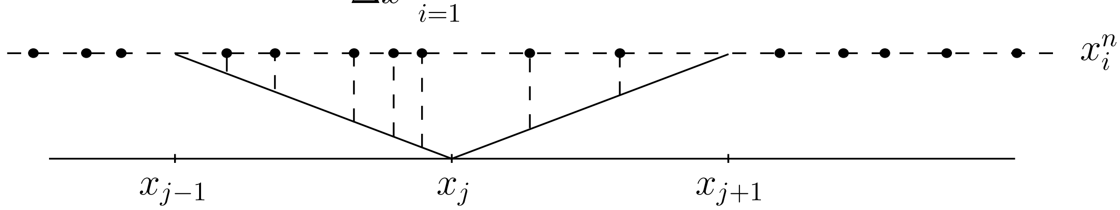
$$c_1 \ = \ W(x_i^n - x_j) \ = \ 1 - \frac{|x_i^n - x_j|}{\Delta x} \ = \ 1 - \frac{x_i^n - x_j}{\Delta x} \ = \ \frac{x_{j+1} - x_i^n}{\Delta x}$$

$$c_2 \ = \ W(x_i^n - x_{j+1}) \ = \ 1 - \frac{|x_i^n - x_{j+1}|}{\Delta x} \ = \ 1 - \frac{x_{j+1} - x_i^n}{\Delta x} \ = \ \frac{x_i^n - x_j}{\Delta x}$$

$0 \le c_1 \le 1\ ,\ 0 \le c_2 \le 1\ ,\ c_1 + c_2 = 1$

$\Rightarrow F_i^n$ is a distance-weighted average of the forces at the 2 nearest mesh points

<u>charge assignment</u> : $\rho_j^n = \dfrac{q}{\Delta x} \sum_{i=1}^{N_p} W(x_i^n - x_j) + \overline{\rho}$



$\Rightarrow \rho_j^n$ is a distance-weighted average of the particle charge in the 2 nearest cells

1. The CIC weight function is continuous and this leads to higher order accuracy.

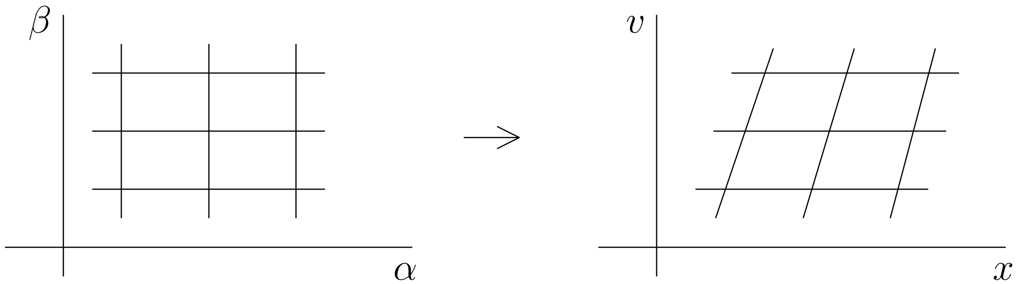
2. If $qN_p + \overline{\rho}N_m\Delta x = 0$, then the NMP and CIC charge assignment schemes satisfy discrete charge neutrality. (hw3)

Vlasov-Poisson method 3 : Lagrangian particle method

recall : $f_t + vf_x + \frac{F}{m}f_v = 0$, $F = qE$, $E = -\phi_x$, $-\phi_{xx} = \rho$, PBC

$$\rho = \rho(x,t) = q\int_{-\infty}^{\infty} f(x,v,t)\,dv + \overline{\rho} \text{ , charge neutrality}$$

define : $\begin{pmatrix}\alpha\\ \beta\end{pmatrix} \to \begin{pmatrix}x(\alpha,\beta,t)\\ v(\alpha,\beta,t)\end{pmatrix}$: flow map of particle distribution



(α,β) : Lagrangian coordinates , particle labels

Newton's equation : $x_t(\alpha,\beta,t) = v(\alpha,\beta,t)$, $v_t(\alpha,\beta,t) = F(x(\alpha,\beta,t))$

PBC : $x(\alpha+1,\beta,t) = x(\alpha,\beta,t)$, $v(\alpha+1,\beta,t) = v(\alpha,\beta,t)$

claim

1. $f(x(\alpha,\beta,t), v(\alpha,\beta,t), t) = f_0(\alpha,\beta)$

2. $J(\alpha,\beta,t) = \det\begin{pmatrix}x_\alpha(\alpha,\beta,t) & x_\beta(\alpha,\beta,t)\\ y_\alpha(\alpha,\beta,t) & y_\beta(\alpha,\beta,t)\end{pmatrix} \Rightarrow J(\alpha,\beta,t) = J_0(\alpha,\beta)$

pf

1. $\frac{d}{dt}f(x(\alpha,\beta,t), v(\alpha,\beta,t), t) = f_x x_t + f_v v_t + f_t = f_x v + f_v F + f_t = 0$ ok

This says that $f(x,v,t)$ is constant on characteristics of the Vlasov equation.

2. $J(t+h) = \det\begin{pmatrix}x_\alpha(t+h) & x_\beta(t+h)\\ v_\alpha(t+h) & v_\beta(t+h)\end{pmatrix} = \det\begin{pmatrix}x_\alpha + hx_{\alpha t} & x_\beta + hx_{\beta t}\\ v_\alpha + hv_{\alpha t} & v_\beta + hv_{\beta t}\end{pmatrix} + O(h^2)$

$$= J(t) + h(x_\alpha v_{\beta t} + x_{\alpha t}v_\beta - (v_\alpha x_{\beta t} + v_{\alpha t}x_\beta)) + O(h^2)$$

$$= J(t) + h(x_\alpha F_x x_\beta + v_\alpha v_\beta - (v_\alpha v_\beta + F_x x_\alpha x_\beta)) + O(h^2) = J(t) + O(h^2)$$

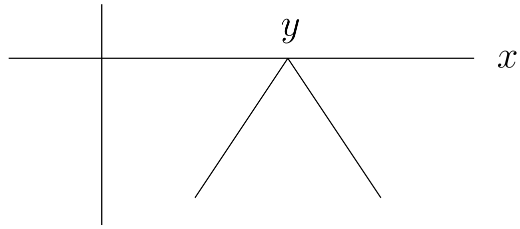
$J'(t) = \lim_{h\to 0}\frac{J(t+h)-J(t)}{h} = 0$ ok

We may choose $x_0(\alpha,\beta) = \alpha, v_0(\alpha,\beta) = \beta$, so $J(t) = 1$; this implies that the phase flow is incompressible.

integral expression for $\phi(x,t)$

$g(x,y) \;=\; -\frac{1}{2}|x-y|$: free-space Green's function in 1d

$$= \begin{cases} -\frac{1}{2}(x-y) \text{ if } x > y \\ \frac{1}{2}(x-y) \text{ if } x < y \end{cases}$$



1. $-g_{xx}(x,y) = 0$ for $x \neq y$, $g(y^+,y) = g(y^-,y)$, $g_x(y^+,y) - g_x(y^-,y) = -1$

These properties are equivalent to $-g_{xx}(x,y) = \delta(x-y)$, i.e. $g(x,y)$ is the potential function due to a point charge at $x = y$.

2. $\phi = \phi_p + \phi_h$, $\phi_p(x,t) = \displaystyle\int_0^1 g(x,y)\rho(y,t)dy$, $\phi_h(x,t) = ax + b$

3. PBC

Since $\phi(x,t)$ is determined up to an additive constant, we choose $b = 0$.

$$\phi_x(1,t) - \phi_x(0,t) = \int_0^1 \phi_{xx}(x,t)dx = \int_0^1 -\rho(x,t)dx = 0 \text{ by charge neutrality}$$

$$\phi(0,t) = \phi(1,t) \;\Rightarrow\; \phi_p(0,t) + \phi_h(0,t) = \phi_p(1,t) + \phi_h(1,t)$$

$$\Rightarrow\; \phi_p(0,t) = \phi_p(1,t) + a$$

$$a \;=\; \phi_p(0,t) - \phi_p(1,t) \;=\; \int_0^1 (\underbrace{g(0,y)}_{-\frac{1}{2}y} - \underbrace{g(1,y)}_{-\frac{1}{2}(1-y)})\,\rho(y,t)dy \;=\; -\int_0^1 y\rho(y,t)dy$$

$$\Rightarrow\; \phi(x,t) \;= \int_0^1 (g(x,y) - xy)\,\rho(y,t)\,dy \quad , \quad \text{check : hw}$$

note : This approach generalizes to 2d and 3d using the free-space Green's function for ϕ_p, and a boundary integral representation for ϕ_h.

force evaluation : $F(x(\alpha,\beta,t))$

$$E(x,t) = -\phi_x(x,t) = \int_0^1 (k(x,y) + y)\rho(y,t)dy \;,\; k(x,y) = \tfrac{1}{2}\text{sign}(x-y)$$

$$= \int_0^1 (k(x,y) + y)\Big(q\int_{-\infty}^{\infty} f(y,v,t)dv + \overline{\rho}\Big)dy$$

$$= q\int_0^1\int_{-\infty}^{\infty} (k(x,y) + y)f(y,v,t)dvdy \;+ \overline{\rho}\int_0^1 (k(x,y) + y)dy$$

$\int_0^1 (k(x,y)+y)\,dy \;=\; x$: hw

$\int_{-\infty}^{\infty}\int_0^1 (k(x,y)+y)f(y,v,t)dydv$: change variables using flow map

$$= \int_{-\infty}^{\infty}\int_0^1 (k(x,x(\alpha,\beta,t))+x(\alpha,\beta,t))f(x(\alpha,\beta,t),v(\alpha,\beta,t),t)J(\alpha,\beta,t)d\alpha d\beta$$

$$= \int_{-\infty}^{\infty}\int_0^1 (k(x,x(\alpha,\beta,t))+x(\alpha,\beta,t))f_0(\alpha,\beta)J_0(\alpha,\beta)d\alpha d\beta$$

<u>summary</u>

$x_t(\alpha,\beta,t) = v(\alpha,\beta,t)\ ,\ x_0(\alpha,\beta) = \alpha$

$v_t(\alpha,\beta,t) \;=\; F(x(\alpha,\beta,t),t)\ ,\ v_0(\alpha,\beta) = \beta$

$$= q^2\int_{-\infty}^{\infty}\int_0^1 \Big(k(x(\alpha,\beta,t),x(\tilde\alpha,\tilde\beta,t))+x(\tilde\alpha,\tilde\beta,t)\Big)f_0(\tilde\alpha,\tilde\beta)d\tilde\alpha d\tilde\beta \;+\; q\,\overline{\rho}\,x(\alpha,\beta,t)$$

This is an integro-differential equation for the flow map.

<u>discretization</u>

$(\alpha,\beta)\;\to\;(\alpha_i,\beta_i)\ ,\ i=1:N$

$x(\alpha_i,\beta_i,t)\,,\,v(\alpha_i,\beta_i,t)\;\to\;x_i(t)\,,\,v_i(t)$: particles moving in phase space

$x_i' = v_i$

$$v_i' = F(x_i) = q^2\sum_{j=1}^{N}(k(x_i,x_j)+x_j)f_0(\alpha_j,\beta_j)\Delta\alpha\,\Delta\beta \;+\; q\,\overline{\rho}\,x_i$$

This is a finite-dimensional system of ODEs.

Three issues arise.

1. evaluating the RHS by direct summation requires $O(N^2)$ ops/timestep

2. $k(x,y)$ is singular for $x=y$

3. The particle distribution typically becomes disordered and remeshing is required.

<u>fluid dynamics in 2d</u>

(u, v) : velocity field , $u = u(x, y, t)$, $v = v(x, y, t)$

We consider <u>incompressible</u> flow, i.e. $u_x + v_y = 0$.

1. An incompressible flow is <u>area-preserving</u>. (hw)

2. If (u, v) is incompressible, then there exists a <u>stream function</u>, $\psi(x, y)$, such that $u = \psi_y$, $v = -\psi_x$.

note : If ψ exists, then $u_x + v_y = (\psi_y)_x + (-\psi_x)_y = 0$.

<u>def</u> : A <u>streamline</u> is a level curve of the stream function, i.e. $\psi(x, y) = c$.

<u>claim</u> : The velocity field is parallel to the streamlines.

<u>pf</u>

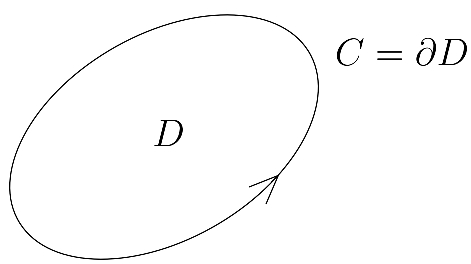
$(x(s), y(s))$: streamline $\Rightarrow \psi(x(s), y(s)) = c \Rightarrow \psi_x \cdot x' + \psi_y \cdot y' = 0$

$\Rightarrow (-v, u) \cdot (x', y') = 0 \Rightarrow (u, v) \cdot (y', -x') = 0$ <u>ok</u>

<u>def</u> : $\omega = v_x - u_y$: <u>vorticity</u> , units $= T^{-1}$

<u>interpretation</u>

Consider the line integral of the velocity around a closed curve C bounding a domain D.



$\displaystyle\int_C u \cdot ds$: <u>circulation</u>

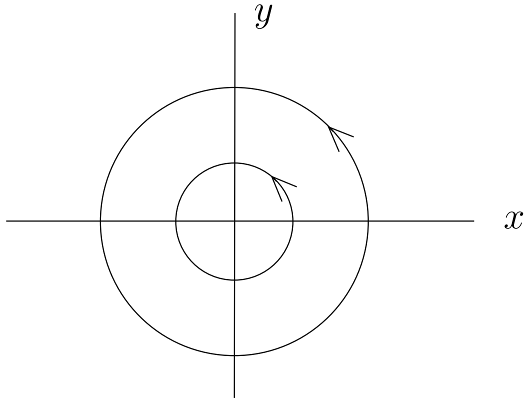
$$\int_C u \cdot ds = \int_{\partial D} u\,dx + v\,dy = \int_D (v_x - u_y)\,dx\,dy = \int_D \omega\,dx\,dy$$

$\Rightarrow$ vorticity = circulation density , local rotation rate

<u>note</u> : $\omega = v_x - u_y = (-\psi_x)_x - (\psi_y)_y \Rightarrow -\nabla^2\psi = \omega$: Poisson equation

ex : point vortex

$\psi(x,y) = -\frac{1}{2\pi}\log r\ ,\ r = \sqrt{x^2+y^2} \ \Rightarrow$ streamlines are circles



$$u(x,y) = \frac{-y}{2\pi(x^2+y^2)}\ ,\ v(x,y) = \frac{x}{2\pi(x^2+y^2)} \ \Rightarrow\ \sqrt{u^2+v^2} = \frac{1}{2\pi r}$$

$$\omega = -\nabla^2\psi = -\left(\psi_{rr} + \frac{1}{r}\psi_r + \frac{1}{r^2}\psi_{\theta\theta}\right) = \frac{1}{2\pi}\left(-\frac{1}{r^2} + \frac{1}{r}\cdot\frac{1}{r}\right) = 0 \quad ,\ \text{if } r \neq 0$$

However, consider the circulation around a circle of radius R.

$C\ :\ x = R\cos\theta\ ,\ y = R\sin\theta$

$$\int_C u\cdot ds = \int_C u\,dx + v\,dy = \int_0^{2\pi}\left(\frac{-R\sin\theta}{2\pi R^2}\cdot -R\sin\theta + \frac{R\cos\theta}{2\pi R^2}\cdot R\cos\theta\right)d\theta$$

$$= \frac{1}{2\pi}\int_0^{2\pi} d\theta = 1 : \text{ independent of } R$$

claim : The vorticity associated with a point vortex is a delta function, i.e. if $\psi = -\frac{1}{2\pi}\log r$, then $\omega = -\nabla^2\psi = \delta$ in the sense of distributions.

note : Let $<f,g> = \int_{\mathbb{R}^2} f(x,y)\,g(x,y)\,dx\,dy$.

The delta function $\delta(x,y)$ is the distribution satisfying

$$<\delta,f> = \int_{\mathbb{R}^2}\delta(x,y)\,f(x,y)\,dx\,dy = f(0,0) \text{ for all test functions } f\in C_0^\infty(\mathbb{R}^2).$$

The weak form of the equation $-\nabla^2\psi = \delta$ says that

$$<-\nabla^2\psi, f> \underset{\substack{\uparrow\\ \text{definition}}}{=} <\psi, -\nabla^2 f> \underset{\substack{\uparrow\\ \text{must be proven}}}{=} <\delta,f> \text{ for all test functions } f.$$

$$\underline{\text{pf}}:\ <\psi, -\nabla^2 f> \,=\, \int_0^{2\pi}\int_0^{\infty} \psi(r)\cdot -\left(\frac{1}{r}(rf_r)_r + \frac{1}{r^2}f_{\theta\theta}\right) r\,dr\,d\theta$$

$$= \int_0^{2\pi}\int_0^{\infty} \frac{1}{2\pi}\log r\cdot(rf_r)_r\,dr\,d\theta$$

$$= \frac{1}{2\pi}\int_0^{2\pi}\left(\log r\cdot rf_r\Big|_{r=0}^{r=\infty} - \int_0^{\infty}\frac{1}{r}\cdot rf_r\,dr\right)d\theta$$

$$= -\frac{1}{2\pi}\int_0^{2\pi}\int_0^{\infty} f_r\,dr\,d\theta \,=\, -\frac{1}{2\pi}\int_0^{2\pi} f\Big|_{r=0}^{r=\infty} d\theta$$

$$= -\frac{1}{2\pi}\int_0^{2\pi} -f(0,0)\,d\theta \,=\, f(0,0) \,=\, <\delta, f> \qquad \underline{\text{ok}}$$

<u>note</u>

1. A function satisfying $-\Delta g = \delta$ is a <u>Green's function</u> for the Laplace operator; the RHS represents a point vortex/charge/mass and g is the corresponding stream function/potential function.

2. We've shown that $g(x,y) = -\frac{1}{2\pi}\log(x^2+y^2)^{1/2}$ is a Green's function for the Laplace operator in 2d; in 3d a Green's function is given by $g(x,y,z) = \frac{1}{4\pi}(x^2+y^2+z^2)^{-1/2}$. (hw)

3. The stream function can be obtained from the vorticity.

$$\psi(x,y) = (g*\omega)(x,y) = \int_{\mathbb{R}^2} g(x-\widetilde{x}, y-\widetilde{y}\,)\,\omega(\widetilde{x},\widetilde{y}\,)\,d\widetilde{x}\,d\widetilde{y}$$

check : $-\nabla^2\psi \,=\, -\nabla^2(g*\omega) \,=\, (-\nabla^2 g)*\omega \,=\, \delta*\omega \,=\, \omega$ $\quad$ <u>ok</u>

4. The velocity can also be obtained from the vorticity.

$\psi = g*\omega \;\Rightarrow\; (u,v) = (\psi_y, -\psi_x) = (g_y*\omega, -g_x*\omega)$

$$u(x,y) = \frac{1}{2\pi}\int_{\mathbb{R}^2}\frac{-(y-\widetilde{y})}{(x-\widetilde{x})^2+(y-\widetilde{y})^2}\omega(\widetilde{x},\widetilde{y}\,)d\widetilde{x}d\widetilde{y}$$

$$v(x,y) = \frac{1}{2\pi}\int_{\mathbb{R}^2}\frac{(x-\widetilde{x})}{(x-\widetilde{x})^2+(y-\widetilde{y})^2}\omega(\widetilde{x},\widetilde{y})d\widetilde{x}d\widetilde{y}$$

In electromagnetic theory this is called the <u>Biot-Savart law</u>, where ω is a current density and (u,v) is the induced magnetic field.

2d incompressible Euler equations

$\vec{u}_t + (\vec{u} \cdot \nabla)\vec{u} = -\nabla p \ , \ \nabla \cdot \vec{u} = 0 \ :$ velocity/pressure

$u_t + uu_x + vu_y = -p_x \ \Rightarrow \ u_{yt} + uu_{xy} + u_y u_x + vu_{yy} + v_y u_y = -p_{xy}$

$v_t + uv_x + vv_y = -p_y \ \Rightarrow \ v_{xt} + uv_{xx} + u_x v_x + vv_{xy} + v_x v_y = -p_{xy}$

$(u_y - v_x)_t + u(u_y - v_x)_x + v(u_y - v_x) + u_y(u_x + v_y) - v_x(u_x + v_y) = 0$

$\omega_t + u\omega_x + v\omega_y = 0 \ , \ -\nabla^2\psi = \omega \ , \ u = \psi_y \ , \ v = -\psi_x \ :$ vorticity/stream function

recall 1d Vlasov-Poisson

$$f_t + vf_x + Ff_v = 0 \ , \ -\phi_{xx} = \rho = q\int_{-\infty}^{\infty} f(x,v,t)\,dv + \overline{\rho} \ , \ F = -q\phi_x$$

Similar considerations hold for these two systems, e.g. numerical methods (the analog of PIC is VIC = vortex-in-cell), flow map, Lagrangian form.

Lagrangian particle method

$(x_i(t), y_i(t)) \, , \, i = 1 : N$

discretize the Biot-Savart law , $\omega(x,y)dxdy \ \rightarrow \ \Gamma_i$

$$\frac{dx_i}{dt} = \frac{1}{2\pi}\sum_{j=1}^{N} \frac{-(y_i - y_j)}{(x_i - x_j)^2 + (y_i - y_j)^2 + \delta^2}\,\Gamma_j \quad , \quad \delta \ : \ \underline{\text{smoothing parameter}}$$

$$\frac{dy_i}{dt} = \frac{1}{2\pi}\sum_{j=1}^{N} \frac{(x_i - x_j)}{(x_i - x_j)^2 + (y_i - y_j)^2 + \delta^2}\,\Gamma_j$$

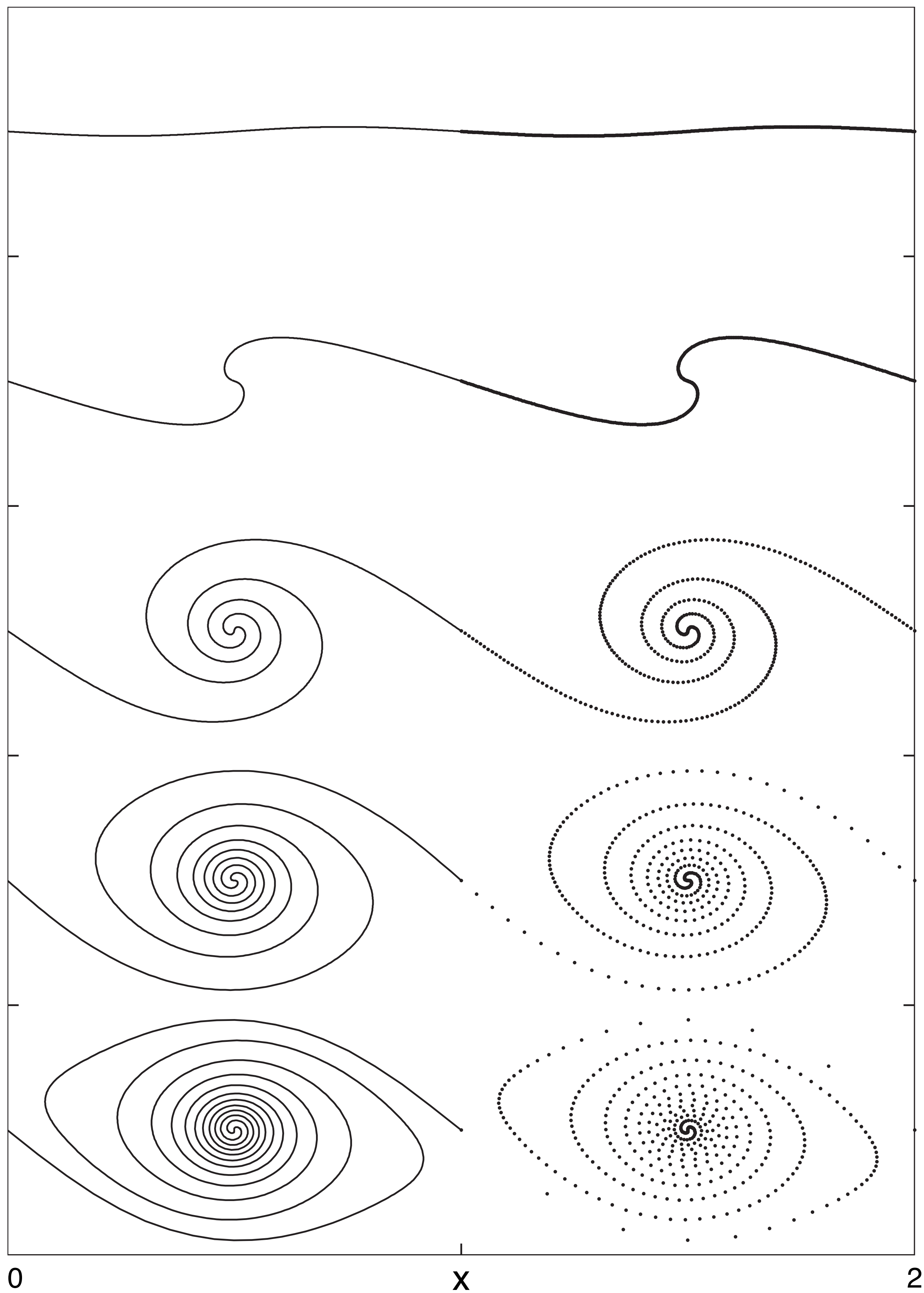
1. If $\delta = 0$ and we take $j \neq i$, then these are the point vortex equations.

2. We can think of the case $\delta > 0$ as arising from a regularized Green's function, $g_\delta(x,y) = -\frac{1}{2\pi}\log(x^2 + y^2 + \delta^2)^{1/2}$; then each particle carries a smooth vorticity distribution called a vortex-blob.

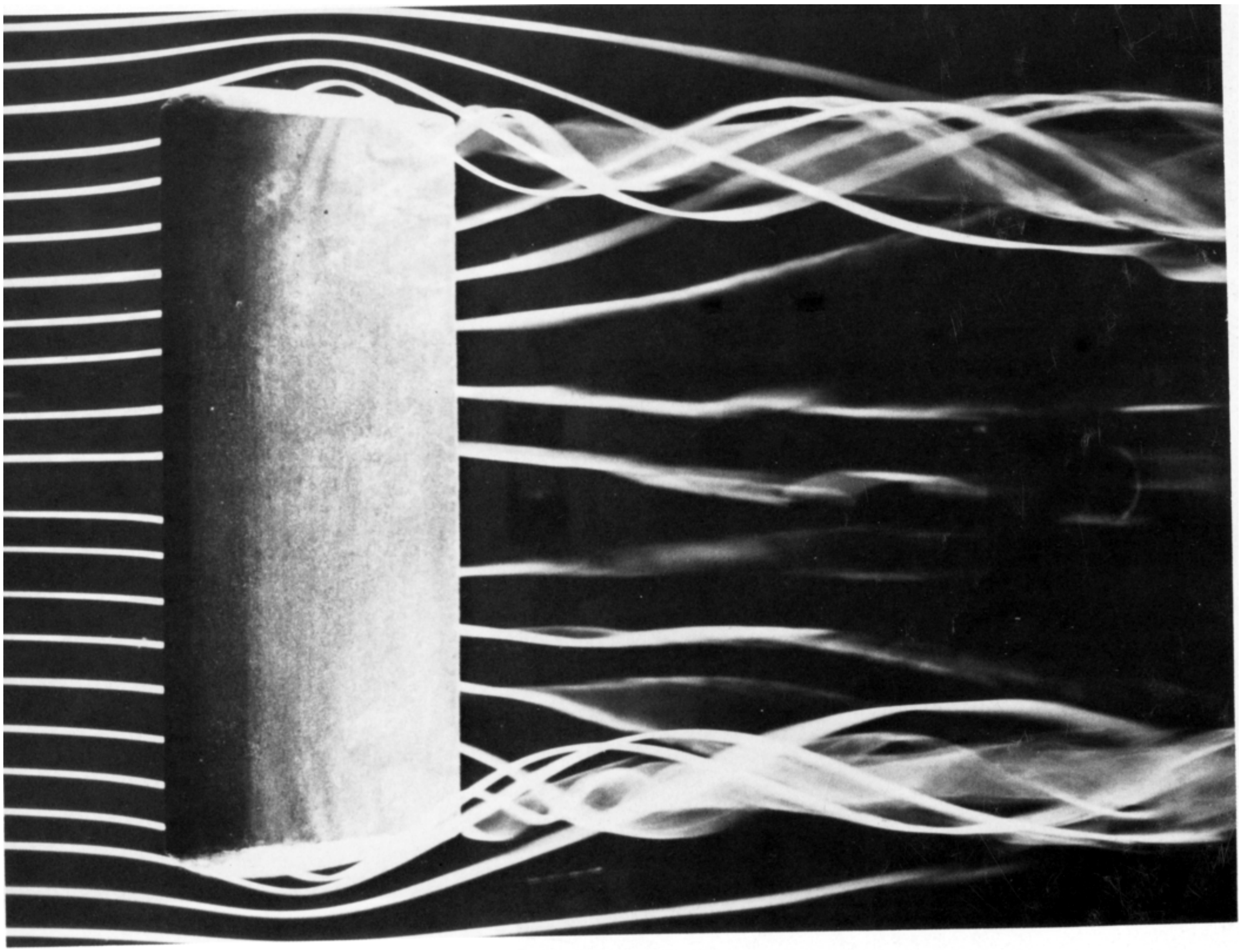
3. The vortex-blob method has no mesh-related artifacts such as artificial diffusion, but it does have artificial smoothing.

4. The vortex-blob method requires $O(N^2)$ ops/timestep if direct summation is used, but the cost can be reduced to $O(N \log N)$ using a treecode.

periodic vortex sheet roll-up/Kelvin-Helmholtz instability ($N = 400\,, \delta = 0.25$)



tip vortices/airfoil wake



vortex sheet model of an airplane wake (Prandtl)

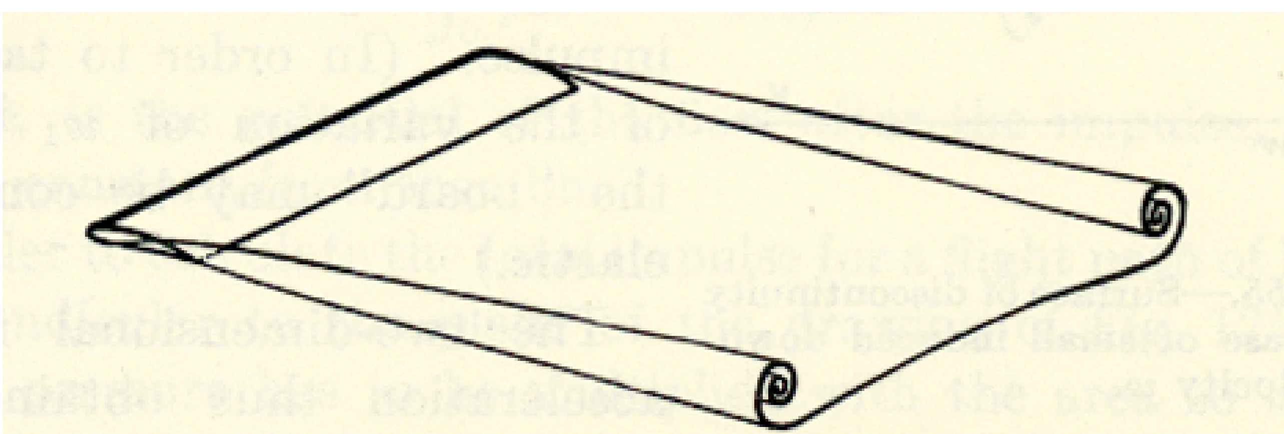
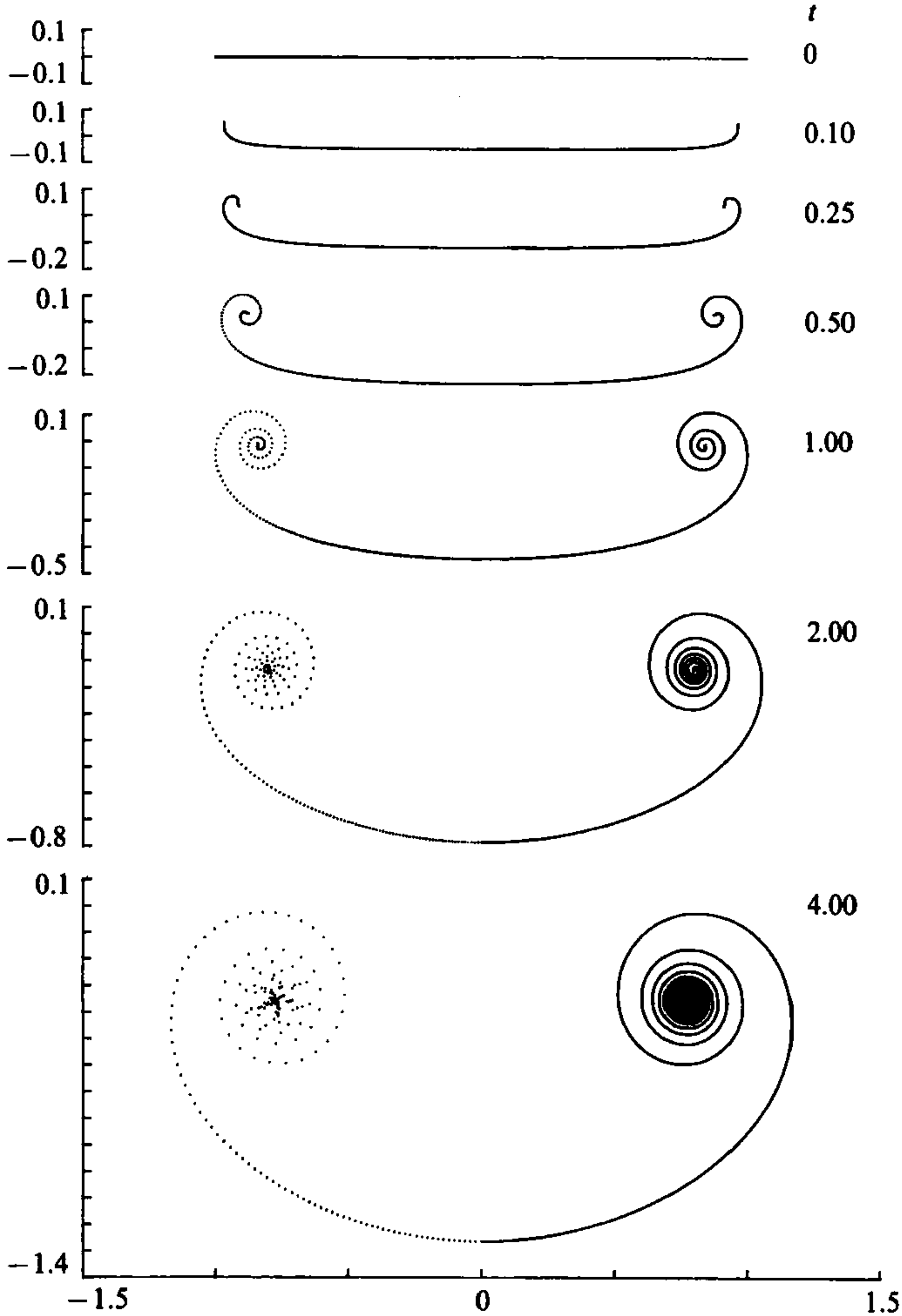
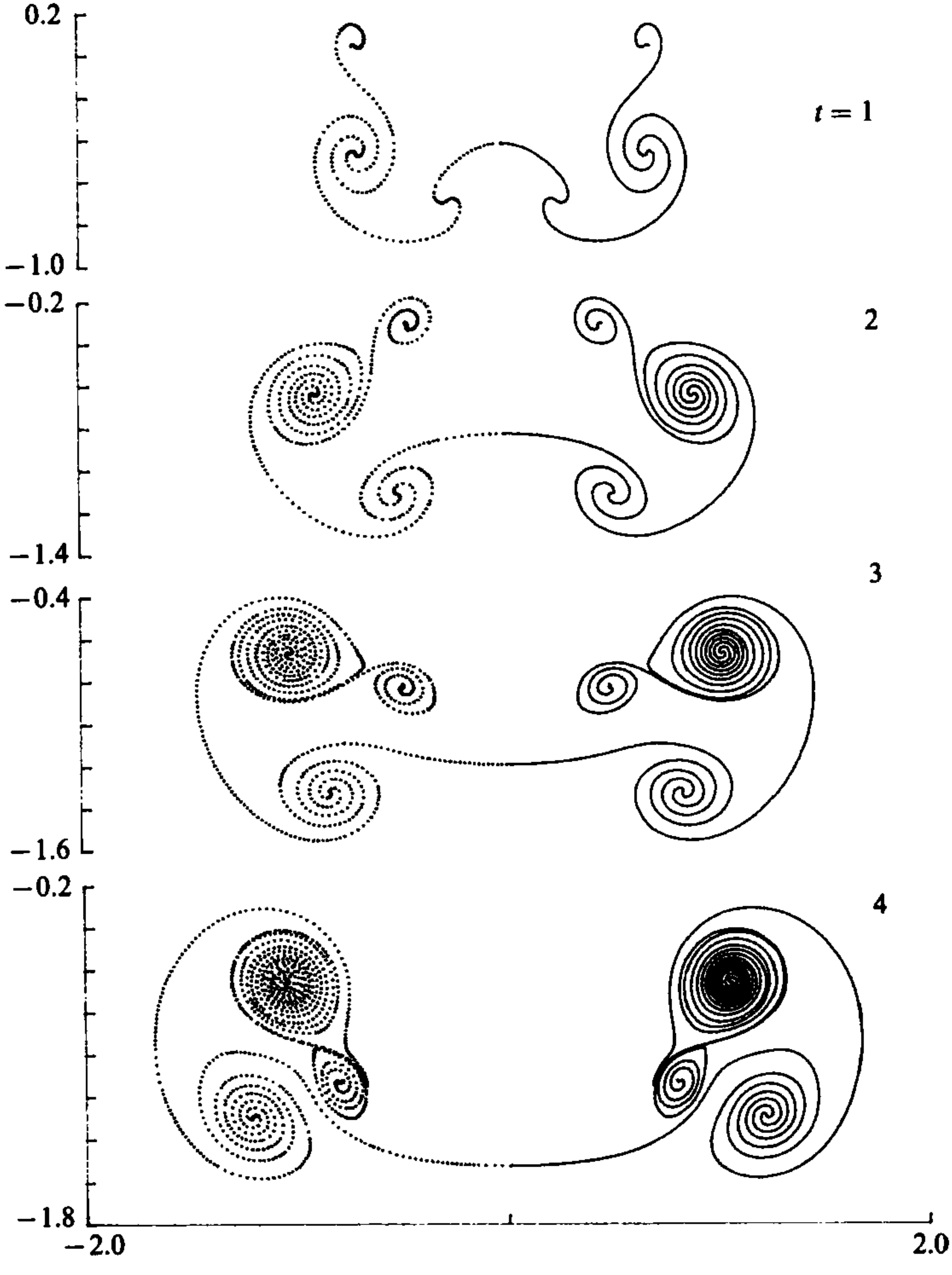


FIG. 154.—Surface of discontinuity behind a wing.

elliptically loaded wing ($N = 200\,, \delta = 0.05$)



fuselage/flap loading



charged particle systems

$x_i \in \mathbb{R}^3$: location , q_i : charge , $i = 1 : N$

$$\phi(x) = \sum_{i=1}^{N} \frac{q_i}{|x - x_i|} \ : \ \text{electrostatic potential} \ , \ -\nabla^2\phi(x) = \sum_{i=1}^{N} 4\pi q_i \delta(x - x_i)$$

$$F_i = q_i E_i = -q_i \nabla\phi(x_i) = q_i \sum_{\substack{j=1 \\ j\neq i}}^{N} q_j \frac{x_i - x_j}{|x_i - x_j|^3} \ : \ \text{force on particle } x_i \ , \ \ldots$$

$$V = \frac{1}{2} \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{q_i q_j}{|x_i - x_j|} \ : \ \text{total potential energy}$$

note : $\phi(x), F_i, V$ can be computed using mesh-based methods, e.g. PIC, but we want to consider mesh-free methods.

direct summation : particle-particle interactions

$$V = \frac{1}{2} \sum_{i=1}^{N} q_i \phi_i \ , \ \phi_i = \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{q_j}{|x_i - x_j|} \ : \ O(N^2) \text{ ops}$$

cutoff method

$$\sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{q_j}{|x_i - x_j|} \approx \sum_{x_j \in B_R(x_i)} \frac{q_j}{|x_i - x_j|} \ , \ B_R(x_i) = \{x : |x - x_i| \leq R\} \ : \ O(N) \text{ ops}$$

The cutoff method is useful for short-range interactions (e.g. Lennard-Jones, Ewald), but it's not recommended for electrostatics since the Coulomb potential decays slowly in space and the cutoff introduces numerical artifacts.

Barnes-Hut treecode : particle-cluster interactions

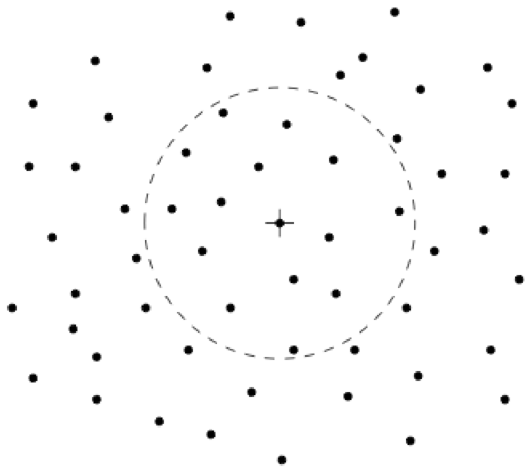
tree = hierarchical subdivision of the particles into clusters c

$$V = \frac{1}{2} \sum_{i=1}^{N} q_i \phi_i \ , \ \phi_i = \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{q_j}{|x_i - x_j|} = \sum_{c} \sum_{x_j \in c} \frac{q_j}{|x_i - x_j|} \ , \ \text{for suitable clusters } c$$

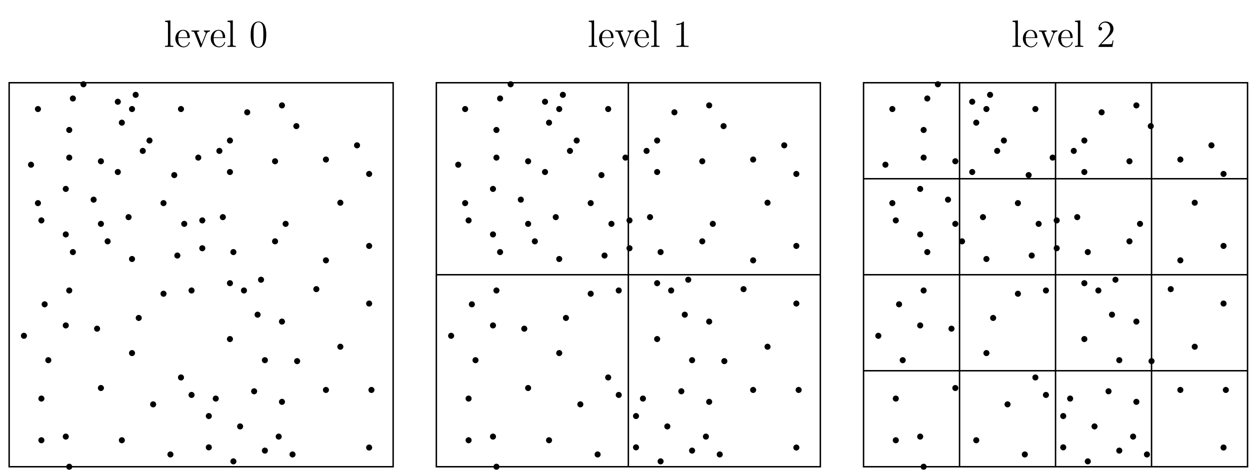
BH uses a monopole approximation to evaluate well-separated particle-cluster interactions.

$$\sum_{x_j \in c} \frac{q_j}{|x_i - x_j|} \approx \frac{Q_c}{|x_i - x_c|} \ , \ Q_c = \sum_{x_j \in c} q_j \ : \ \text{total charge in } c \ , \ x_c : \text{cluster center}$$

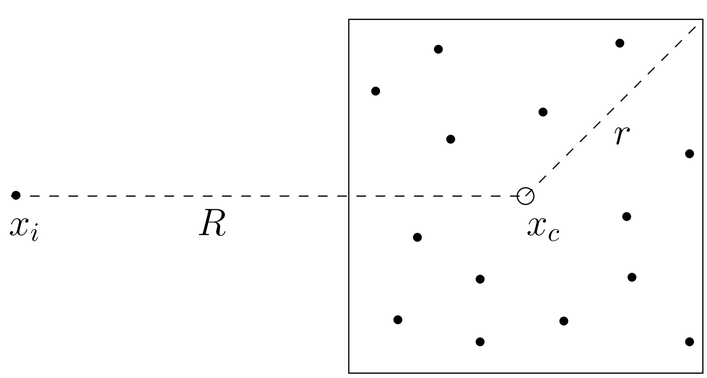
cutoff method



tree structure



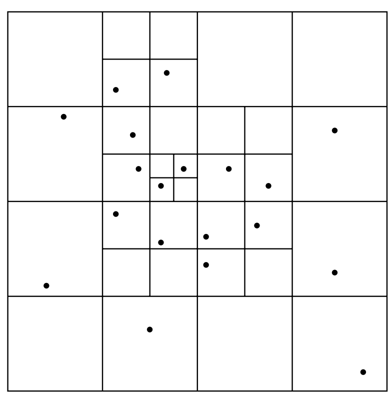
particle-cluster interaction



r : cluster radius , R : particle-cluster distance

<u>program</u> potential_energy
% input : x_i , q_i , $i = 1 : N$
% θ : accuracy parameter
% N_0 : maximum number of particles in a leaf of the tree
% output : V
construct tree
for $i = 1 : N$, compute_interaction(x_i , root), end
<u>function</u> compute_interaction(x_i , c)
if $r/R \le \theta$
    compute and store Q_c , x_c (unless done before)
    compute interaction by monopole approximation
else
    if c is a leaf, compute interaction by direct summation
    else, for each child c' of cluster c, compute_interaction(x_i , c')
end

<u>ex</u> : $N_0 = 1$



<u>operation count</u> : assume uniform particle density

N = number of particles in each box at level 0

$N/8$ = ... " 1

$N/8^L$ = ... " L

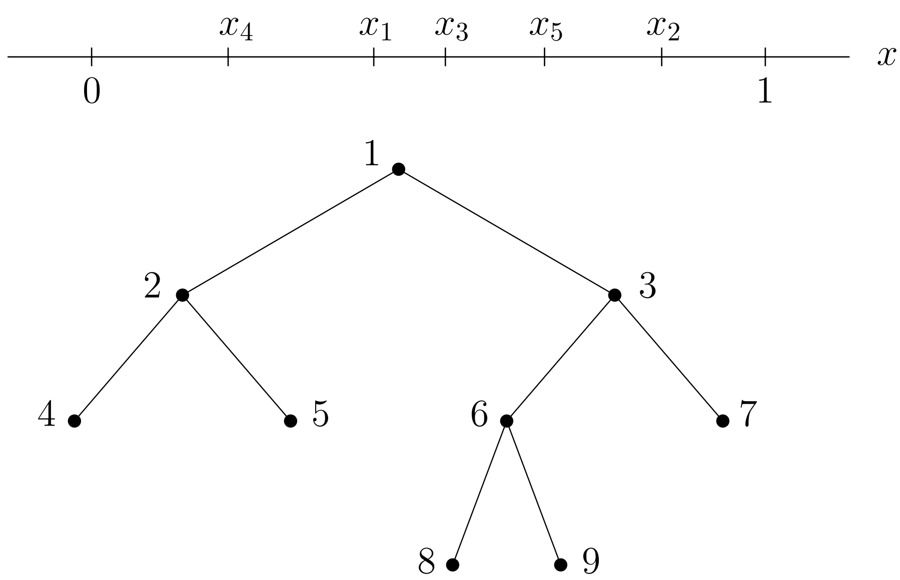
N/N = ... " .... $\log_8 N$

Hence there are $\log_8 N$ levels in the tree, and since each particle requires $O(1)$ ops at each level, BH requires $O(N \log N)$ ops.

1. forces : $F_i = q_i \sum_{\substack{j=1 \\ j \ne i}}^{N} q_j \frac{x_i - x_j}{|x_i - x_j|^3} \approx q_i \sum_c Q_c \frac{x_i - x_c}{|x_i - x_c|^3}$, ...

2. The monopole approximation is the 1st term in a <u>multipole expansion</u> of the particle-cluster interaction; the accuracy is improved using higher-order terms.

<u>ex</u> : $N = 5$, $N_0 = 1$, particles = [0.4186 0.8462 0.5252 0.2026 0.6721]



>> tree = m671b_build_tree
tree =
1×9 **struct** array with fields:
    interval
    members
    children

>> tree(1)
ans =
    interval: [0 1]
    members: [1 2 3 4 5]
    children: [2 3]

>> tree(2)
ans =
    interval: [0 0.5000]
    members: [1 4]
    children: [4 5]

>> tree(3)
ans =
    interval: [0.5000 1]
    members: [2 3 5]
    children: [6 7]

>> tree(4)
ans =
    interval: [0 0.2500]
    members: 4
    children: [ ]

>> tree(5)
ans =
    interval: [0.2500 0.5000]
    members: 1
    children: [ ]

>> tree(6)
ans =
    interval: [0.5000 0.7500]
    members: [3 5]
    children: [8 9]

>> tree(7)
ans =
    interval: [0.7500 1]
    members: 2
    children: [ ]

>> tree(8)
ans =
    interval: [0.5000 0.6250]
    members: 3
    children: [ ]

>> tree(9)
ans =
    interval: [0.6250 0.7500]
    members: 5
    children: [ ]

```
function tree_out = m671b_build_tree % Barnes-Hut
global tree particles node_count N0
% N = 100; N0 = 1; rand_N = rand(N,1); particles = rand_N(:,1);
N = 5; N0 = 1; particles = [0.4186 0.8462 0.5252 0.2026 0.6721];
tree = struct( 'interval' , [] , 'members' , [] , 'children' , [] );
tree(1).interval = [0,1];
tree(1).members = 1:N;
node_count = 1;
root = 1; build_tree(root); tree_out = tree;
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function build_tree(cluster_index)
global tree particles node_count N0
child = struct( 'interval' , [] , 'members' , [] , 'children' , [] );
n = length(tree(cluster_index).members);
if (n > N0)
  %
  % step 1 : define intervals for child clusters
  %
  a = tree(cluster_index).interval(1); b = tree(cluster_index).interval(2);
  midpoint = (a+b)/2;
  child(1).interval = [a midpoint]; child(2).interval = [midpoint b];
  %
  % step 2 : insert particles from parent into child clusters
  %
  count(1) = 0; count(2) = 0;
  for j = 1:n
    particle_index = tree(cluster_index).members(j);
    index = 1; if particles(particle_index) > midpoint; index = 2; end
    child(index).members = [child(index).members particle_index];
    count(index) = count(index) + 1;
  end
  %
  % step 3 : add non-empty children to tree
  %
  for j = 1:2
    if (count(j) >= 1)
      node_count = node_count + 1;
      tree(cluster_index).children = [tree(cluster_index).children node_count];
      tree = [tree child(j)];
    end
  end
  %
  % step 4 : recursive call to build next level of children
  %
  for i = 1:length(tree(cluster_index).children)
    cluster_index_new = tree(cluster_index).children(i);
    build_tree(cluster_index_new);
  end
end
```

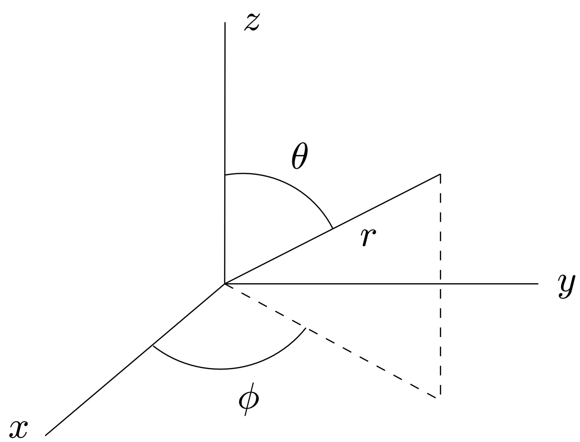
goal : multipole expansion (Folland, Wallace)

Let $x_1, \ldots, x_N \in \mathbb{R}^3$ be a set of point charges.

$$\Phi(x) = \sum_{i=1}^{N} \frac{q_i}{|x - x_i|} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \frac{M_n^m}{r^{n+1}} Y_n^m(\theta, \phi)$$

$Y_n^m(\theta, \phi)$: spherical harmonics , $M_n^m = \sum_{i=1}^{N} q_i \, r_i^n \, Y_n^{-m}(\theta_i, \phi_i)$: moments

$x = (r, \theta, \phi)$, $x_i = (r_i, \theta_i, \phi_i)$: spherical coordinates



$x = r \sin\theta \cos\phi$, $y = r \sin\theta \sin\phi$, $z = r \cos\theta$

$r = \sqrt{x^2 + y^2 + z^2}$, $r \geq 0$

θ : co-latitude , $0 \leq \theta \leq \pi$

ϕ : longitude , $0 \leq \phi \leq 2\pi$

we want to solve $-\nabla^2 \Phi = \rho$, but first consider $\nabla^2 \Phi = 0$

$$\Phi = \Phi(r, \theta, \phi) \Rightarrow \nabla^2 \Phi = \frac{1}{r^2}(r^2 \Phi_r)_r + \frac{1}{r^2 \sin\theta}(\sin\theta \, \Phi_\theta)_\theta + \frac{1}{r^2 \sin^2\theta} \Phi_{\phi\phi} = 0$$

separation of variables

$$\Phi(r, \theta, \phi) = R(r) S(\theta, \phi)$$

$$\frac{1}{R}(r^2 R_r)_r + \frac{1}{S \sin\theta}(\sin\theta \, S_\theta)_\theta + \frac{1}{S \sin^2\theta} S_{\phi\phi} = 0$$

$$\Rightarrow \frac{1}{R}(r^2 R_r)_r = \lambda \, , \quad \frac{1}{S \sin\theta}(\sin\theta \, S_\theta)_\theta + \frac{1}{S \sin^2\theta} S_{\phi\phi} = -\lambda$$

$S(\theta,\phi) = f(\theta)g(\phi)$

$$\frac{1}{f}\sin\theta(\,\sin\theta\, f_\theta)_\theta + \lambda\sin^2\!\theta + \frac{1}{g}g_{\phi\phi} = 0$$

$$\Rightarrow\ \frac{1}{f}\sin\theta(\,\sin\theta\, f_\theta)_\theta + \lambda\sin^2\!\theta = m^2\ ,\ \frac{1}{g}g_{\phi\phi} = -m^2$$

$g_{\phi\phi} + m^2 g = 0$ + PBC $\Rightarrow\ g(\phi) = \frac{1}{\sqrt{2\pi}}\, e^{im\phi}\,,\ m = 0,\,\pm1,\,\pm2,\,\ldots$: Fourier series

$$f_{\theta\theta} + \frac{\cos\theta}{\sin\theta}f_\theta + \Big(\lambda - \frac{m^2}{\sin^2\!\theta}\Big)f = 0\ :\ \text{e-value problem}$$

The equation for f has <u>regular singular points</u> at $\theta = 0\,,\pi$ (more later); there are no explicit BCs; instead, the e-function f is required to have a finite limit at $\theta = 0,\pi$; for each integer m, there exists an infinite sequence of e-values λ; the corresponding e-spaces are one-dimensional and mutually orthogonal.

<u>special case</u> : $m = 0$, we will verify these claims in this case

Then $\Phi(r,\theta,\phi)$ is independent of ϕ and hence is axisymmetric wrt z-axis.

$$f_{\theta\theta} + \frac{\cos\theta}{\sin\theta}f_\theta + \lambda f = 0$$

set $s = \cos\theta\,,\ f(\theta) = F(s)$

$$f_\theta = F_s s_\theta = F_s\cdot -\sin\theta = -\sin\theta F_s$$

$$f_{\theta\theta} = -\sin\theta F_{ss}\cdot -\sin\theta - \cos\theta F_s = \sin^2\!\theta F_{ss} - \cos\theta F_s$$

$$\Rightarrow\ \sin^2\!\theta F_{ss} - \cos\theta F_s + \frac{\cos\theta}{\sin\theta}\cdot -\sin\theta F_s + \lambda F = 0$$

$\Rightarrow\ (1-s^2)F_{ss} - 2sF_s + \lambda F = 0$: <u>Legendre equation</u>

$\Rightarrow\ ((1-s^2)F_s)_s + \lambda F = 0$: <u>Sturm-Liouville problem</u>

The Legendre equation has regular singular points at $s = \pm1$. (more later)

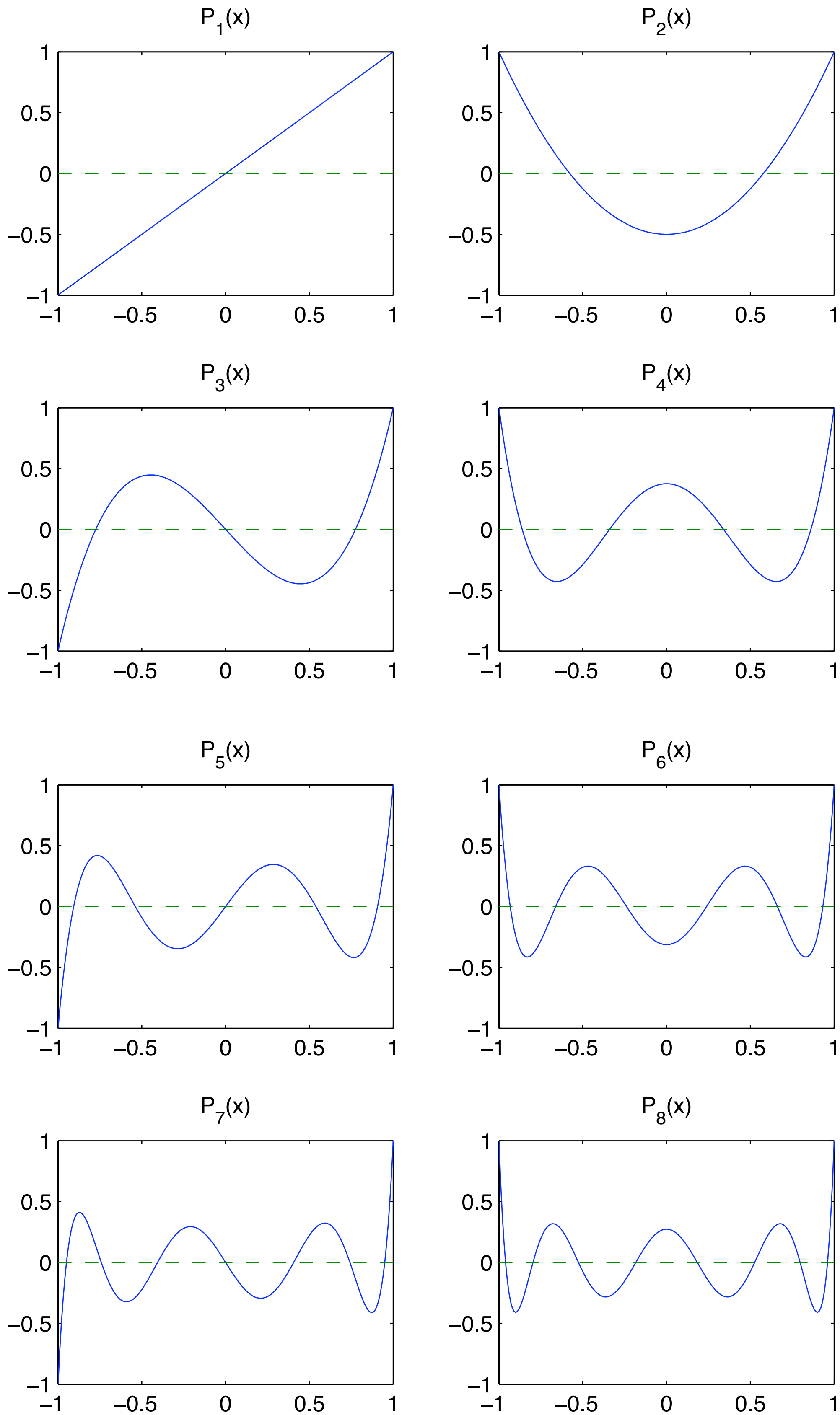
<u>def</u> : $P_n(x) = \dfrac{1}{2^n n!}\dfrac{d^n}{dx^n}(x^2-1)^n$: <u>Rodrigues formula</u>

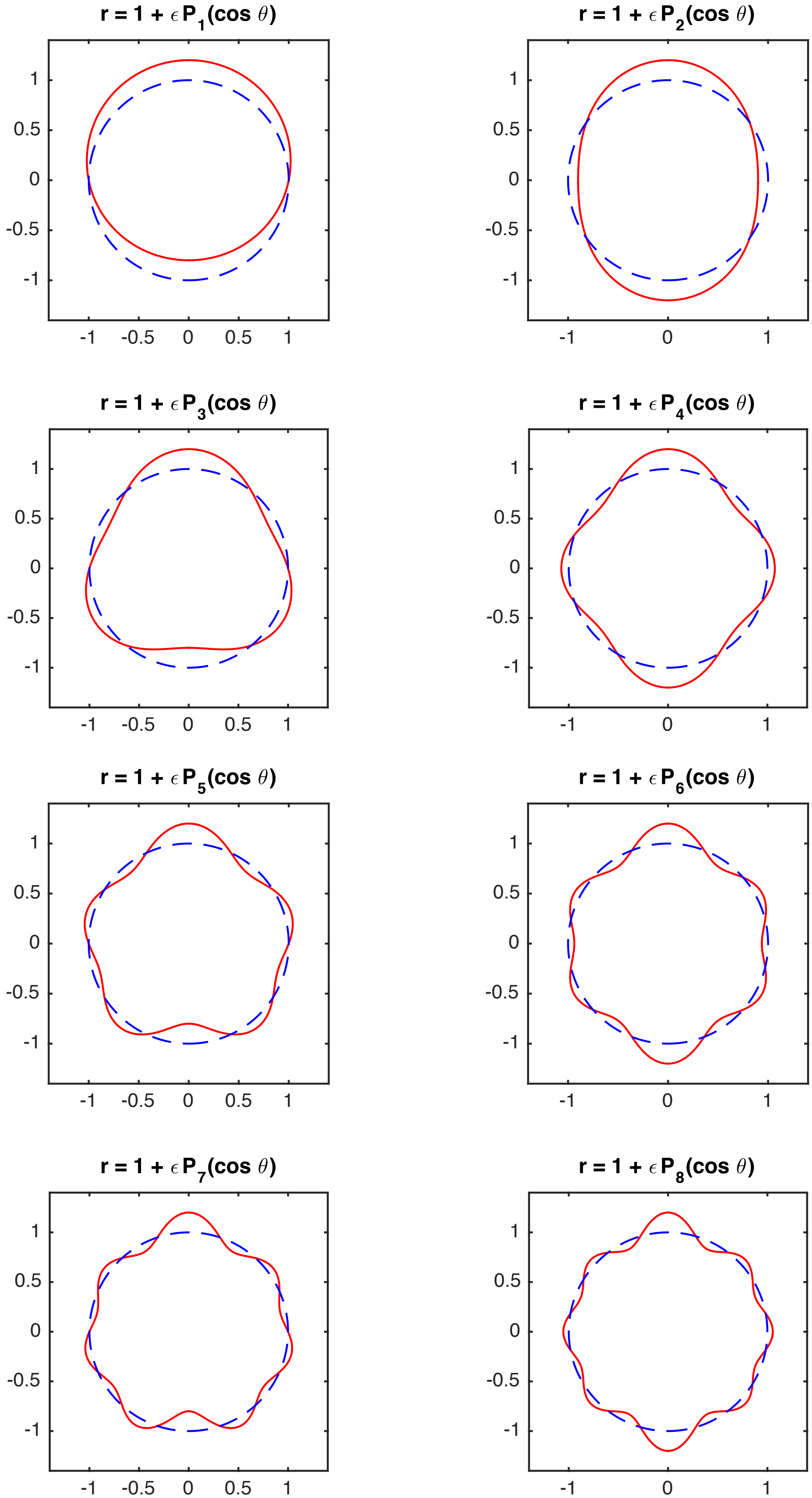
$P_n(x)$ is the <u>Legendre polynomial</u> of degree n

$P_0(x) = 1$

$P_1(x) = \frac{1}{2}\frac{d}{dx}(x^2-1) = \frac{1}{2}(2x) = x$

$P_2(x) = \frac{1}{4\cdot2}\frac{d^2}{dx^2}(x^2-1)^2 = \frac{1}{8}\frac{d^2}{dx^2}(x^4-2x^2+1) = \frac{1}{8}(12x^2-4) = \frac{3}{2}x^2 - \frac{1}{2}$


P_1(x)
P_2(x)
P_3(x)
P_4(x)
P_5(x)
P_6(x)
P_7(x)
P_8(x)
1
0.5
0
−0.5
−1
−1
−0.5
0
0.5
1


r = 1 + ϵP1(cos θ)
r = 1 + ϵP2(cos θ)
r = 1 + ϵP3(cos θ)
r = 1 + ϵP4(cos θ)
r = 1 + ϵP5(cos θ)
r = 1 + ϵP6(cos θ)
r = 1 + ϵP7(cos θ)
r = 1 + ϵP8(cos θ)

<u>properties of Legendre polynomials</u>

1. $((1-x^2)P_n'(x))' + n(n+1)P_n(x) = 0$: Legendre equation , $\lambda = n(n+1)$

2. $\int_{-1}^{1} P_n(x)P_m(x)dx = 0$ if $n \neq m$: orthogonality

<u>pf</u>

1. $n = 0, 1$: ok , consider $n \geq 2$

set $y = (x^2-1)^n \Rightarrow y' = n(x^2-1)^{n-1} \cdot 2x \Rightarrow (x^2-1)y' = 2nxy$

differentiate both sides $n+1$ times

recall : $(fg)^{(n)} = fg^{(n)} + nf^{(1)}g^{(n-1)} + \frac{1}{2}n(n-1)f^{(2)}g^{(n-2)} + \cdots$

$(x^2-1)y^{(n+2)} + (n+1)2xy^{(n+1)} + \frac{1}{2}(n+1)n2y^{(n)} = 2n(xy^{(n+1)} + (n+1)y^{(n)})$

$\Rightarrow (x^2-1)y^{(n+2)} + 2xy^{(n+1)} - n(n+1)y^{(n)} = 0$

$\Rightarrow (1-x^2)y^{(n+2)} - 2xy^{(n+1)} + n(n+1)y^{(n)} = 0$

note : $y^{(n)} = \dfrac{d^n}{dx^n}(x^2-1)^n = 2^n n! P_n(x)$

$\Rightarrow (1-x^2)P_n''(x) - 2xP_n'(x) + n(n+1)P_n(x) = 0$ <u>ok</u>

2. $((1-x^2)P_n'(x))' + n(n+1)P_n(x) = 0$

$\Rightarrow \int_{-1}^{1} \left[((1-x^2)P_n'(x))'P_m(x) + n(n+1)P_n(x)P_m(x)\right] dx = 0$

note : $(1-x^2)P_n'(x)P_m(x)\Big|_{-1}^{1} = 0$

$\Rightarrow -\int_{-1}^{1}(1-x^2)P_n'(x)P_m'(x)dx + n(n+1)\int_{-1}^{1} P_n(x)P_m(x)dx = 0$

now reverse m and n

$\Rightarrow -\int_{-1}^{1}(1-x^2)P_m'(x)P_n'(x)dx + m(m+1)\int_{-1}^{1} P_m(x)P_n(x)dx = 0$

subtract $\Rightarrow ((n(n+1) - m(m+1))\int_{-1}^{1} P_n(x)P_m(x)dx = 0$ <u>ok</u>

<u>note</u> : The Legendre equation has e-values $\lambda = n(n+1)$ for $n = 0, 1, 2, \ldots,$ and the corresponding e-functions $P_n(x)$ form an orthogonal basis for $L^2(-1, 1)$.

<u>background</u> : series solutions of differential equations

<u>def</u> : A function $f(x)$ is <u>analytic</u> at x_0 if it has a convergent power series expansion in a neighborhood of x_0, i.e. $f(x) = \sum_{k=0}^{\infty} b_k(x-x_0)^k$ for $|x-x_0| < R$, where $R > 0$; otherwise $f(x)$ is <u>singular</u> at x_0.

Consider $y'' + a_1(x)y' + a_2(x)y = 0$: 2nd order, linear, variable coefficient ODE.

question : are the solutions $y(x)$ analytic or singular at a given x_0?

<u>thm</u> : classification of x_0

1. <u>ordinary point</u> : $a_1(x)$ and $a_2(x)$ are analytic at x_0

$\Rightarrow$ there are two linearly independent analytic solutions at x_0

<u>ex</u> : $y'' + y = 0$

$a_1(x) = 0\,,\ a_2(x) = 1$: all points x_0 are ordinary

$y(x) = c_1 \sin x + c_2 \cos x$ <u>ok</u>

2. <u>singular point</u> : $a_1(x)$ or $a_2(x)$ is singular at x_0

2a. <u>regular singular point</u> : $(x-x_0)a_1(x)$ and $(x-x_0)^2 a_2(x)$ are analytic at x_0,

i.e. $y'' + \dfrac{\tilde{a}_1(x)}{x-x_0}\,y' + \dfrac{\tilde{a}_2(x)}{(x-x_0)^2}\,y = 0$, where $\tilde{a}_1(x), \tilde{a}_2(x)$ are analytic at x_0

$\Rightarrow$ there is at least one nonzero solution of the form $y(x) = \sum_{k=0}^{\infty} b_k(x-x_0)^{k+s}$,

where $s \in \mathbb{C}$, and $y(x)$ is analytic at $x_0 \Leftrightarrow s = 0, 1, 2, \ldots$

<u>ex</u> : $(1-x^2)y'' - 2xy' = 0$: Legendre equation , $n = 0$

$y'' - \dfrac{2x}{1-x^2}\,y' = 0$: regular singular points at $x_0 = \pm 1$

$y(x) = c_1 + c_2 \log \frac{1+x}{1-x}$ <u>ok</u>

2b. <u>irregular singular point</u> : x_0 is singular, but not regular singular

$\Rightarrow$ a nonzero analytic solution at x_0 may or may not exist

<u>ex</u> : $x^4 y'' + 2x^3 y' + y = 0$

$y'' + \dfrac{2}{x}\,y' + \dfrac{1}{x^4}\,y = 0$: irregular singular point at $x_0 = 0$

$y(x) = c_1 \sin \frac{1}{x} + c_2 \cos \frac{1}{x}$ <u>ok</u>

<u>ex</u> : $(1-x^2)y'' - 2xy' + n(n+1)y = 0$: Legendre equation , $n = 0, 1, 2, \ldots$

$x_0 = 0$ is an ordinary point , we want to verify the theorem

$$y = \sum_{k=0}^{\infty} b_k x^k \ , \ y' = \sum_{k=0}^{\infty} b_k k x^{k-1} \ , \ y'' = \sum_{k=0}^{\infty} b_k k(k-1) x^{k-2}$$

$$\sum_{k=0}^{\infty} b_k k(k-1)x^{k-2} - \sum_{k=0}^{\infty} b_k k(k-1)x^k - 2\sum_{k=0}^{\infty} b_k k x^k + n(n+1)\sum_{k=0}^{\infty} b_k x^k = 0$$

$$\Rightarrow \sum_{k=0}^{\infty} b_k k(k-1)x^{k-2} - \sum_{k=0}^{\infty} b_k (k(k-1) + 2k - n(n+1))x^k = 0$$

set $f(k) = k(k-1)$, note : $k(k-1) + 2k = k(k+1) = f(k+1)$

$$\Rightarrow \sum_{k=0}^{\infty} b_k f(k) x^{k-2} - \sum_{k=0}^{\infty} b_k (f(k+1) - f(n+1))x^k = 0$$

$$\Rightarrow \sum_{k=0}^{\infty} b_k f(k) x^{k-2} - \sum_{k=2}^{\infty} b_{k-2} (f(k-1) - f(n+1))x^{k-2} = 0$$

$b_0 f(0) x^{-2} + b_1 f(1) x^{-1} = 0$ because $f(0) = f(1) = 0$

$$\Rightarrow \sum_{k=2}^{\infty} [b_k f(k) - b_{k-2}(f(k-1) - f(n+1))] x^{k-2} = 0$$

$\Rightarrow b_k f(k) = b_{k-2}(f(k-1) - f(n+1))$, $k \geq 2$

<u>case 1</u> : $b_0 \neq 0$, $b_1 = 0$

$\Rightarrow b_3 = b_5 = b_7 = \cdots = 0 \Rightarrow$ we may assume k is even

<u>case 1a</u> : n is even $\Rightarrow f(k-1) = f(n+1)$ for $k = n+2 \Rightarrow b_k = 0$ for $k \geq n+2$

$\Rightarrow y(x)$ is an even polynomial of degree n , $P_n(x)$

<u>case 1b</u> : n is odd $\Rightarrow f(k-1) \neq f(n+1)$ for $k \geq 2$

$\Rightarrow y(x)$ is an even non-terminating power series , $Q_n(x)$

<u>case 2</u> : $b_0 = 0$, $b_1 \neq 0$

$\Rightarrow b_2 = b_4 = b_6 = \cdots = 0 \Rightarrow$ we may assume k is odd , $\ldots \begin{cases} n : \text{even} \Rightarrow Q_n(x) \\ n : \text{odd} \ \Rightarrow P_n(x) \end{cases}$

<u>general solution</u> : $y(x) = c_1 P_n(x) + c_2 Q_n(x)$

<u>note</u> : We saw that $Q_0(x) = \log \frac{1+x}{1-x}$, which is analytic at $x_0 = 0$; in fact, $Q_n(x)$ is singular at $x = \pm 1$ for all $n \geq 0$.

more properties of Legendre polynomials

1. $\displaystyle\sum_{n=0}^{\infty} P_n(x)t^n = \frac{1}{\sqrt{1-2xt+t^2}}$: generating function , holds for $|x| \le 1\,, |t| < 1$

2. $P_n(1) = 1$

3. $\displaystyle ||P_n||^2 = \int_{-1}^{1} P_n(x)^2 dx \; = \; \frac{2}{2n+1}$

4. $(n+1)P_{n+1}(x) - (2n+1)xP_n(x) + nP_{n-1}(x) = 0$: recurrence relation , $n \ge 1$

pf

1. recall : $\displaystyle \frac{1}{2\pi i}\int_C \frac{f(z)}{(z-z_0)^{n+1}}\,dz = \frac{f^{(n)}(z_0)}{n!}$: Cauchy integral formula

set $f(z) = \left(\dfrac{z^2-1}{2}\right)^n$, $z_0 = x$, $C = \{z : |z-x| = 1\}$

$$\Rightarrow\; \frac{1}{2\pi i}\int_C \frac{(z^2-1)^n}{2^n(z-x)^{n+1}}\,dz = \frac{1}{n!}\frac{d^n}{dx^n}\left(\frac{x^2-1}{2}\right)^n = P_n(x)$$

$$\Rightarrow \sum_{n=0}^{\infty} P_n(x)t^n = \frac{1}{2\pi i}\int_C \sum_{n=0}^{\infty}\left(\frac{t}{2}\right)^n \frac{(z^2-1)^n}{(z-x)^{n+1}}\,dz : \begin{cases} \text{geometric series,} \\ \text{for small } t \text{ the series} \\ \text{converges uniformly for } z \in C \end{cases}$$

$$= \frac{1}{2\pi i}\int_C \frac{1}{z-x}\left(1 - \frac{t(z^2-1)}{2(z-x)}\right)^{-1} dz$$

$$= \frac{1}{2\pi i}\int_C \frac{2}{2(z-x)-t(z^2-1)}\,dz \;:\; \text{evaluate by residue theorem}$$

$$-tz^2 + 2z + t - 2x = 0 \;\Rightarrow\; z = \frac{-2 \pm \sqrt{4-4(-t)(t-2x)}}{-2t} = \frac{1 \pm \sqrt{1-2xt+t^2}}{t}$$

$z_1 = \dfrac{1-\sqrt{1-2xt+t^2}}{t}$, $\displaystyle\lim_{t\to 0} z_1 = x \;\Rightarrow\; z_1$ is inside C , ... z_2 is outside C

$$\sum_{n=0}^{\infty} P_n(x)t^n = \mathrm{Res}\left(\frac{2}{-t(z-z_1)(z-z_2)}\,; z = z_1\right) = \frac{2}{-t(z_1-z_2)} = \frac{1}{\sqrt{1-2xt+t^2}}$$

This proves the result for small t, but the series is the Taylor series of a function which is analytic at $t = 0$ and whose only singularities are at $t = x \pm i\sqrt{1-x^2}$, which satisfy $|t| = 1$, so the series converges for $|t| < 1$. ok

2. $\displaystyle x = 1 \;\Rightarrow\; \sum_{n=0}^{\infty} P_n(1)t^n = \frac{1}{\sqrt{1-2t+t^2}} \;=\; \frac{1}{1-t} = \sum_{n=0}^{\infty} t^n$ ok

3. square and integrate

$$\int_{-1}^{1} \frac{dx}{1-2xt+t^2} = \int_{-1}^{1}\left(\sum_{n=0}^{\infty} P_n(x)t^n\right)^2 dx = \sum_{n=0}^{\infty}\int_{-1}^{1} P_n(x)^2 dx \cdot t^{2n}$$

$$= \frac{\log(1-2xt+t^2)}{-2t}\Big|_{-1}^{1} = -\frac{1}{2t}\log\left(\frac{1-2t+t^2}{1+2t+t^2}\right) = \frac{1}{t}\log\frac{1+t}{1-t}$$

$$\frac{1}{1+t} = \sum_{l=0}^{\infty}(-t)^n \Rightarrow \log(1+t) = \sum_{n=0}^{\infty}\frac{(-1)^n t^{n+1}}{n+1}$$

$$\frac{1}{1-t} = \sum_{n=0}^{\infty} t^n \Rightarrow -\log(1-t) = \sum_{n=0}^{\infty}\frac{t^{n+1}}{n+1}$$

$$\Rightarrow \frac{1}{t}\log\frac{1+t}{1-t} = \sum_{n=0}^{\infty}\frac{2}{2n+1}t^{2n} \quad \underline{\text{ok}}$$

4. set $f(t) = (1-2xt+t^2)^{-1/2}$, then $P_n(x) = \dfrac{f^{(n)}(0)}{n!}$

$f'(t) = -\frac{1}{2}(1-2xt+t^2)^{-3/2}\cdot(-2x+2t) \Rightarrow (1-2xt+t^2)f'(t) = (x-t)f(t)$

differentiate n times wrt t

$$(1-2xt+t^2)f^{(n+1)}(t) + n(-2x+2t)f^{(n)}(t) + \tfrac{1}{2}n(n-1)2f^{(n-1)}(t)$$
$$= (x-t)f^{(n)}(t) + n(-1)f^{(n-1)}(t)$$

set $t=0$: $f^{(n+1)}(0) - 2nxf^{(n)}(0) + n(n-1)f^{(n-1)}(0) = xf^{(n)}(0) - nf^{(n-1)}(0)$

divide by $(n+1)!$: $\dfrac{f^{(n+1)}(0)}{(n+1)!} - \dfrac{(2n+1)xf^{(n)}(0)}{(n+1)!} + \dfrac{n^2 f^{(n-1)}(0)}{(n+1)!} = 0$ <u>ok</u>

<u>check</u>

1. generating function

recall : $(1+x)^k = 1 + kx + \frac{1}{2}k(k-1)x^2 + \frac{1}{3!}k(k-1)(k-2)x^3 + \cdots$

set $k = -\frac{1}{2}$, $x \to -2xt+t^2$

$(1-2xt+t^2)^{-1/2} = 1 + \frac{1}{2}(2xt-t^2) + \frac{3}{8}(2xt-t^2)^2 + \frac{5}{16}(2xt-t^2)^3 + \cdots$

$P_0(x) = 1$, $P_1(x) = x$, $P_2(x) = \frac{3}{2}x^2 - \frac{1}{2}$, $P_3(x) = \frac{5}{2}x^3 - \frac{3}{2}x$ <u>ok</u>

2. recurrence relation

$P_0(x) = 1$, $P_1(x) = x$

$n=1 \Rightarrow 2P_2(x) - 3xP_1(x) + P_0(x) = 0 \Rightarrow P_2(x) = \frac{3}{2}x^2 - \frac{1}{2}$

$n=2 \Rightarrow 3P_3(x) - 5xP_2(x) + 2P_1(x) = 0 \Rightarrow P_3(x) = \frac{5}{2}x^3 - \frac{3}{2}x$ <u>ok</u>

recall : radial equation , $\frac{1}{R}(r^2R_r)_r = \lambda = n(n+1)$

$r^2R_{rr} + 2rR_r - n(n+1)R = 0$

$a_1(r) = \frac{2}{r}$, $a_2(r) = -\frac{n(n+1)}{r^2}$: singular point at $r = 0$

$ra_1(r) = 2$, $r^2a_2(r) = -n(n+1)$: regular singular point

$$R(r) = r^s \Rightarrow s(s-1)r^s + 2sr^s - n(n+1)r^s = 0$$
$$\Rightarrow s^2 + s - n(n+1) = (s-n)(s+(n+1)) = 0 \Rightarrow s = n\,, -(n+1)$$
$$\Rightarrow R(r) = ar^n + \frac{b}{r^{n+1}}$$

general axisymmetric solution of $\nabla^2\Phi = 0$

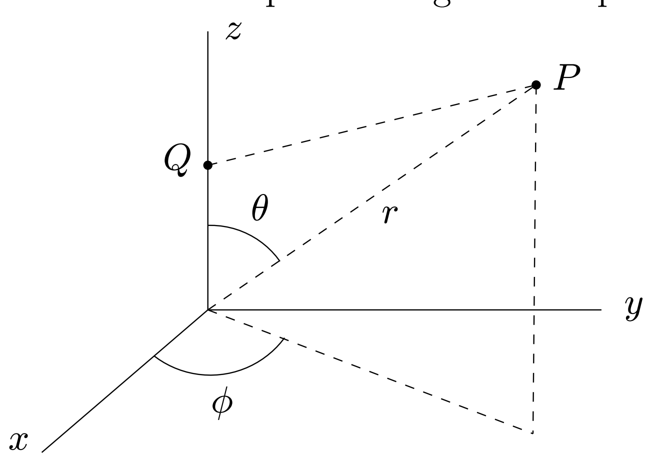
$$\Phi(r,\theta,\phi) = \sum_{n=0}^{\infty}\left(a_nr^n + \frac{b_n}{r^{n+1}}\right)P_n(\cos\theta) \ : \ \text{axisymmetric wrt } z\text{-axis}$$

We allow a singularity at $r = 0$, but not at $\theta = 0, \pi$.

ex 1 : potential due to a point charge at the origin

$$\Phi(r,\theta,\phi) = \frac{1}{r} \ , \ -\nabla^2\left(\frac{1}{r}\right) = 4\pi\delta(r) \ : \ \text{hw}$$

ex 2 : potential due to a point charge on the positive z-axis



$Q = (0,0,z_0)$, $P = (x,y,z) = (r\sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta)$

$$\Phi(r,\theta,\phi) = \frac{1}{|P-Q|} = \frac{1}{\sqrt{x^2+y^2+(z-z_0)^2}} = \frac{1}{\sqrt{r^2 - 2rz_0\cos\theta + z_0^2}}$$

$$z_0 < r \Rightarrow \Phi(r,\theta,\phi) = \frac{1}{r}\frac{1}{\sqrt{1-2\cos\theta(z_0/r) + (z_0/r)^2}} = \sum_{n=0}^{\infty}\frac{z_0^n}{r^{n+1}}P_n(\cos\theta)$$

note : 1. If $z_0 \to 0$, then ex 2 $\to$ ex 1.

2. $z_0 > r \Rightarrow \Phi(r,\theta,\phi) = \sum_{n=0}^{\infty}\frac{r^n}{z_0^{n+1}}P_n(\cos\theta)$

alternative viewpoint

Consider again the potential due to a point charge on the positive z-axis.

$$\Phi(x,y,z;z_0) \;=\; \frac{1}{\sqrt{x^2+y^2+(z-z_0)^2}} \;\;,\;\text{Taylor expand wrt } z_0 \text{ about } z_0=0$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!}\partial_{z_0}^n \Phi|_{z_0=0}\, z_0^n \;\;,\; \text{where } \partial_{z_0}\Phi|_{z_0=0} \;=\; -\partial_z\Phi|_{z_0=0} \;=\; -\partial_z\left(\frac{1}{r}\right)$$

$$= \sum_{n=0}^{\infty} z_0^n \,\frac{(-1)^n}{n!}\partial_z^n\left(\frac{1}{r}\right) = \sum_{n=0}^{\infty} \frac{z_0^n}{r^{n+1}}\, P_n(\cos\theta) \;:\; \text{converges for } z_0 < r$$

$$\Rightarrow P_n(\cos\theta) = \frac{(-1)^n}{n!}\, r^{n+1}\, \partial_z^n\left(\frac{1}{r}\right) \;:\; \text{another definition of Legendre polynomials}$$

$$\text{define } \Phi_n(x,y,z;0) \;=\; \frac{(-1)^n}{n!}\partial_z^n\left(\frac{1}{r}\right) \;=\; \frac{P_n(\cos\theta)}{r^{n+1}} \;:\; \text{axisymmetric potential}$$

$$\Phi_0(x,y,z;0) = \frac{1}{r} = \frac{P_0(\cos\theta)}{r} \;,\; \nabla^2\Phi_0 = -4\pi\delta \;:\; \text{monopole potential}$$

$$\Phi_1(x,y,z;0) = -\partial_z\left(\frac{1}{r}\right) = \frac{z}{r^3} = \frac{P_1(\cos\theta)}{r^2} \;,\; \nabla^2\Phi_1 = 4\pi\partial_z\delta \;:\; \text{dipole potential}$$

$$= \partial_{z_0}\Phi_0 \;=\; \lim_{\epsilon\to 0}\left(\frac{\Phi_0(x,y,z;\epsilon)-\Phi_0(x,y,z;-\epsilon)}{2\epsilon}\right)$$

$$\Phi_2(x,y,z;0) = \frac{1}{2}\,\partial_z^2\left(\frac{1}{r}\right) = \frac{1}{2}\cdot -\partial_z\left(\frac{z}{r^3}\right) = \frac{1}{2}\cdot -\left(\frac{r^3 - z\cdot 3r^2\cdot z/r}{r^6}\right)$$

$$= \frac{3z^2-r^2}{2r^5} = \frac{P_2(\cos\theta)}{r^3} \;,\; \nabla^2\Phi_2 = -4\pi\partial_z^2\delta \;:\; \text{quadrupole potential}$$

summary

$$\Phi(x,y,z;z_0) = \sum_{n=0}^{\infty} M_n(z_0)\Phi_n(x,y,z;0) \;:\; \text{multipole expansion}$$

$\Phi_n(x,y,z;0)$: multipole potential of order 2^n along the z-axis at $z_0=0$

$M_n(z_0) = z_0^n$: multipole moment

Hence for $r > z_0$, a monopole charge at $(0,0,z_0)$ is equivalent to a multipole charge at $(0,0,0)$.

$$\delta_{z_0} = \sum_{n=0}^{\infty} z_0^n \frac{(-1)^n}{n!}\,\partial_z^n\delta_0$$

<u>recall</u> : separation of variables , $S(\theta,\phi) = f(\theta)g(\phi)$

$g(\phi) = \frac{1}{\sqrt{2\pi}}\, e^{im\phi}$, $m = 0, \pm 1, \pm 2, \ldots$: Fourier series

$f_{\theta\theta} + \dfrac{\cos\theta}{\sin\theta} f_\theta + \Big(\lambda - \dfrac{m^2}{\sin^2\theta}\Big) f = 0$ + BC : e-value problem

$s = \cos\theta\,,\ f(\theta) = F(s)$

$((1-s^2)F_s)_s + \Big(\lambda - \dfrac{m^2}{1-s^2}\Big)F = 0$: <u>associated Legendre equation</u>

special case : $m = 0$

$((1-s^2)F_s)_s + \lambda F = 0$: Legendre equation

$\lambda = n(n+1)\,,\ F(s) = P_n(s)\,,\ f(\theta) = P_n(\cos\theta)\,,\ n = 0, 1, 2, \ldots$

---

now consider $m = 1, 2, \ldots$

<u>claim</u>: If $w(s)$ satisfies LE, then $F(s) = (1-s^2)^{m/2} w^{(m)}(s)$ satisfies ALE.

<u>pf</u> : given $((1-s^2)w_s)_s + \lambda w = 0$, differentiate m times

$\Rightarrow\ ((1-s^2)w_s)^{(m+1)} + \lambda w^{(m)} = 0$

$\Rightarrow\ (1-s^2)w^{(m+2)} + (m+1)(-2s)w^{(m+1)} + \frac{1}{2}(m+1)m(-2)w^{(m)} + \lambda w^{(m)} = 0$

set $F(s) = (1-s^2)^{m/2} w^{(m)}(s)$

$\Rightarrow\ F_s = (1-s^2)^{m/2} w^{(m+1)} + \frac{m}{2}(1-s^2)^{(m/2)-1}(-2s)w^{(m)}$

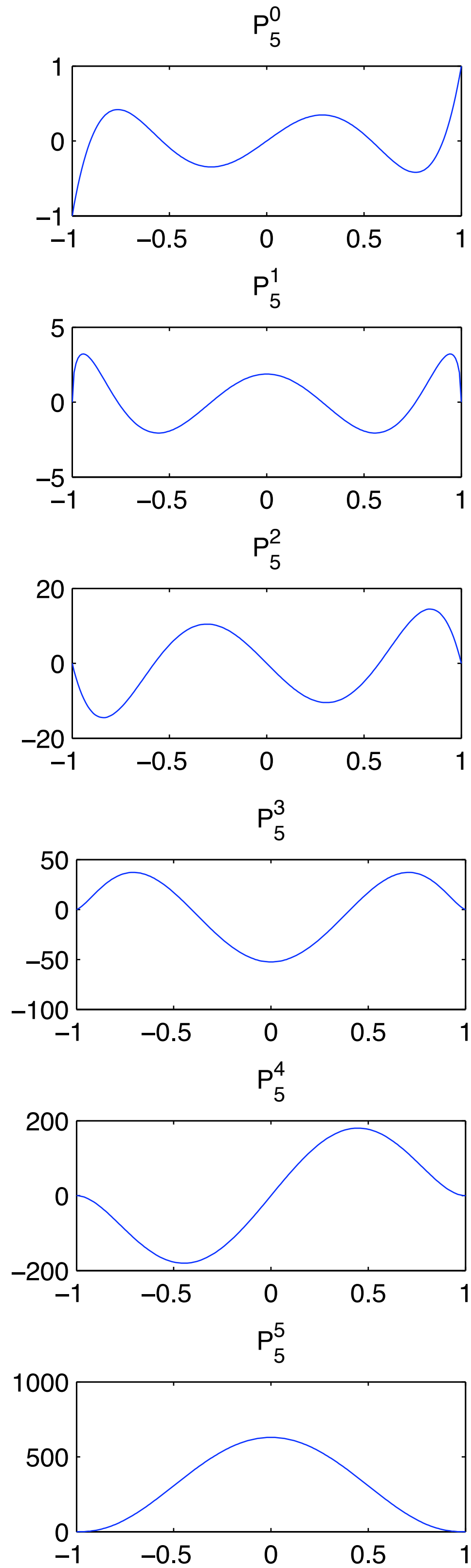
$\Rightarrow\ (1-s^2)F_s = (1-s^2)^{(m/2)+1} w^{(m+1)} - ms(1-s^2)^{m/2} w^{(m)}$

$$\begin{aligned}
\Rightarrow\ ((1-s^2)F_s)_s &= (1-s^2)^{(m/2)+1} w^{(m+2)} + (\tfrac{m}{2}+1)(1-s^2)^{m/2}(-2s)w^{(m+1)} \\
&\quad - ms(1-s^2)^{m/2} w^{(m+1)} - ms\tfrac{m}{2}(1-s^2)^{(m/2)-1}(-2s)w^{(m)} - m(1-s^2)^{m/2} w^{(m)} \\
&= (1-s^2)^{m/2}\,[(1-s^2)w^{(m+2)} - 2(m+1)sw^{(m+1)} + (\tfrac{m^2 s^2}{1-s^2} - m)w^{(m)}] \\
&= (1-s^2)^{m/2}\,[(m+1)mw^{(m)} - \lambda w^{(m)} + (\tfrac{m^2 s^2}{1-s^2} - m)w^{(m)}] \\
&= [m^2(1 + \tfrac{s^2}{1-s^2}) - \lambda]F = (\tfrac{m^2}{1-s^2} - \lambda)F \qquad \underline{\text{ok}}
\end{aligned}$$

Now choose $\lambda = n(n+1)\,, w(s) = P_n(s)$.

<u>def</u>: $P_n^m(s) = (1-s^2)^{m/2} \dfrac{d^m}{ds^m} P_n(s)$, for $m = 0 : n$

$$= \frac{(1-s^2)^{m/2}}{2^n n!} \frac{d^{n+m}}{ds^{n+m}}(s^2-1)^n$$: <u>associated Legendre function</u>



associated Legendre functions

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n\,,\ n = 0, 1, 2, \dots$$

$$P_n^m(x) = (1-x^2)^{m/2}\frac{d^m}{dx^m}P_n(x)\,,\ m = 0 : n$$

n	P_n^0
0	1
1	x
2	$\frac{1}{2}(3x^2-1)$
3	$\frac{1}{2}(5x^3-3x)$
4	$\frac{1}{8}(35x^4-30x^2+3)$
5	$\frac{1}{8}(63x^5-70x^3+15x)$
n	P_n^1
1	$(1-x^2)^{1/2}$
2	$3x(1-x^2)^{1/2}$
3	$\frac{3}{2}(5x^2-1)(1-x^2)^{1/2}$
4	$\frac{5}{2}(7x^3-3x)(1-x^2)^{1/2}$
5	$\frac{15}{8}(21x^4-14x^2+1)(1-x^2)^{1/2}$
n	P_n^2
2	$3(1-x^2)$
3	$15x(1-x^2)$
4	$\frac{15}{2}(7x^2-1)(1-x^2)$
5	$\frac{105}{2}(3x^3-x)(1-x^2)$
n	P_n^3
3	$15(1-x^2)^{3/2}$
4	$105x(1-x^2)^{3/2}$
5	$\frac{105}{2}(6x^2-1)(1-x^2)^{3/2}$
n	P_n^4
4	$105(1-x^2)^2$
5	$630x(1-x^2)^2$
n	P_n^5
5	$630(1-x^2)^{5/2}$

1. $P_n^m(x)$ satisfies the following BVP for $m = 1 : n$

   $((1-x^2)y')' + (n(n+1) - \frac{m^2}{1-x^2})y = 0\,,\ y(-1) = y(1) = 0$

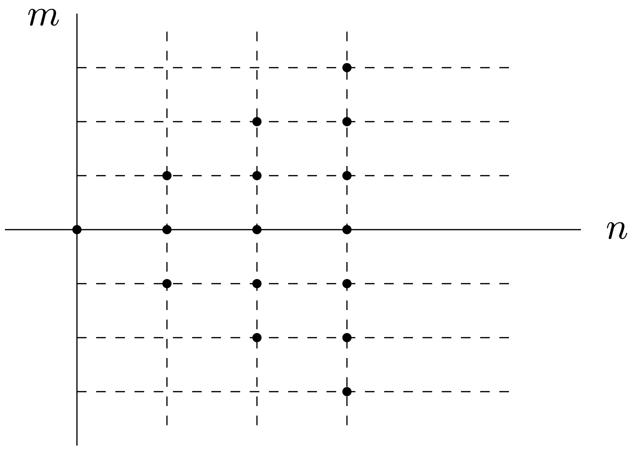
2. $s = \pm 1$ are irregular singular points

3. For $m \to n$, $P_n^m(x)$ becomes flatter near $x = \pm 1$ and concentrated near $x = 0$.

claim

1. For each $m = 0, 1, 2, \ldots$, $\{P_n^m(s)\}_{n=m}^\infty$ is an orthogonal basis for $L^2(-1,1)$.

2. $||P_n^m||^2 = \dfrac{(n+m)!}{(n-m)!}\dfrac{2}{2n+1}$, $n = 0, 1, 2, \ldots$, $m = 0 : n$



pf : the case $m = 0$ is already done, so assume $m = 1, 2, \ldots$

1. Orthogonality follows as usual for solutions of a self-adjoint e-value problem. To show completeness, let $q_k(s) = (1-s^2)^{-m/2}P_{m+k}^m(s)$ for $k = 0, 1, 2, \ldots$, so q_k is a polynomial of degree k, and the set $\{q_k\}_{k=0}^\infty$ is an orthogonal basis for $L_w^2(-1,1)$ with weight $(1-s^2)^m$. Now suppose $f \in L^2(-1,1)$ is orthogonal to $\{P_{m+k}^m\}_{k=0}^\infty$ in $L^2(-1,1)$; then $g = (1-s^2)^{-m/2}f \in L_w^2(-1,1)$ is orthogonal to $\{q_k\}_{k=0}^\infty$ in $L_w^2(-1,1)$; so $g = 0$ in $L_w^2(-1,1)$, and hence $f = 0$ in $L^2(-1,1)$. ok

2. set $y_m(s) = P_n^m(s) = (1-s^2)^{m/2}\dfrac{d^m}{ds^m}P_n(s)$, $y_0(s) = P_n(s)$

we will derive a relation between y_m and y_{m-1}

case a : $m = 1$

$y_1 = (1-s^2)^{1/2}y_0'$

$$||y_1||^2 = \int_{-1}^{1}(1-s^2)(y_0')^2 ds = \cancelto{0}{(1-s^2)y_0'y_0\Big|_{-1}^{1}} - \int_{-1}^{1}\left[(1-s^2)y_0'\right]'y_0 ds$$

$$= \int_{-1}^{1} n(n+1)y_0^2 ds = n(n+1)||y_0||^2 \quad \text{ok}$$

case b : $m = 2, 3, \ldots$

$$y_{m-1}' = \frac{d}{ds}\left[(1-s^2)^{(m-1)/2}\frac{d^{m-1}}{ds^{m-1}}P_n\right]$$

$$= (1-s^2)^{(m-1)/2}\frac{d^m}{ds^m}P_n + \frac{m-1}{2}(1-s^2)^{(m-3)/2}(-2s)\frac{d^{m-1}}{ds^{m-1}}P_n$$

$$= (1-s^2)^{-1/2}y_m - (m-1)s(1-s^2)^{-1}y_{m-1}$$

$$y_m = \frac{(m-1)s}{(1-s^2)^{1/2}}\, y_{m-1} + (1-s^2)^{1/2}y'_{m-1}$$

$$||y_m||^2 = \int_{-1}^{1}\left[\frac{(m-1)^2s^2}{1-s^2}y_{m-1}^2 + (1-s^2)(y'_{m-1})^2 + 2(m-1)sy_{m-1}y'_{m-1}\right]ds$$

integrate 2nd and 3rd terms by parts

$$\int_{-1}^{1}(1-s^2)(y'_{m-1})^2ds = \cancelto{0}{(1-s^2)y'_{m-1}y_{m-1}\Big|_{-1}^{1}} - \int_{-1}^{1}\left[(1-s^2)y'_{m-1}\right]'y_{m-1}ds$$

$$= \int_{-1}^{1}\left[n(n+1) - \frac{(m-1)^2}{1-s^2}\right]y_{m-1}^2ds$$

$$\int_{-1}^{1}sy_{m-1}y'_{m-1}ds = \cancelto{0}{sy_{m-1}^2\Big|_{-1}^{1}} - \int_{-1}^{1}[sy_{m-1}]'y_{m-1}ds$$

$$= -\int_{-1}^{1}\left[sy'_{m-1}y_{m-1} + y_{m-1}^2\right]ds \;\Rightarrow\; 2\int_{-1}^{1}sy_{m-1}y'_{m-1}ds = -\int_{-1}^{1}y_{m-1}^2ds$$

$$||y_m||^2 = \int_{-1}^{1}\left[\frac{(m-1)^2s^2}{1-s^2} + n(n+1) - \frac{(m-1)^2}{1-s^2} - (m-1)\right]y_{m-1}^2ds$$

$$= (n(n+1)-(m-1)^2-(m-1))||y_{m-1}||^2 = (n(n+1)-(m-1)m)||y_{m-1}||^2$$

$$||y_m||^2 = (n+m)(n-m+1)||y_{m-1}||^2$$

replace m by $m-1,\dots,1$

$$||y_m||^2 = (n+m)(n+m-1)\cdots(n+1)\cdot(n-m+1)(n-m+2)\cdots n||y_0||^2$$

$$= (n+m)(n+m-1)\cdots(n+1)\cdot n(n-1)\cdots(n-m+1)||y_0||^2$$

$$= \frac{(n+m)!}{(n-m)!}||y_0||^2 \quad \underline{\text{ok}}$$

<u>note</u>

1. $s=\cos\theta \Rightarrow \displaystyle\int_{-1}^{1}f(s)\overline{g(s)}ds = \int_0^{\pi}f(\cos\theta)\overline{g(\cos\theta)}\sin\theta d\theta$

2. The unit sphere is a product space, $S=[0,\pi]\times[-\pi,\pi]$.

define $Y_n^m(\theta,\phi) = \sqrt{\dfrac{2n+1}{4\pi}\dfrac{(n-|m|)!}{(n+|m|)!}}\,P_n^{|m|}(\cos\theta)e^{im\phi}$: <u>spherical harmonics</u>

Then $\{Y_n^m(\theta,\phi): n=0,1,2,\dots, m=-n:n\}$ is an orthonormal basis for $L_2(S)$ wrt the measure $dS(\theta,\phi)=\sin\theta d\theta d\phi$.

<u>general solution of $\nabla^2\Phi = 0$</u> (allowing a singularity at $r = 0$)

$$\Phi(r,\theta,\phi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\left(a_{mn}r^n + \frac{b_{mn}}{r^{n+1}}\right)Y_n^m(\theta,\phi)$$

<u>ex</u>: interior Dirichlet problem for the unit ball in $\mathbb{R}^3$

$\nabla^2\Phi = 0$ for $r < 1$, $\Phi = f$ for $r = 1$

$$f(\theta,\phi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} c_{mn}Y_n^m(\theta,\phi) \ , \ c_{mn} = \langle f, Y_n^m\rangle = \int_{-\pi}^{\pi}\int_0^{\pi} f(\theta,\phi)Y_n^{-m}(\theta,\phi)\sin\theta d\theta d\phi$$

$$\Phi(r,\theta,\phi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} c_{mn}r^nY_n^m(\theta,\phi) \quad \underline{\text{ok}}$$

<u>alternative form</u>

$$\Phi(x) = \frac{1}{4\pi}\int_S \frac{1-|x|^2}{|x-y|^3}f(y)dS(y) \, , \, |x| < 1 \, , \, |y| = 1$$

<u>pf</u> : Assume that $x = (r, 0, *)$ lies on the positive z-axis.

$$\Phi(r,0,*) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} c_{mn}r^nY_n^m(0,*) \ , \ \text{recall : } P_n(1) = 1 \, , \, P_n^m(1) = 0, m \neq 1$$

$$= \sum_{n=0}^{\infty}\sum_{m=-n}^{n} c_{mn}r^n\sqrt{\frac{2n+1}{4\pi}\frac{(n-|m|)!}{(n+|m|)!}}P_n^{|m|}(1)e^{im*} = \sum_{n=0}^{\infty} c_{0n}r^n\sqrt{\frac{2n+1}{4\pi}}$$

$$c_{0n} = \langle f, Y_n^0\rangle = \int_{-\pi}^{\pi}\int_0^{\pi} f(\theta,\phi)\sqrt{\frac{2n+1}{4\pi}}P_n(\cos\theta)\sin\theta d\theta d\phi$$

$$\Phi(r,0,*) = \frac{1}{4\pi}\int_{-\pi}^{\pi}\int_0^{\pi}\sum_{n=0}^{\infty}(2n+1)P_n(\cos\theta)r^nf(\theta,\phi)\sin\theta d\theta d\phi$$

$$\sum_{n=0}^{\infty}(2n+1)P_n(\cos\theta)r^n = \left(2r\frac{d}{dr}+1\right)\sum_{n=0}^{\infty}P_n(\cos\theta)r^n$$

$$= \left(2r\frac{d}{dr}+1\right)\frac{1}{(1-2r\cos\theta+r^2)^{1/2}}$$

$$= 2r\cdot\frac{-\frac{1}{2}(-2\cos\theta+2r)}{(1-2r\cos\theta+r^2)^{3/2}} + \frac{1}{(1-2r\cos\theta+r^2)^{1/2}}$$

$$= \frac{2r\cos\theta - 2r^2 + 1 - 2r\cos\theta + r^2}{(1-2r\cos\theta+r^2)^{3/2}} = \frac{1-r^2}{(1-2r\cos\theta+r^2)^{3/2}} \quad \underline{\text{ok}}$$