

Bachelor Project

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1 Motivation

2 Dense Simulation

We want to simulate applying the QFT to some state, for this we need a way to represent the QFT and the state. In this section we will work towards representing the QFT circuit as a matrix and the state as a vector.

2.1 Representing a one qubit state

In classical computation a bit can either be 1 or 0, in quantum systems however a qubit has a certain probability of collapsing to either one or zero at a given time. To simulate this we use a vector to represent a qubit or a system of qubits, we denote this using Dirac notation. In Dirac notation we have a bra $\langle|$ and a ket $| \rangle$, generally a bra denotes a row vector and a ket denotes a column vector. To extract the probabilities of a qubit or system of qubits collapsing to one state or the other we take the norm squared of the entries in the vector, the sum of these must be 1 to be a valid state.

$$|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Figure 1: A qubit with a probability of 1 of collapsing to one

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Figure 2: A qubit with a probability of 1 of collapsing to zero

$$\begin{aligned} |+\rangle &= \sqrt{0.5}(|0\rangle + |1\rangle) = \begin{bmatrix} \sqrt{0.5} \\ \sqrt{0.5} \end{bmatrix} \\ |-\rangle &= \sqrt{0.5}(|0\rangle - |1\rangle) = \begin{bmatrix} \sqrt{0.5} \\ -\sqrt{0.5} \end{bmatrix} \end{aligned}$$

Figure 3: Qubits with a probability of 0.5 of collapsing to zero and one

In general a qubit $\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \alpha |0\rangle + \beta |1\rangle$ has a probability of $|\alpha|^2$ of collapsing to zero and $|\beta|^2$ of collapsing to one. Since we use a vector of complex numbers $|x|^2 = xx^*$ denotes the norm squared, where if $x = a + bi$ then x^* is the complex

conjugate of x , $x^* = a - bi$. For readability sake we will not write $+bi$ after a number if $b = 0$, you can assume all numbers in vectors and matrices are complex.

If we look at these vectors in a coordinate system, where the z axis is the imaginary axis, they all lie on a unit circle.

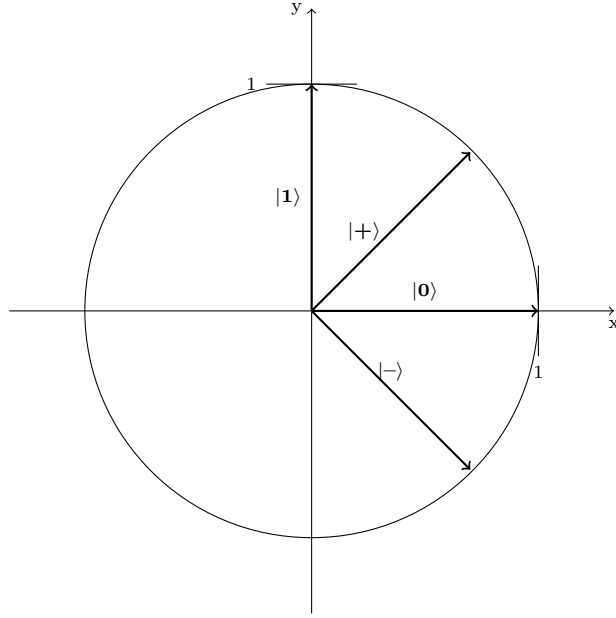


Figure 4: 'Bloch circle' with vectors $|1\rangle$, $|+\rangle$, $|0\rangle$ and $|-\rangle$ plotted

In reality we often use complex numbers with a non-zero imaginary part in the vectors, which results in the qubit states instead lying on the unit sphere, this is known as the Bloch sphere. The z axis is called the phase and generally has no impact on the probabilities of collapsing to a certain state, however it can be used to hold extra information before the qubit is collapsed, this can be useful in computations.

2.2 Multiple qubit states

$|1+-\rangle$ denotes a system collapsing to either $|100\rangle$, $|101\rangle$, $|110\rangle$ or $|111\rangle$ with probability 0.25. If we want to compute the state vector for the whole system we take the Kronecker product, sometimes called the tensor product, of the vectors representing the individual qubits in the system. The Kronecker product of two matrix like objects consists of duplicating the second object for every entry in the first object and then scaling every value in the duplicate by the entry in the first object.

$$\begin{aligned}
& \begin{bmatrix} a_{00} & a_{01} & a_{02} \\ a_{10} & a_{11} & a_{12} \end{bmatrix} \otimes \begin{bmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \\ b_{20} & b_{21} \end{bmatrix} = \\
& \begin{bmatrix} a_{00} \begin{bmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \\ b_{20} & b_{21} \end{bmatrix} & a_{01} \begin{bmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \\ b_{20} & b_{21} \end{bmatrix} & a_{02} \begin{bmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \\ b_{20} & b_{21} \end{bmatrix} \\ a_{10} \begin{bmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \\ b_{20} & b_{21} \end{bmatrix} & a_{11} \begin{bmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \\ b_{20} & b_{21} \end{bmatrix} & a_{12} \begin{bmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \\ b_{20} & b_{21} \end{bmatrix} \end{bmatrix} = \\
& \begin{bmatrix} a_{00}b_{00} & a_{00}b_{01} & a_{01}b_{00} & a_{01}b_{01} & a_{02}b_{00} & a_{02}b_{01} \\ a_{00}b_{10} & a_{00}b_{11} & a_{01}b_{10} & a_{01}b_{11} & a_{02}b_{10} & a_{02}b_{11} \\ a_{00}b_{20} & a_{00}b_{21} & a_{01}b_{20} & a_{01}b_{21} & a_{02}b_{20} & a_{02}b_{21} \\ a_{10}b_{00} & a_{10}b_{01} & a_{11}b_{00} & a_{11}b_{01} & a_{12}b_{00} & a_{12}b_{01} \\ a_{10}b_{10} & a_{10}b_{11} & a_{11}b_{10} & a_{11}b_{11} & a_{12}b_{10} & a_{12}b_{11} \\ a_{10}b_{20} & a_{10}b_{21} & a_{11}b_{20} & a_{11}b_{21} & a_{12}b_{20} & a_{12}b_{21} \end{bmatrix}
\end{aligned}$$

Figure 5: Example of taking the Kronecker product of two matrices

$$\begin{aligned}
& |\mathbf{1}+-\rangle = |\mathbf{1}\rangle \otimes |+\rangle \otimes |-\rangle = \\
& \begin{bmatrix} 0 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} \sqrt{0.5} \\ \sqrt{0.5} \end{bmatrix} \otimes \begin{bmatrix} \sqrt{0.5} \\ -\sqrt{0.5} \end{bmatrix} = \\
& \begin{bmatrix} 0 \begin{bmatrix} \sqrt{0.5} \begin{bmatrix} \sqrt{0.5} \\ -\sqrt{0.5} \end{bmatrix} \\ \sqrt{0.5} \begin{bmatrix} \sqrt{0.5} \\ -\sqrt{0.5} \end{bmatrix} \\ \sqrt{0.5} \begin{bmatrix} \sqrt{0.5} \\ -\sqrt{0.5} \end{bmatrix} \end{bmatrix} \\ 1 \begin{bmatrix} \sqrt{0.5} \begin{bmatrix} \sqrt{0.5} \\ -\sqrt{0.5} \end{bmatrix} \\ \sqrt{0.5} \begin{bmatrix} \sqrt{0.5} \\ -\sqrt{0.5} \end{bmatrix} \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 0 \begin{bmatrix} 0.5 \\ -0.5 \\ 0.5 \\ -0.5 \\ 0.5 \\ -0.5 \end{bmatrix} \\ 1 \begin{bmatrix} 0.5 \\ -0.5 \\ 0.5 \\ -0.5 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0.5 \\ -0.5 \\ 0.5 \\ -0.5 \end{bmatrix} = \\
& 0 \cdot |\mathbf{000}\rangle + 0 \cdot |\mathbf{001}\rangle + 0 \cdot |\mathbf{010}\rangle + 0 \cdot |\mathbf{011}\rangle + \\
& 0.5 \cdot |\mathbf{100}\rangle - 0.5 \cdot |\mathbf{101}\rangle + 0.5 \cdot |\mathbf{110}\rangle - 0.5 \cdot |\mathbf{111}\rangle
\end{aligned}$$

Figure 6: Using the Kronecker product to compute the state vector for the system in state $|\mathbf{1}+-\rangle$

If we square this vector, equivalent to taking the norm squared when the imaginary parts are zero, we get the probability corresponding to each state.

$$|1+-\rangle^2 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0.5 \\ -0.5 \\ 0.5 \\ -0.5 \end{bmatrix}^2 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \end{bmatrix}$$

Figure 7: Squaring entries the in state vector to obtain probabilities of the system being in each state, the i 'th entry in the vector is the probability of the system being in state $|i\rangle$ if you write i in binary using 3 digits

2.3 The Quantum Fourier Transform

Now we can represent a state as a vector. The QFT_n circuit applies the QFT to a n qubit state and looks like this:

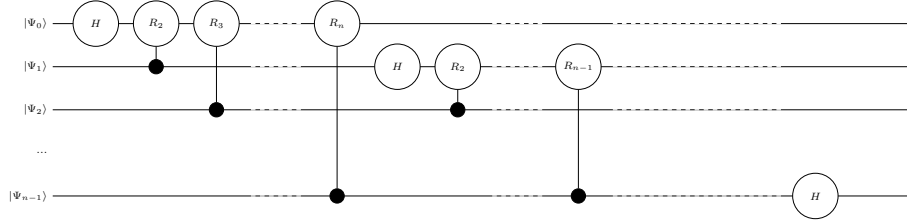


Figure 8: circuit diagram of QFT_n

In essence this circuit diagram can be read:

1. apply the **H** gate to the first qubit.
2. apply the **R₂** gate to the first qubit controlled by the second qubit.
3. apply the **R₃** gate to the first qubit controlled by the third qubit.
4. ...
5. apply the **R_n** gate to the first qubit controlled by the last qubit.
6. apply the **H** gate to the second qubit.
7. apply the **R₂** gate to the second qubit controlled by the third qubit.
8. ...

9. apply the \mathbf{R}_{n-1} gate to the second qubit controlled by the last qubit.
10. ...
11. apply the \mathbf{H} gate to the last qubit.

2.4 Manipulating qubits

In traditional electrical circuits we use logic gates such as NOT, AND, OR, NAND, etc. to manipulate bits. In quantum circuits some common gates are Pauli-X (X, bit flip or NOT), I (identity), H (Hadamard), CNOT (CX or controlled not), etc. In the same way we represent the state of a quantum system as a vector, we can represent a gate that operates on a state as a matrix.

$$\begin{aligned}\mathbf{I} &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \\ \mathbf{X} &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ \mathbf{H} &= \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} \\ \mathbf{R}_n &= \begin{bmatrix} 1 & 0 \\ 0 & e^{\frac{2\pi i}{2^n}} \end{bmatrix}\end{aligned}$$

Figure 9: Matrixes corresponding to \mathbf{I} , \mathbf{X} , \mathbf{H} and \mathbf{R}_n gates, which act on a single cubit

If we wish to apply a gate to a qubit in a system we do so by doing matrix multiplication between the state and the gate.

$$\begin{aligned}\mathbf{I}|\mathbf{0}\rangle &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \cdot 1 + 0 \cdot 0 \\ 0 \cdot 1 + 1 \cdot 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = |\mathbf{0}\rangle \\ \mathbf{I}|\mathbf{1}\rangle &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \cdot 0 + 0 \cdot 1 \\ 0 \cdot 0 + 1 \cdot 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |\mathbf{1}\rangle\end{aligned}$$

Figure 10: Applying \mathbf{I} gate to the states $|\mathbf{0}\rangle$ and $|\mathbf{1}\rangle$

$$\begin{aligned}
\mathbf{X} |0\rangle &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \cdot 1 + 1 \cdot 0 \\ 1 \cdot 1 + 0 \cdot 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |1\rangle \\
\mathbf{X} |1\rangle &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \cdot 0 + 1 \cdot 1 \\ 1 \cdot 0 + 0 \cdot 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = |0\rangle
\end{aligned}$$

Figure 11: Applying \mathbf{X} gate to the states $|0\rangle$ and $|1\rangle$

$$\begin{aligned}
\mathbf{H} |0\rangle &= \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \sqrt{0.5} \cdot 1 + \sqrt{0.5} \cdot 0 \\ \sqrt{0.5} \cdot 1 - \sqrt{0.5} \cdot 0 \end{bmatrix} = \begin{bmatrix} \sqrt{0.5} \\ \sqrt{0.5} \end{bmatrix} = |+\rangle \\
\mathbf{H} |1\rangle &= \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \sqrt{0.5} \cdot 0 + \sqrt{0.5} \cdot 1 \\ \sqrt{0.5} \cdot 0 - \sqrt{0.5} \cdot 1 \end{bmatrix} = \begin{bmatrix} \sqrt{0.5} \\ -\sqrt{0.5} \end{bmatrix} = |-\rangle
\end{aligned}$$

Figure 12: Applying \mathbf{H} gate to the states $|0\rangle$ and $|1\rangle$

$$\begin{aligned}
\mathbf{R}_2 |0\rangle &= \begin{bmatrix} 1 & 0 \\ 0 & e^{\frac{2\pi i}{2^2}} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \cdot 1 + 0 \cdot 0 \\ 0 \cdot 1 + e^{\frac{2\pi i}{2^2}} \cdot 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = |0\rangle \\
\mathbf{R}_2 |1\rangle &= \begin{bmatrix} 1 & 0 \\ 0 & e^{\frac{2\pi i}{2^2}} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \cdot 0 + 0 \cdot 1 \\ 0 \cdot 0 + e^{\frac{2\pi i}{2^2}} \cdot 1 \end{bmatrix} = \begin{bmatrix} 0 \\ e^{\frac{2\pi i}{2^2}} \end{bmatrix} = \begin{bmatrix} 0 \\ i \end{bmatrix}
\end{aligned}$$

Figure 13: Applying \mathbf{R}_2 gate to the states $|0\rangle$ and $|1\rangle$

$$\begin{aligned}
\mathbf{CX}|\mathbf{00}\rangle &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = |\mathbf{00}\rangle \\
\mathbf{CX}|\mathbf{01}\rangle &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \cdot 0 + 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 0 + 1 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 0 + 0 \cdot 1 + 0 \cdot 0 + 1 \cdot 0 \\ 0 \cdot 0 + 0 \cdot 1 + 1 \cdot 0 + 0 \cdot 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = |\mathbf{01}\rangle \\
\mathbf{CX}|\mathbf{11}\rangle &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 1 + 0 \cdot 0 \\ 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 1 + 0 \cdot 0 \\ 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 1 + 1 \cdot 0 \\ 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 1 + 0 \cdot 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = |\mathbf{11}\rangle \\
\mathbf{CX}|\mathbf{11}\rangle &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 1 \\ 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 1 \\ 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 1 \\ 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = |\mathbf{10}\rangle
\end{aligned}$$

Figure 14: Applying **CX** gate to the states $|\mathbf{00}\rangle$, $|\mathbf{01}\rangle$, $|\mathbf{10}\rangle$ and $|\mathbf{11}\rangle$

Here we see that applying **I** does not change the state. Applying **X** takes the state to the same state but reversed. Applying **H** takes the state into a superposition of $|1\rangle$ and $|0\rangle$. Applying **R_n** changes the phase of the cubit but not the chance of it collapsing to something. A key property of quantum gates is that they are reversible, and in fact their own inverses.

$$\begin{aligned}\mathbf{I}(\mathbf{I}|0\rangle) &= \mathbf{I}|0\rangle = |0\rangle \\ \mathbf{I}(\mathbf{I}|1\rangle) &= \mathbf{I}|1\rangle = |1\rangle\end{aligned}$$

Figure 15: Applying **I** gate to the states $|0\rangle$ and $|1\rangle$ twice

$$\begin{aligned}\mathbf{X}(\mathbf{X}|0\rangle) &= \mathbf{X}|1\rangle = |0\rangle \\ \mathbf{X}(\mathbf{X}|1\rangle) &= \mathbf{X}|0\rangle = |1\rangle\end{aligned}$$

Figure 16: Applying **X** gate to the states $|0\rangle$ and $|1\rangle$ twice

$$\begin{aligned}\mathbf{H}(\mathbf{H}|0\rangle) &= \mathbf{H}|+\rangle = |0\rangle \\ \mathbf{H}(\mathbf{H}|1\rangle) &= \mathbf{H}|-\rangle = |1\rangle\end{aligned}$$

Figure 17: Applying **H** gate to the states $|0\rangle$ and $|1\rangle$ twice

$$\begin{aligned}\mathbf{R}_2(\mathbf{R}_2|0\rangle) &= \mathbf{R}_2|0\rangle = |0\rangle \\ \mathbf{R}_2(\mathbf{R}_2|1\rangle) &= \mathbf{R}_2\begin{bmatrix} 0 \\ i \end{bmatrix} = |1\rangle\end{aligned}$$

Figure 18: Applying **R₂** gate to the states $|0\rangle$ and $|1\rangle$ twice

$$\begin{aligned}
\mathbf{CX}(\mathbf{CX} |00\rangle) &= \mathbf{CX} |00\rangle = |00\rangle \\
\mathbf{CX}(\mathbf{CX} |01\rangle) &= \mathbf{CX} |01\rangle = |01\rangle \\
\mathbf{CX}(\mathbf{CX} |10\rangle) &= \mathbf{CX} |11\rangle = |10\rangle \\
\mathbf{CX}(\mathbf{CX} |11\rangle) &= \mathbf{CX} |10\rangle = |11\rangle
\end{aligned}$$

Figure 19: Applying \mathbf{CX} gate to the states $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$ twice

This makes any quantum circuit constructed using these gates reversible.

2.5 Manipulating qubits individually

We have seen how we apply a gate to a system of qubits the same size as the gate. If we want to apply a gate to the i 'th qubit we construct a gate the same size as the system which acts with identity on every other qubit. We again use the Kronecker product for this.

$$\begin{bmatrix} 0 \cdot 1 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 1 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Figure 20: Applying \mathbf{X} to the first qubit in a 3 qubit system

$$\begin{aligned}
(\mathbf{I} \otimes \mathbf{X} \otimes \mathbf{I})|000\rangle &= \left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right) \left(\begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix} \right) = \\
&= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \\
&= \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \\
&= \begin{bmatrix} 0 \cdot 1 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 1 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = |010\rangle
\end{aligned}$$

Figure 21: Applying \mathbf{X} to the second qubit in a 3 qubit system

$$\begin{bmatrix} 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 \\ 1 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Figure 22: Applying \mathbf{X} to the thrid qubit in a 3 qubit system

If we want to apply multiple gates at a time we just replace the corresponding \mathbf{I} gates.

[illegible]

Figure 23: Applying \mathbf{X} to the third qubit and \mathbf{H} to the first qubit in a 3 qubit system

In general we can construct and apply any number of gates, U_0, U_1, \dots, U_n , to a state $|\Psi\rangle$ in sequence, this is in essence our quantum circuit. And because of the associative nature of matrix multiplication we can combine the entire circuit before applying it to different states! This saves tremendously when doing repetitive computations.

$$U_0 U_1 \dots U_n |\Psi\rangle = \left(\prod_{i=0}^n U_i \right) |\Psi\rangle$$

Figure 24: Associative nature of matrix multiplication

$$\begin{aligned}
\mathbf{U} &= \mathbf{CX} (\mathbf{I} \otimes \mathbf{H}) (\mathbf{I} \otimes \mathbf{X}) = \\
&\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} & 0 \\ 0 & \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} & 1 \end{bmatrix} \begin{bmatrix} \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} & \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} \\ 0 & \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} \end{bmatrix} \begin{bmatrix} 1 & \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} & 0 \\ 0 & \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} & 1 \end{bmatrix} = \\
&\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ \sqrt{0.5} & -\sqrt{0.5} & 0 & 0 \\ 0 & 0 & \sqrt{0.5} & \sqrt{0.5} \\ 0 & 0 & \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} & \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \\ \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ \sqrt{0.5} & -\sqrt{0.5} & 0 & 0 \\ 0 & 0 & \sqrt{0.5} & -\sqrt{0.5} \\ 0 & 0 & \sqrt{0.5} & \sqrt{0.5} \end{bmatrix} & \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \end{bmatrix} = \\
&\begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ -\sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ 0 & 0 & -\sqrt{0.5} & \sqrt{0.5} \\ 0 & 0 & \sqrt{0.5} & \sqrt{0.5} \end{bmatrix}
\end{aligned}$$

Figure 25: Computing a matrix representation of a circuit, \mathbf{U} , that first applies \mathbf{X} then \mathbf{H} to the first qubit then \mathbf{CX} to the first and second qubit

$$\begin{aligned}
\mathbf{U}|\mathbf{00}\rangle &= \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ -\sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ 0 & 0 & -\sqrt{0.5} & \sqrt{0.5} \\ 0 & 0 & \sqrt{0.5} & \sqrt{0.5} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \sqrt{0.5} \\ -\sqrt{0.5} \\ 0 \\ 0 \end{bmatrix} = |\mathbf{0-}\rangle \\
\mathbf{U}|\mathbf{01}\rangle &= \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ -\sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ 0 & 0 & -\sqrt{0.5} & \sqrt{0.5} \\ 0 & 0 & \sqrt{0.5} & \sqrt{0.5} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \sqrt{0.5} \\ \sqrt{0.5} \\ 0 \\ 0 \end{bmatrix} = |\mathbf{0+}\rangle \\
\mathbf{U}|\mathbf{10}\rangle &= \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ -\sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ 0 & 0 & -\sqrt{0.5} & \sqrt{0.5} \\ 0 & 0 & \sqrt{0.5} & \sqrt{0.5} \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -\sqrt{0.5} \\ \sqrt{0.5} \end{bmatrix} = -|\mathbf{1-}\rangle \\
\mathbf{U}|\mathbf{11}\rangle &= \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ -\sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ 0 & 0 & -\sqrt{0.5} & \sqrt{0.5} \\ 0 & 0 & \sqrt{0.5} & \sqrt{0.5} \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \sqrt{0.5} \\ \sqrt{0.5} \end{bmatrix} = |\mathbf{1+}\rangle
\end{aligned}$$

Figure 26: Applying the circuit represented by the matrix \mathbf{U} from figure 25 to different states

2.6 Controlled gates

We have described the \mathbf{R}_n gate but for the QFT circuit we need it controlled by another qubit. We can construct a controlled gate out of any other gate we simply take the gate that should happen if the control qubit is $|\mathbf{0}\rangle$ and place it in the top left quadrant of a matrix, then place what should happen if it is $|\mathbf{1}\rangle$ in the bottom right quadrant. This can be expressed like so:

$$\begin{aligned}
\mathbf{CU}_{1,2} &= |\mathbf{0}\rangle\langle\mathbf{0}| \otimes \mathbf{I} + |\mathbf{1}\rangle\langle\mathbf{1}| \otimes \mathbf{U} = \\
&\begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} \otimes \mathbf{I} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} \otimes \mathbf{U} = \\
&\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \otimes \mathbf{I} + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \otimes \mathbf{U}
\end{aligned}$$

Figure 27: Constructing a controlled gate $\mathbf{CU}_{1,2}$ from a gate \mathbf{U} where the first qubit controls the second

$$\begin{aligned}
\mathbf{CU}_{2,1} &= \mathbf{I} \otimes |0\rangle \langle 0| + \mathbf{U} \otimes |1\rangle \langle 1| = \\
&\mathbf{I} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \mathbf{U} \otimes \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \\
&\mathbf{I} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \mathbf{U} \otimes \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}
\end{aligned}$$

Figure 28: Constructing a controlled gate $\mathbf{CU}_{2,1}$ from a gate \mathbf{U} where the second qubit controls the first

In our case the controlling qubit is always after the \mathbf{R}_n gate so we only need the second formula. It is important to note that the controlled gate, \mathbf{U} in the examples, can be of any size, therefore it is not an issue that some of the controlled gates have 'empty' wires between them for example here is the result for a $\mathbf{CR}_{3,1}$ gate.

$$\begin{aligned}
\mathbf{CR}_{3,1} &= \mathbf{I} \otimes \mathbf{I} \otimes |0\rangle \langle 0| + \mathbf{R}_3 \otimes \mathbf{I} \otimes |1\rangle \langle 1| = \\
&\mathbf{I} \otimes \mathbf{I} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \mathbf{R}_3 \otimes \mathbf{I} \otimes \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \\
&\mathbf{I} \otimes \mathbf{I} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \mathbf{R}_3 \otimes \mathbf{I} \otimes \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}
\end{aligned}$$

Figure 29: Constructing a controlled gate $\mathbf{CR}_{3,1}$ from a gate \mathbf{R}_3 where the second qubit controls the first

2.7 Putting it all together

With these tools we can now create a formula for constructing a n qubit state and a n qubit QFT circuit.

$$|\Psi\rangle = |\Psi_1 \Psi_2 \dots \Psi_n\rangle = \bigotimes_{i=1}^n |\Psi_i\rangle$$

Figure 30: Constructing the state vector for the n qubit state $|\Psi\rangle$

$$\begin{aligned}
I(k) &= \begin{cases} \bigotimes_{i=k}^1 \mathbf{I} & \text{if } k \geq 1 \\ [1] & \text{otherwise} \end{cases} \\
STEP(i, n) &= \begin{cases} \prod_{j=i}^2 (I(i) \otimes (\mathbf{I} \otimes I(j-2) \otimes |\mathbf{0}\rangle \langle \mathbf{0}| + \mathbf{R}_j \otimes I(j-2) \otimes |\mathbf{1}\rangle \langle \mathbf{1}|) \otimes I(n-i-j)) & \text{if } i \geq 2 \\ [1] & \text{otherwise} \end{cases} \\
QFT(n) &= \prod_{i=n-1}^0 (STEP(n-i, n) (I(i) \otimes \mathbf{H} \otimes I(n-i-1)))
\end{aligned}$$

Figure 31: Constructing the matrix for the n qubit QFT

This can be turned into pseudo code:

```

STATE(psi)
1  r = [1]
2  for each digit d in psi do:
3      if d = 1
4          r = r ⊗  $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ 
5      else if d = 0
6          r = r ⊗  $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ 
7  return r

```

```

I(k)
1  r =  $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ 
2  id =  $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ 
3  while k ≥ 1 do:
4      r = r ⊗ id
5      k = k - 1
6  return r

```

```

STEP( $i, n$ )
1   $j = i$ 
2   $r = [1]$ 
3   $id = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ 
4   $p0 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ 
5   $p1 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$ 
6  while  $j \geq 2$  do:
7       $r_j = \begin{bmatrix} 1 & 0 \\ 0 & e^{\frac{2\pi i}{2^j}} \end{bmatrix}$ 
8       $r = r \cdot (I(i) \otimes (id \otimes I(j-2) \otimes p0 + r_j \otimes I(j-2) \otimes p0) \otimes I(n-i-j))$ 
9       $j = j - 1$ 
10 return  $r$ 

QTF( $n$ )
1   $r = I(n)$ 
2   $had = \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix}$ 
3   $i = n - 1$ 
4  while  $i \geq 0$  do:
5       $r = r \cdot STEP(n-i, n) \cdot (I(i) \otimes had \otimes I(n-i-1))$ 
6       $i = i - 1$ 
7  return  $r$ 

```

An example application could be $QFT(4) \cdot STATE(0010)$. Now we move on to show how we construct and apply the circuit using tensor networks.

3 Tensor Network Simulation

tensors are mathematical objects have a lot in common with nd-arrays, some examples of tensors you are probably familiar with, a rank 0 tensor is just a scalar, a rank 1 tensor is a vector, a rank 2 tensor is a matrix, and so on. The rank of the tensor tells you how many indices you need to describe a single element in the tensor, e.g. you need 1 index to tell which element in a vector you are talking about and you need 2, namely a column and row index to uniquely specify an element in a matrix. Each index has a dimension, for example a rank 2 tensor that is m by n would have one index i taking one of n values and another index j taking one of m values, typically $i \in \{0, 1, \dots, n-1\}, j \in \{0, 1, \dots, m-1\}$, we can then describe an element by a_{ij} , if we have more indices they are sometimes written as a_{ij}^{kl} .



Figure 32: rank 0 tensor.

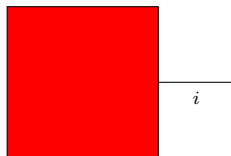


Figure 33: rank 1 tensor. Each index is represented by a line



Figure 34: rank 2 tensor. Each index is represented by a line

Often the indices are not numbered on these drawings. If we have two tensors we can make them share an index if they have the same dimension, so if we have two rank 3 tensors, one where the dimensions of the indices are 2, 3, 5 and another where it is 1, 4, 3. We can see that they both have an index of size 3 so if we wish we can make them share a label for this index. Thus they could have the indices i, j, k and l, m, j , notice the reuse of j .

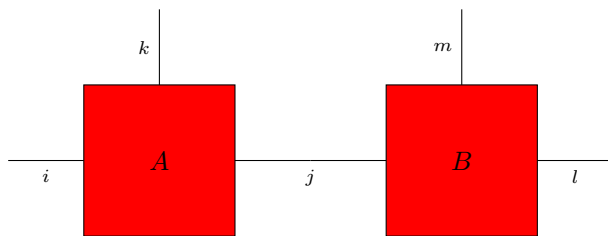


Figure 35: rank 3 tensors sharing index j .

But what is this good for? In essence, when we make tensors share indices it is a way to symbolise that we are multiplying them, matrix multiplication style. The actual computation of the multiplication can be done at a later point we are just marking our intention. This is important as we might want to build an entire network of tensors and then be strategic about which shared indices we choose to *contract*. Contracting a shared index is synonymous with computing the product of the two tensors.

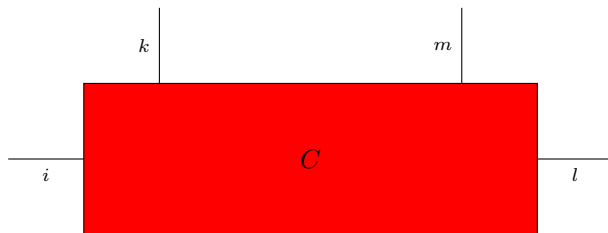


Figure 36: rank 4 tensor after contracting shared index j from Figure 35.

in this example we have two tensors A and B where each have elements of the form a_{ijk}, b_{lmj} resulting in a single tensor C with the elements

$$c_{iklm} = \sum_{x=0}^{dim(j)-1} a_{ixk} b_{lmx}$$

here $dim(j) = 3$ and we subtract 1 since the elements are 0 indexed. In *tensor notation* the summation is implicit if there is a shared index in such an equation so we would just write $c_{iklm} = a_{ijk} b_{lmj}$

4 Conclusion