How to Write Fast Numerical Code

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Lecture: Discrete Fourier transform, fast Fourier transforms

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Linear Transforms

- **Overview: Transforms and algorithms**
- **Discrete Fourier transform**
- **Fast Fourier transforms**
- **After that:**
  - Optimized implementation and autotuning (FFTW)
  - Automatic program synthesis (Spiral)

Blackboard

- **Linear Transforms**
- **Discrete Fourier transform (DFT)**
- **Transform algorithms**
- **Fast Fourier transform, size 4**

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FFT References

- **Complexity:** *Bürgisser, Clausen, Shokrollahi,* ***Algebraic Complexity Theory****, Springer, 1997*
- **History:** *Heideman, Johnson, Burrus:* ***Gauss and the History of the Fast Fourier Transform****, Arch. Hist. Sc. 34(3) 1985*
- **FFTs:**
  - *Cooley and Tukey,* ***An algorithm for the machine calculation of complex Fourier series****," Math. of Computation, vol. 19, pp. 297–301, 1965*
  - *Nussbaumer,* ***Fast Fourier Transform and Convolution Algorithms****, 2nd ed., Springer, 1982*
  - *van Loan,* ***Computational Frameworks for the Fast Fourier Transform****, SIAM, 1992*
  - *Tolimieri, An, Lu,* ***Algorithms for Discrete Fourier Transforms and Convolution****, Springer, 2nd edition, 1997*
  - *Franchetti, Püschel, Voronenko, Chellappa and Moura,* ***Discrete Fourier Transform on Multicore****, IEEE Signal Processing Magazine, special issue on ``Signal Processing on Platforms with Multiple Cores'', Vol. 26, No. 6, pp. 90-102, 2009*

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Linear Transforms

- Very important class of functions: signal processing, scientific computing, …
- *Mathematically:* Change of basis = Multiplication by a fixed matrix T

$$\begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{n-1} \end{pmatrix} = y = Tx$$

$$x = \begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_{n-1} \end{pmatrix}$$

$$T = [t_{k,\ell}]_{0 \le k,\ell < n}$$

Output *Input*

- Equivalent definition: Summation form

$$y_k = \sum_{\ell=0}^{n-1} t_{k,\ell} x_\ell, \quad 0 \le k < n$$

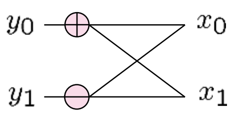
Smallest Relevant Example: DFT, Size 2

Transform (matrix): $T = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$

Computation: $y = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} x$ *or*

$$\begin{aligned} y_0 &= x_0 + x_1 \\ y_1 &= x_0 - x_1 \end{aligned}$$

As graph (direct acyclic graph or DAG):



called a butterfly

http://charlottesmartypants.blogspot.com/2011_02_01_archive.html

Transforms: Examples

- A few dozen transforms are relevant
- Some examples

$$\mathbf{DFT}_n = [e^{-2k\ell\pi i/n}]_{0\le k,\ell<n}$$

$$\mathbf{RDFT}_n = [r_{k\ell}]_{0\le k,\ell<n}, \quad r_{k\ell} = \begin{cases} \cos\frac{2\pi k\ell}{n}, & k \le \lfloor\frac{n}{2}\rfloor \\ -\sin\frac{2\pi k\ell}{n}, & k > \lfloor\frac{n}{2}\rfloor \end{cases}$$

universal tool

$$\mathbf{DHT} = \left[\cos(2k\ell\pi/n) + \sin(2k\ell\pi/n)\right]_{0\le k,\ell<n}$$

$$\mathbf{WHT}_n = \begin{bmatrix} \mathbf{WHT}_{n/2} & \mathbf{WHT}_{n/2} \\ \mathbf{WHT}_{n/2} & -\mathbf{WHT}_{n/2} \end{bmatrix}, \quad \mathbf{WHT}_2 = \mathbf{DFT}_2$$

$$\mathbf{IMDCT}_n = \left[\cos((2k+1)(2\ell+1+n)\pi/4n)\right]_{0\le k<2n, 0\le\ell<n}$$

MPEG

$$\mathbf{DCT\text{-}2}_n = \left[\cos(k(2\ell+1)\pi/2n)\right]_{0\le k,\ell<n}$$

JPEG

$$\mathbf{DCT\text{-}3}_n = \mathbf{DCT\text{-}2}_n^T \quad \text{(transpose)}$$

$$\mathbf{DCT\text{-}4}_n = \left[\cos((2k+1)(2\ell+1)\pi/4n)\right]_{0\le k,\ell<n}$$

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Linear Transforms: DFT

$$\begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{n-1} \end{pmatrix} = y = Tx$$

$$x = \begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_{n-1} \end{pmatrix}$$

$$T = [t_{k,\ell}]_{0\le k,\ell<n}$$

Output *Input*

Example: $T = \mathbf{DFT}_n = [e^{-2k\ell\pi i/n}]_{0\le k,\ell<n}$

$$= [\omega_n^{k\ell}]_{0\le k,\ell<n}, \quad \omega_n = e^{-2\pi i/n}$$

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Algorithms: Example FFT, n = 4

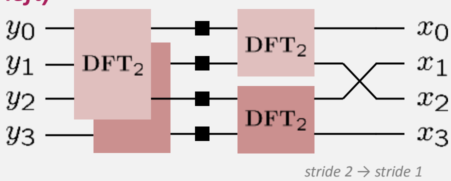
Fast Fourier transform (FFT)

$$\begin{bmatrix}1&1&1&1\\1&i&-1&-i\\1&-1&1&-1\\1&-i&-1&i\end{bmatrix}x=\begin{bmatrix}1&\cdot&1&\cdot\\\cdot&1&\cdot&1\\1&\cdot&-1&\cdot\\\cdot&1&\cdot&-1\end{bmatrix}\begin{bmatrix}1&\cdot&\cdot&\cdot\\\cdot&1&\cdot&\cdot\\\cdot&\cdot&1&\cdot\\\cdot&\cdot&\cdot&i\end{bmatrix}\begin{bmatrix}1&1&\cdot&\cdot\\1&-1&\cdot&\cdot\\\cdot&\cdot&1&1\\\cdot&\cdot&1&-1\end{bmatrix}\begin{bmatrix}1&\cdot&\cdot&\cdot\\\cdot&\cdot&1&\cdot\\\cdot&1&\cdot&\cdot\\\cdot&\cdot&\cdot&1\end{bmatrix}x$$

Representation using matrix algebra

$$\mathbf{DFT}_4=(\mathbf{DFT}_2\otimes \mathrm{I}_2)\,\mathrm{diag}(1,1,1,i)(\mathrm{I}_2\otimes\mathbf{DFT}_2)\,\mathrm{L}^4_2$$

Data flow graph (right to left)



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Cooley-Tukey FFT (Recursive, General-Radix)

- **Blackboard**
- **Kronecker products**
- **Stride permutations**

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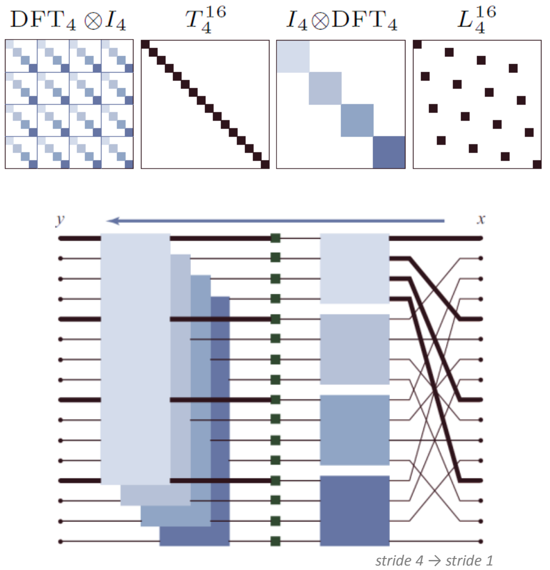
Example FFT, n = 16 *(Recursive, Radix 4)*

$\mathrm{DFT}_{16} =$



Recursive Cooley-Tukey FFT

radix

$$\mathbf{DFT}_{km} = (\mathbf{DFT}_k \otimes \mathrm{I}_m) T^{km}_m (\mathrm{I}_k \otimes \mathbf{DFT}_m) L^{km}_k$$ *decimation-in-time*

$$\mathbf{DFT}_{km} = L^{km}_m (\mathrm{I}_k \otimes \mathbf{DFT}_m) T^{km}_m (\mathbf{DFT}_k \otimes \mathrm{I}_m)$$ *decimation-in-frequency*

- **For powers of two n = 2^t sufficient together with base case**

$$\mathbf{DFT}_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

- **Cost:**
  - (complex adds, complex mults) = (n $\log_2$(n), n $\log_2$(n)/2)
    independent of recursion
  - (real adds, real mults) ≤ (2n $\log_2$(n), 3n $\log_2$(n)) = 5n $\log_2$(n) flops
    depends on recursion: best is at least radix-8

Recursive vs. Iterative FFT

- **Recursive, radix-k Cooley-Tukey FFT**

$$\mathbf{DFT}_{km} = (\mathbf{DFT}_k \otimes \mathrm{I}_m) T_m^{km} (\mathrm{I}_k \otimes \mathbf{DFT}_m) L_k^{km}$$

$$\mathbf{DFT}_{km} = L_m^{km} (\mathrm{I}_k \otimes \mathbf{DFT}_m) T_m^{km} (\mathbf{DFT}_k \otimes \mathrm{I}_m)$$

- **Iterative, radix 2, decimation-in-time/decimation-in-frequency**

$$\mathbf{DFT}_{2^t} = \left(\prod_{j=1}^{t} (\mathrm{I}_{2^{j-1}} \otimes \mathbf{DFT}_2 \otimes \mathrm{I}_{2^{t-j}}) \cdot (\mathrm{I}_{2^{j-1}} \otimes T_{2^{t-j}}^{2^{t-j+1}}) \right) \cdot R_{2^t}$$

$$\mathbf{DFT}_{2^t} = R_{2^t} \cdot \left(\prod_{j=1}^{t} (\mathrm{I}_{2^{t-j}} \otimes T_{2^{j-1}}^{2^j}) \cdot (\mathrm{I}_{2^{t-j}} \otimes \mathbf{DFT}_2 \otimes \mathrm{I}_{2^{j-1}}) \right)$$

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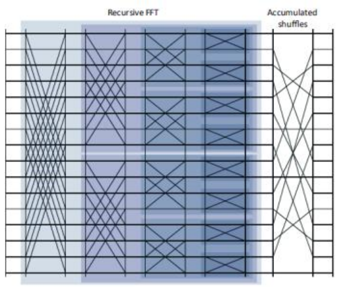
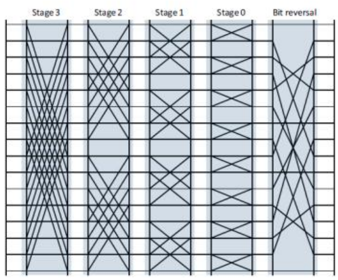
Radix 2, recursive



$$(\mathrm{DFT}_2 \otimes I_8) T_8^{16} \Big(I_2 \otimes \Big((\mathrm{DFT}_2 \otimes I_4) T_4^8 (I_2 \otimes ((\mathrm{DFT}_2 \otimes I_2) T_2^4 (I_2 \otimes \mathrm{DFT}_2) L_2^4)) L_2^8 \Big) \Big) L_2^{16}$$

Radix 2, iterative



$$\Big((I_1 \otimes \mathrm{DFT}_2 \otimes I_8) D_0^{16} \Big) \Big((I_2 \otimes \mathrm{DFT}_2 \otimes I_4) D_1^{16} \Big) \Big((I_4 \otimes \mathrm{DFT}_2 \otimes I_2) D_2^{16} \Big) \Big((I_8 \otimes \mathrm{DFT}_2 \otimes I_1) D_3^{16} \Big) R_2^{16}$$

Recursive vs. Iterative

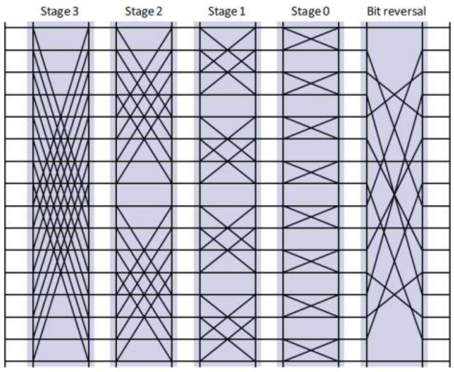
- **Iterative FFT computes in stages of butterflies =**
  $\log_2(n)$ passes through the data
- **Recursive FFT reduces passes through data =**
  better locality
- **Same computation graph but different topological sorting**

- **Rough analogy:**

MMM	DFT
Triple loop	Iterative FFT
Blocked	Recursive FFT

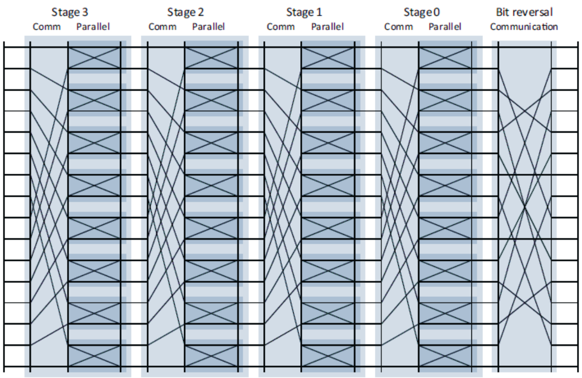
The FFT Is Very Malleable

Iterative FFT, Radix 2



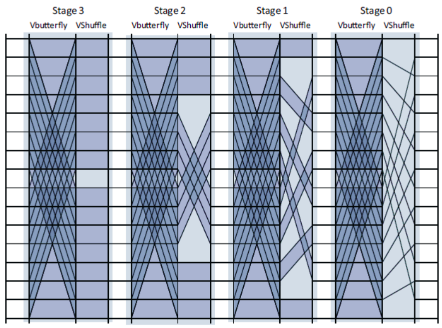
$$\left((I_1 \otimes \mathrm{DFT}_2 \otimes I_8) D_0^{16}\right)\left((I_2 \otimes \mathrm{DFT}_2 \otimes I_4) D_1^{16}\right)\left((I_4 \otimes \mathrm{DFT}_2 \otimes I_2) D_2^{16}\right)\left((I_8 \otimes \mathrm{DFT}_2 \otimes I_1) D_3^{16}\right) R_2^{16}$$

Pease FFT, Radix 2



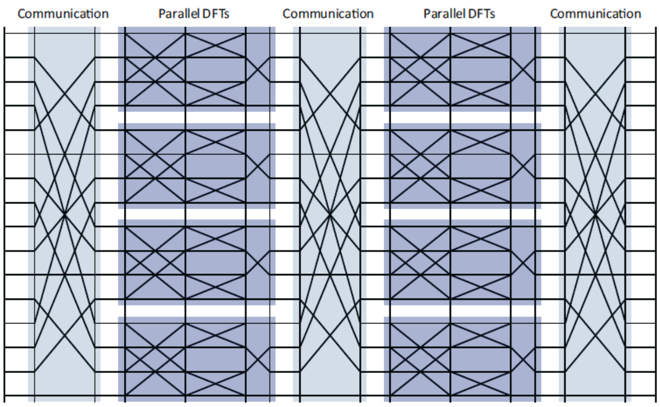
$$\left(L_2^{16}(I_8 \otimes \mathrm{DFT}_2) D_0^{16}\right)\left(L_2^{16}(I_8 \otimes \mathrm{DFT}_2) D_1^{16}\right)\left(L_2^{16}(I_8 \otimes \mathrm{DFT}_2) D_2^{16}\right)\left(L_2^{16}(I_8 \otimes \mathrm{DFT}_2) D_3^{16}\right) R_2^{16}$$

Stockham FFT, Radix 2



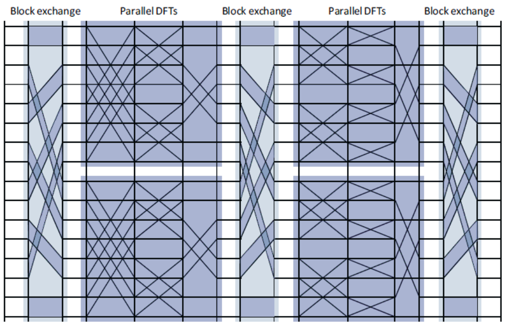
$$\Big((\mathrm{DFT}_2 \otimes I_8) D_0^{16} (L_2^2 \otimes I_8)\Big)\Big((\mathrm{DFT}_2 \otimes I_8) D_1^{16} (L_2^4 \otimes I_4)\Big)\Big((\mathrm{DFT}_2 \otimes I_8) D_2^{16} (L_2^8 \otimes I_2)\Big)\Big((\mathrm{DFT}_2 \otimes I_8) D_3^{16} (L_2^{16} \otimes I_1)\Big)$$

Six-Step FFT



$$L_4^{16}\Big(I_4 \otimes \big((\mathrm{DFT}_2 \otimes I_2) T_2^4 (I_2 \otimes \mathrm{DFT}_2) L_2^4\big)\Big) L_4^{16} T_4^{16} \Big(I_4 \otimes \big((\mathrm{DFT}_2 \otimes I_2) T_2^4 (I_2 \otimes \mathrm{DFT}_2) L_2^4\big)\Big) L_4^{16}$$

Multi-Core FFT



$$(L_4^8 \otimes I_2)\left(I_2 \otimes \left((\mathrm{DFT}_2 \otimes I_2) T_2^4 (I_2 \otimes \mathrm{DFT}_2) L_2^4\right) \otimes I_2\right)(L_2^8 \otimes I_2)\, T_4^{16}\left(I_2 \otimes \left(I_2 \otimes (\mathrm{DFT}_2 \otimes I_2) T_2^4 (I_2 \otimes \mathrm{DFT}_2)\right) R_2^8\right)(L_2^8 \otimes I_2)$$

Transform Algorithms

$$\mathbf{DFT}_n \to P_{k/2,2m}^\top \left(\mathbf{DFT}_{2m} \oplus \left(I_{k/2-1} \otimes_i C_{2m}\, \mathbf{rDFT}_{2m}(i/k)\right)\right)\left(\mathbf{RDFT}'_k \otimes I_m\right), \quad k \text{ even},$$

$$\begin{vmatrix}\mathbf{RDFT}_n\\ \mathbf{RDFT}'_n\\ \mathbf{DHT}_n\\ \mathbf{DHT}'_n\end{vmatrix} \to (P_{k/2,m}^\top \otimes I_2)\left(\begin{vmatrix}\mathbf{RDFT}_{2m}\\ \mathbf{RDFT}'_{2m}\\ \mathbf{DHT}_{2m}\\ \mathbf{DHT}'_{2m}\end{vmatrix} \oplus \left(I_{k/2-1} \otimes_i D_{2m} \begin{vmatrix}\mathbf{rDFT}_{2m}(i/k)\\ \mathbf{rDFT}_{2m}(i/k)\\ \mathbf{rDHT}_{2m}(i/k)\\ \mathbf{rDHT}_{2m}(i/k)\end{vmatrix}\right)\right)\left(\begin{vmatrix}\mathbf{RDFT}'_k\\ \mathbf{RDFT}'_k\\ \mathbf{DHT}'_k\\ \mathbf{DHT}'_k\end{vmatrix} \otimes I_m\right), \quad k \text{ even},$$

$$\begin{vmatrix}\mathbf{rDFT}_{2n}(u)\\ \mathbf{rDHT}_{2n}(u)\end{vmatrix} \to L_m^{2n}\left(I_k \otimes_i \begin{vmatrix}\mathbf{rDFT}_{2m}((i+u)/k)\\ \mathbf{rDHT}_{2m}((i+u)/k)\end{vmatrix}\right)\left(\begin{vmatrix}\mathbf{rDFT}_{2k}(u)\\ \mathbf{rDHT}_{2k}(u)\end{vmatrix} \otimes I_m\right),$$

$$\mathbf{RDFT\text{-}3}_n \to (Q_{k/2,m}^\top \otimes I_2)\,(I_k \otimes_i \mathbf{rDFT}_{2m})(i+1/2)/k))\,(\mathbf{RDFT\text{-}3}_k \otimes I_m), \quad k \text{ even},$$

$$\mathbf{DCT\text{-}2}_n \to P_{k/2,2m}^\top\left(\mathbf{DCT\text{-}2}_{2m} K_2^{2m} \oplus \left(I_{k/2-1} \otimes N_{2m}\, \mathbf{RDFT\text{-}3}_{2m}^\top\right)\right) B_n (L_{k/2}^{n/2} \otimes I_2)(I_m \otimes \mathbf{RDFT}'_k) Q_{m/2,k},$$

$$\mathbf{DCT\text{-}3}_n \to \mathbf{DCT\text{-}2}_n^\top,$$

$$\mathbf{DCT\text{-}4}_n \to Q_{k/2,2m}^\top\left(I_{k/2} \otimes N_{2m}\, \mathbf{RDFT\text{-}3}_{2m}^\top\right) B'_n (L_{k/2}^{n/2} \otimes I_2)(I_m \otimes \mathbf{RDFT\text{-}3}_k) Q_{m/2,k}.$$

$$\mathbf{DFT}_n \to (\mathbf{DFT}_k \otimes \mathrm{I}_m)\, \mathsf{T}_m^n (\mathrm{I}_k \otimes \mathbf{DFT}_m)\, \mathsf{L}_k^n, \quad n = km$$ — *Cooley-Tukey FFT*

$$\mathbf{DFT}_n \to P_n(\mathbf{DFT}_k \otimes \mathbf{DFT}_m) Q_n, \quad n = km,\ \gcd(k,m) = 1$$ — *Prime-factor FFT*

$$\mathbf{DFT}_p \to R_p^T(\mathrm{I}_1 \oplus \mathbf{DFT}_{p-1}) D_p (\mathrm{I}_1 \oplus \mathbf{DFT}_{p-1}) R_p, \quad p \text{ prime}$$ — *Rader FFT*

$$\mathbf{DCT\text{-}3}_n \to (\mathrm{I}_m \oplus \mathsf{J}_m)\, \mathsf{L}_m^n (\mathbf{DCT\text{-}3}_m(1/4) \oplus \mathbf{DCT\text{-}3}_m(3/4)) \cdot (\mathsf{F}_2 \otimes \mathrm{I}_m) \begin{bmatrix}\mathrm{I}_m & 0 \oplus -\mathsf{J}_{m-1}\\ & \frac{1}{\sqrt{2}}(\mathrm{I}_1 \oplus 2\,\mathrm{I}_m)\end{bmatrix}, \quad n = 2m$$

$$\mathbf{DCT\text{-}4}_n \to S_n \mathbf{DCT\text{-}2}_n\, \mathrm{diag}_{0 \le k < n}(1/(2\cos((2k+1)\pi/4n)))$$

$$\mathbf{IMDCT}_{2m} \to (\mathsf{J}_m \oplus \mathrm{I}_m \oplus \mathrm{I}_m \oplus \mathsf{J}_m)\left(\left(\begin{bmatrix}1\\-1\end{bmatrix} \otimes \mathrm{I}_m\right) \oplus \left(\begin{bmatrix}-1\\-1\end{bmatrix} \otimes \mathrm{I}_m\right)\right) \mathsf{J}_{2m}\, \mathbf{DCT\text{-}4}_{2m}$$

$$\mathbf{WHT}_{2^k} \to \prod_{i=1}^{t} (\mathrm{I}_{2^{k_1+\cdots+k_{i-1}}} \otimes \mathbf{WHT}_{2^{k_i}} \otimes \mathrm{I}_{2^{k_{i+1}+\cdots+k_t}}), \quad k = k_1 + \cdots + k_t$$

$$\mathbf{DFT}_2 \to \mathsf{F}_2$$

$$\mathbf{DCT\text{-}2}_2 \to \mathrm{diag}(1, 1/\sqrt{2})\, \mathsf{F}_2$$

$$\mathbf{DCT\text{-}4}_2 \to \mathsf{J}_2 \mathsf{R}_{13\pi/8}$$

Complexity of the DFT

- **Measure: L_c, $2 \le c$**
  - Complex adds count 1
  - Complex mult by a constant a with $|a| < c$ counts 1
  - L_2 is strictest, L_∞ the loosest (and most natural)
- **Upper bounds:**
  - $n = 2^k$: $L_2(DFT_n) \le 3/2 \, n \log_2(n)$ *(using Cooley-Tukey FFT)*
  - General n: $L_2(DFT_n) \le 8 \, n \log_2(n)$ *(needs Bluestein FFT)*
- **Lower bound:**
  - Theorem by Morgenstern: If $c < \infty$, then $L_c(DFT_n) \ge ½ \, n \log_c(n)$
  - Implies: in the measure L_c, the DFT is $\Theta(n \log(n))$

History of FFTs

- **The advent of digital signal processing is often attributed to the FFT** *(Cooley-Tukey 1965)*
- **History:**
  - Around 1805: FFT discovered by Gauss [1] (Fourier publishes the concept of Fourier analysis in 1807!)
  - 1965: Rediscovered by Cooley-Tukey

[1]: Heideman, Johnson, Burrus: "Gauss and the History of the Fast Fourier Transform" Arch. Hist. Sc. 34(3) 1985

Carl-Friedrich Gauss

1777 - 1855

- **Contender for the greatest mathematician of all times**
- **Some contributions:** Modular arithmetic, least square analysis, normal distribution, fundamental theorem of algebra, Gauss elimination, Gauss quadrature, Gauss-Seidel, non-Euclidean geometry, …