





$N$  charges:  $\{q_i, r_i\}_{i=1}^N$

$$\text{Potential: } \phi_i = \sum_{j \neq i} \frac{q_j}{\|r_i - r_j\|} \text{ for } i \in \{1, 2, \dots, N\}$$

Note that we have  $\phi = Aq$ ,  $\phi$  is the set of potentials,  $q$  is the set of charges and  $A_{ij} = \frac{1}{\|r_i - r_j\|}$  for  $i \neq j$

Matrix-vector product: Given  $q$ , compute  $\phi$ . Cost is  $\mathcal{O}(N^2)$

Solve linear system: Given  $\phi$ , compute  $q$ . Cost is  $\mathcal{O}(N^3)$

Can we reduce the above computational complexity to say  $\mathcal{O}(N)$ ?

Let's look at a slightly easier problem

$N$  charges:  $\{q_i, r_i\}_{i=1}^N$

Potential:  $\phi_i = \sum_{j=1}^N \sin(k(r_i - r_j)) q_j$  for  $i \in \{1, 2, \dots, N\}$

Matrix-vector product:  $Aq$ , where  $A_{ij} = \sin(k(r_i - r_j))$  for  $i \neq j$

Computational cost is  $\mathcal{O}(N^2)$

Can we reduce the computational complexity?

Note that  $\sin(k(r_i - r_j)) = \sin(kr_i) \cos(kr_j) - \cos(kr_i) \sin(kr_j)$

$$\phi_i = \sum_{j=1}^N \sin(kr_i) \cos(kr_j) q_j - \sum_{j=1}^N \cos(kr_i) \sin(kr_j) q_j$$

for  $i \in \{1, 2, \dots, N\}$

$$\phi_i = \left( \sum_{j=1}^N \cos(kr_j) q_j \right) \sin(kr_i) - \left( \sum_{j=1}^N \sin(kr_j) q_j \right) \cos(kr_i)$$

for  $i \in \{1, 2, \dots, N\}$

$$\text{Compute } a = \sum_{j=1}^N \cos(kr_j) q_j; \text{ Cost is } \mathcal{O}(N)$$

$$\text{Compute } b = \sum_{j=1}^N \sin(kr_j) q_j; \text{ Cost is } \mathcal{O}(N)$$

$$\phi_i = a \sin(kr_i) - b \cos(kr_i) \text{ for } i \in \{1, 2, \dots, N\}; \text{ Cost is } \mathcal{O}(N)$$

Total cost is  $\mathcal{O}(N)$

Wait... What happened?

How did we go from  $\mathcal{O}(N^2)$  to  $\mathcal{O}(N)$ ?

In matrix form, we rewrote the matrix  $A$  as

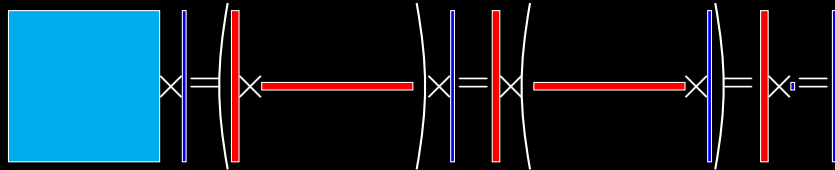
$$\begin{aligned} A &= u_1 v_1^T - v_1 u_1^T \\ A &= \begin{bmatrix} u_1 & -v_1 \end{bmatrix}_{N \times 2} \begin{bmatrix} v_1^T \\ u_1^T \end{bmatrix}_{2 \times N} \\ u_1 &= \begin{bmatrix} \sin(kr_1) \\ \sin(kr_2) \\ \vdots \\ \sin(kr_N) \end{bmatrix} \\ v_1 &= \begin{bmatrix} \cos(kr_1) \\ \cos(kr_2) \\ \vdots \\ \cos(kr_N) \end{bmatrix} \end{aligned}$$

Hence,

$$Aq = u_1 (v_1^T q) - v_1 (u_1^T q)$$

$$\square = \text{—} \times \text{—}$$

The diagram illustrates a mathematical relationship using geometric shapes. On the left is a solid blue square. To its right is an equals sign. Further right is a vertical red line. To the right of the vertical line is a multiplication symbol (×). To the right of the multiplication symbol is a horizontal red line. The vertical and horizontal red lines are of equal length and intersect at their midpoints, forming a cross shape.





Does the same idea work for  $1/\|r_i - r_j\|$  instead of  $\sin(k(r_i - r_j))$ ?

Unfortunately, not.

The “kernel” (Green’s function)  $1/r$  has a singularity at the origin.

Let’s look at other kernel functions; For instance,  $\log(r)$

But what about away from the singularity?

Away from the singularity the matrix looks like low-rank (?)

Can this be proved?

Yes! The matrix is indeed low-rank in finite precision!

Away from the singularity, the kernel is smooth and a separable expansion of the kernel can be obtained

$$K(x, y) = \sum_{i,j=1}^r c_{ij} \phi_i(x) \psi_j(y) + \mathcal{O}(\epsilon)$$

where  $r = \mathcal{O}(\log(1/\epsilon))$  uniformly across the domain of  $x$  and  $y$ .

An appropriate series (Taylor or Eigen-function) expansion of the kernel into separable expansions

We could also rely on polynomial interpolation to construct separable expansions

The rank  $r$  is *independent* of  $N$

Fast Multipole Method - souped version of the previous mentioned

- Relies on hierarchically sub-dividing your domain
- Identifying blocks to leverage low-rank matrix vector products

Total computational complexity is  $\mathcal{O}(rN)$

Fast Multipole Method in Computational Physics

Matrices arising out of N-body problems have an even nicer structure