Algorithms of Scientific Computing

Fast Fourier Transform (FFT)

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The Pair DFT/IDFT as Matrix-Vector Product

DFT and IDFT may be computed in the form

$$F_k = \frac{1}{N} \sum_{n=0}^{N-1} f_n \omega_N^{-nk} \qquad f_n = \sum_{k=0}^{N-1} F_k \omega_N^{nk}$$

or as matrix-vector products

$$\mathbf{F} = \frac{1}{N} \mathbf{W}^H \mathbf{f} \,, \qquad \mathbf{f} = \mathbf{W}\mathbf{F} \,,$$

with a **computational complexity of $\mathcal{O}(N^2)$**.

Note that

$$\mathrm{DFT}(f) = \frac{1}{N} \overline{\mathrm{IDFT}(\bar{f})} \,.$$

A fast computation is possible via the **divide-and-conquer** approach.

Fast Fourier Transform for $N = 2^p$

Basic idea: sum up even and odd indices separately in IDFT

$\rightarrow$ first for $n = 0, 1, \ldots, \frac{N}{2} - 1$:

$$x_n = \sum_{k=0}^{N-1} X_k \omega_N^{nk} = \sum_{k=0}^{\frac{N}{2}-1} \left(X_{2k}\omega_N^{2nk} + X_{2k+1}\omega_N^{(2k+1)n} \right) .$$

We set $Y_k := X_{2k}$ and $Z_k := X_{2k+1}$, use $\omega_N^{2nk} = \omega_{N/2}^{nk}$, and get a sum of two IDFT on $\frac{N}{2}$ coefficients:

$$x_n = \sum_{k=0}^{N-1} X_k \omega_N^{nk} = \underbrace{\sum_{k=0}^{\frac{N}{2}-1} Y_k \omega_{N/2}^{nk}}_{:= y_n} + \omega_N^n \underbrace{\sum_{k=0}^{\frac{N}{2}-1} Z_k \omega_{N/2}^{nk}}_{:= z_n} .$$

Note: this formula is actually valid for all $n = 0, \ldots, N-1$; however, the IDFTs of size $\frac{N}{2}$ will only deliver the y_n and z_n for $n = 0, \ldots, \frac{N}{2} - 1$ (but: y_n and z_n are periodic!)

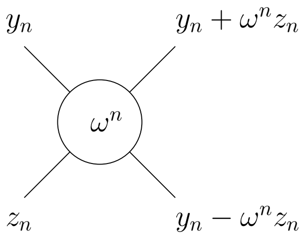
Fast Fourier Transform (FFT)

Do the same even vs. odd separation for indices $\frac{N}{2}, \ldots, N-1$:

$$x_{n+\frac{N}{2}} \quad = \quad y_{n+\frac{N}{2}} + \omega_N^{\left(n+\frac{N}{2}\right)} z_{n+\frac{N}{2}}$$

Since $\omega_N^{\left(n+\frac{N}{2}\right)} = -\omega_N^n$ and y_n and z_n have a period of $\frac{N}{2}$, we obtain the so-called **butterfly scheme**:

$$\begin{aligned} x_n &= y_n + \omega_N^n z_n \\ x_{n+\frac{N}{2}} &= y_n - \omega_N^n z_n \end{aligned}$$



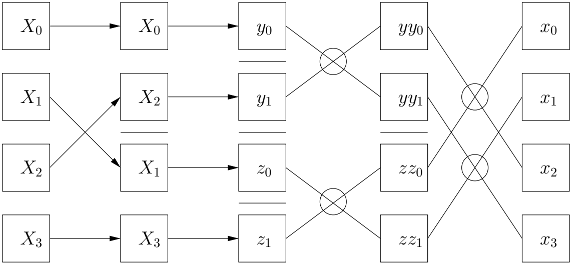
Fast Fourier Transform – Butterfly Scheme

$$(x_0, x_1, \ldots, \ldots, x_{N-1}) = \mathrm{IDFT}(X_0, X_1, \ldots, \ldots, X_{N-1})$$

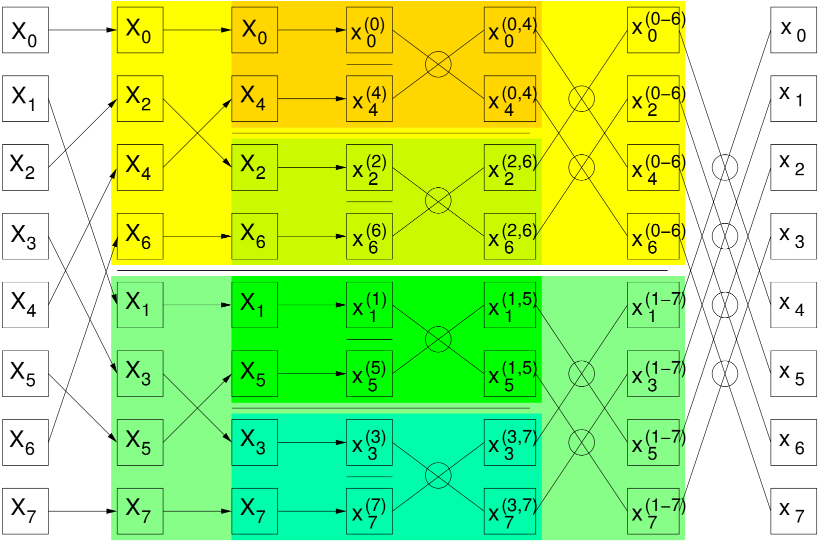
$$\Downarrow$$

$$(y_0, y_1, \ldots, y_{\frac{N}{2}-1}) = \mathrm{IDFT}(X_0, X_2, \ldots, X_{N-2})$$

$$(z_0, z_1, \ldots, z_{\frac{N}{2}-1}) = \mathrm{IDFT}(X_1, X_3, \ldots, X_{N-1})$$



Fast Fourier Transform – Butterfly Scheme (2)



Recursive Implementation of the FFT

$\texttt{rekFFT}(\mathbf{X}) \longrightarrow \mathbf{x}$

(1) Generate vectors **Y** and **Z**:

$$\text{for } n = 0, \ldots, \tfrac{N}{2} - 1: \qquad Y_n := X_{2n} \quad \text{und} \quad Z_n := X_{2n+1}$$

(2) compute 2 FFTs of half size:

$$\texttt{rekFFT}(\mathbf{Y}) \longrightarrow \mathbf{y} \qquad \text{and} \qquad \texttt{rekFFT}(\mathbf{Z}) \longrightarrow \mathbf{z}$$

(3) combine with "butterfly scheme":

$$\text{for } k = 0, \ldots, \tfrac{N}{2} - 1: \quad \left\{ \begin{array}{rcl} x_k & = & y_k + \omega_N^k z_k \\ x_{k+\frac{N}{2}} & = & y_k - \omega_N^k z_k \end{array} \right.$$

Observations on the Recursive FFT

- Computational effort $C(N)$ $(N = 2^p)$ given by recursion equation

$$C(N) = \begin{cases} \mathcal{O}(1) & \text{for} \quad N = 1 \\ \mathcal{O}(N) + 2C\left(\frac{N}{2}\right) & \text{for} \quad N > 1 \end{cases} \quad \Rightarrow \quad C(N) = \mathcal{O}(N \log N)$$

- Algorithm splits up in 2 phases:
  - resorting of input data
  - combination following the "butterfly scheme"

$\Rightarrow$ Anticipation of the resorting enables a simple, iterative algorithm without additional memory requirements.

Sorting Phase of the FFT – Bit Reversal

Observation:

- even indices are sorted into the upper half, odd indices into the lower half.
- distinction even/odd based on least significant bit
- distinction upper/lower based on most significant bit

$\Rightarrow$ An index in the sorted field has the **reversed** (i.e. mirrored) binary representation compared to the original index.

Sorting of a Vector ($N = 2^p$ Entries, Bit Reversal)

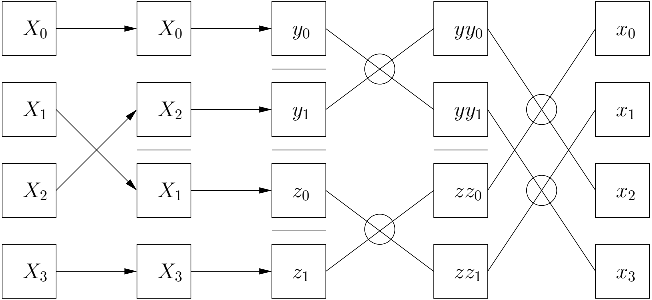
```
/** FFT sorting phase: reorder data in array X */
for(int n=0; n<N; n++) {
   // Compute p-bit bit reversal of n in j
   int j=0; int m=n;
   for(int i=0; i<p; i++) {
      j = 2*j + m%2; m = m/2;
   }
   // if j>n exchange X[j] and X[n]:
   if (j>n) { complex<double> h;
      h = X[j]; X[j] = X[n]; X[n] = h;
   }
}
```

Bit reversal needs $\mathcal{O}(p) = \mathcal{O}(\log N)$ operations

$\Rightarrow$ Sorting results also in a complexity of $\mathcal{O}(N \log N)$

$\Rightarrow$ Sorting may consume up to 10–30 % of the CPU time!

Iterative Implementation of the “Butterflies”



Iterative Implementation of the “Butterflies”

```
{Loop over the size of the IDFT}
for(int L=2; L<=N; L*=2)
   {Loop over the IDFT of one level}
   for(int k=0; k<N; k+=L)
      {perform all butterflies of one level}
      for(int j=0; j<L/2; j++) {
         {complex computation:}
         z ← ω_L^j * X[k+j+L/2]
         X[k+j+L/2] ← X[k+j] - z
         X[k+j] ← X[k+j] + z
      }
```

- k-loop und j-loop are “commutable”!
- How and when are the ω_L^j computed?

Iterative Implementation – Variant 1

```
/** FFT butterfly phase: variant 1 */
for(int L=2; L<=N; L*=2)
   for(int k=0; k<N; k+=L)
      for(int j=0; j<L/2; j++) {
         complex<double> z = omega(L,j) * X[k+j+L/2];
         X[k+j+L/2] = X[k+j] - z;
         X[k+j] = X[k+j] + z;
      }
```

Advantage: consecutive access to data in field `X`

⇒ suitable for vectorisation

⇒ good cache performance due to prefetching (stream access) and usage of cache lines

Disadvantage: multiple computations of ω_L^j

Iterative Implementation – Variant 2

```
/** FFT butterfly phase: variant 2 */
for(int L=2; L<=N; L*=2)
  for(int j=0; j<L/2; j++) {
    complex<double> w = omega(L,j);
    for(int k=0; k<N; k+=L) {
      complex<double> z = w * X[k+j+L/2];
      X[k+j+L/2] = X[k+j] - z;
      X[k+j] = X[k+j] + z;
  } }
```

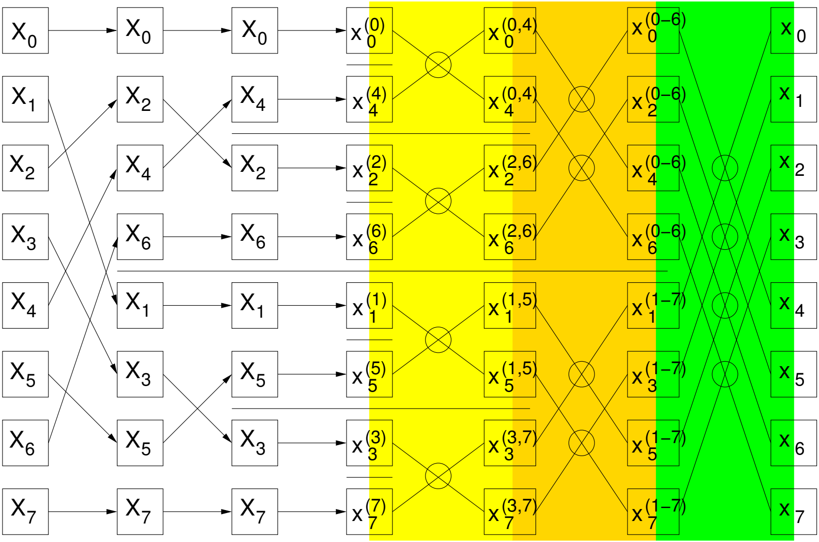
Advantage: each ω_L^j only computed once

Disadvantage: “stride-L”-access to the array `X`

$\Rightarrow$ worse cache performance (inefficient use of cache lines)

$\Rightarrow$ not suitable for vectorisation

L-Oriented Implementation – Illustration



Separate Computation of $\omega_{\mathtt{L}}^{\mathtt{j}}$

- necessary: $N-1$ factors

$$\omega_2^0, \omega_4^0, \omega_4^1, \ldots, \omega_L^0, \ldots, \omega_L^{L/2-1}, \ldots, \omega_N^0, \ldots, \omega_N^{N/2-1}$$

- are computed in advance, and stored in an array `w`, e.g.:

```
for(int L=2; L<=N; L*=2)
   for(int j=0; j<L/2; j++)
      w[L-j-1] ← ω_L^j;
```

- Variant 2: access on `w` in sequential order
- Variant 1: access on `w` local (but repeated)

Cache Efficiency – Variant 1 Revisited

```
/** FFT butterfly phase: variant 1 */
for(int L=2; L<=N; L*=2)
   for(int k=0; k<N; k+=L)
      for(int j=0; j<L/2; j++) {
         complex<double> z = w[L-j-1] * X[k+j+L/2];
         X[k+j+L/2] = X[k+j] - z;
         X[k+j] = X[k+j] + z;
      }
```

Observation:

- each L-loop traverses entire array X
- in the ideal case $(N \log N)/B$ cache line transfers (B the size of the cache line)

Compare with recursive scheme:

- if $L < M$ (M the cache size), entire FFT of size L could be computed in cache
- ideal case then only $L/(MB)$ cache line transfers

Butterfly Phase with Loop Blocking

```
/** FFT butterfly phase: loop blocking for k */
for(int L=2; L<=N; L*=2)
  for(int kb=0; kb<N; kb+=M)
    for(int k=kb; k<kb+M; k+=L)
      for(int j=0; j<L/2; j++) {
         complex<double> z = w[L-j-1] * X[k+j+L/2];
         X[k+j+L/2] = X[k+j] - z;
         X[k+j] = X[k+j] + z;
      }
```

Question: can we make the L-loop an inner loop?

- kb-loop and L-loop may be swapped, if $M > L$
- however, we assumed that $N > M$ (“data does not fit into cache”)
- we thus need to split the L-loop into a phase L=2..M (in cache) and a phase L=2∗M..N (out of cache)

Butterfly Phase with Loop Blocking (2)

```
/** perform all butterfly phases of size M */
for(int kb=0; kb<N; kb+=M)
  for(int L=2; L<=M; L*=2)
    for(int k=kb; k<kb+M; k+=L)
      for(int j=0; j<L/2; j++) {
         complex<double> z = w[L-j-1] * X[k+j+L/2];
         X[k+j+L/2] = X[k+j] - z;
         X[k+j] = X[k+j] + z;
      }
/** perform remaining butterfly levels of size L>M */
for(int L=2*M; L<=N; L*=2)
   for(int k=0; k<N; k+=L)
      for(int j=0; j<L/2; j++) {
         complex<double> z = w[L-j-1] * X[k+j+L/2];
         X[k+j+L/2] = X[k+j] - z;
         X[k+j] = X[k+j] + z;
      }
```

Loop Blocking and Recursion – Illustration