



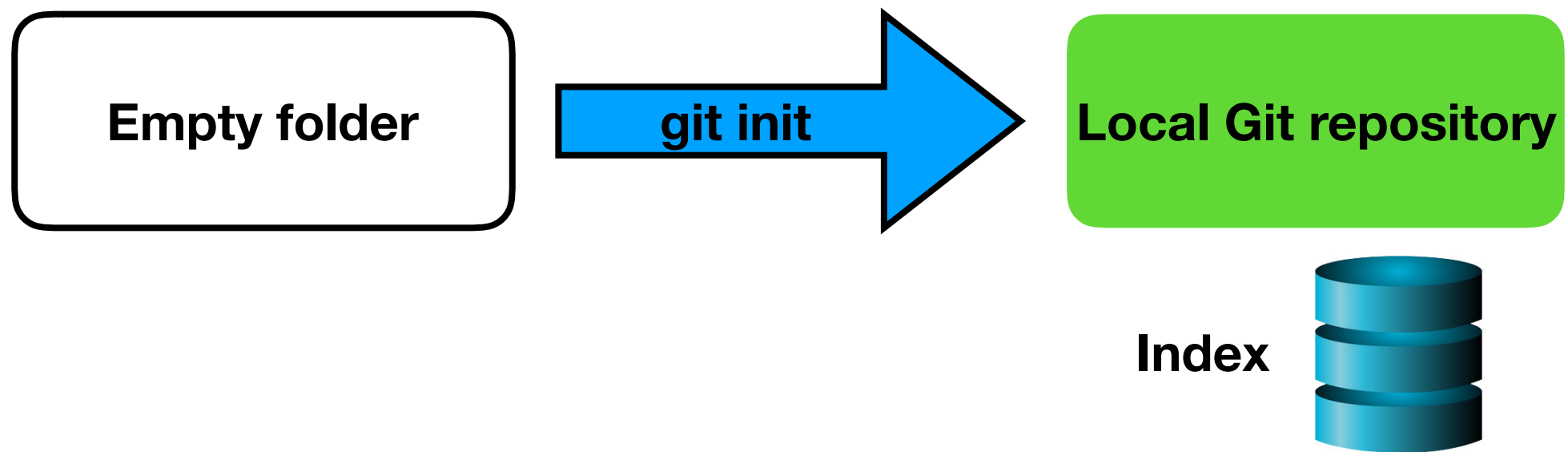
Introduction to Scientific Computation

Lecture 1

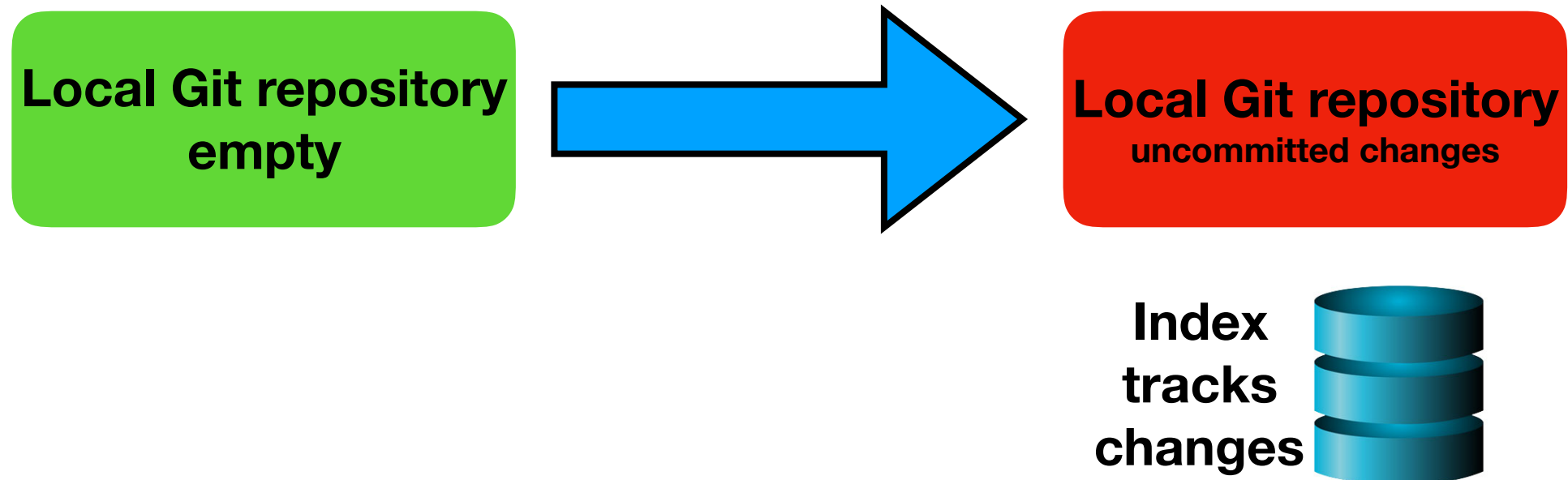
Fall 2019

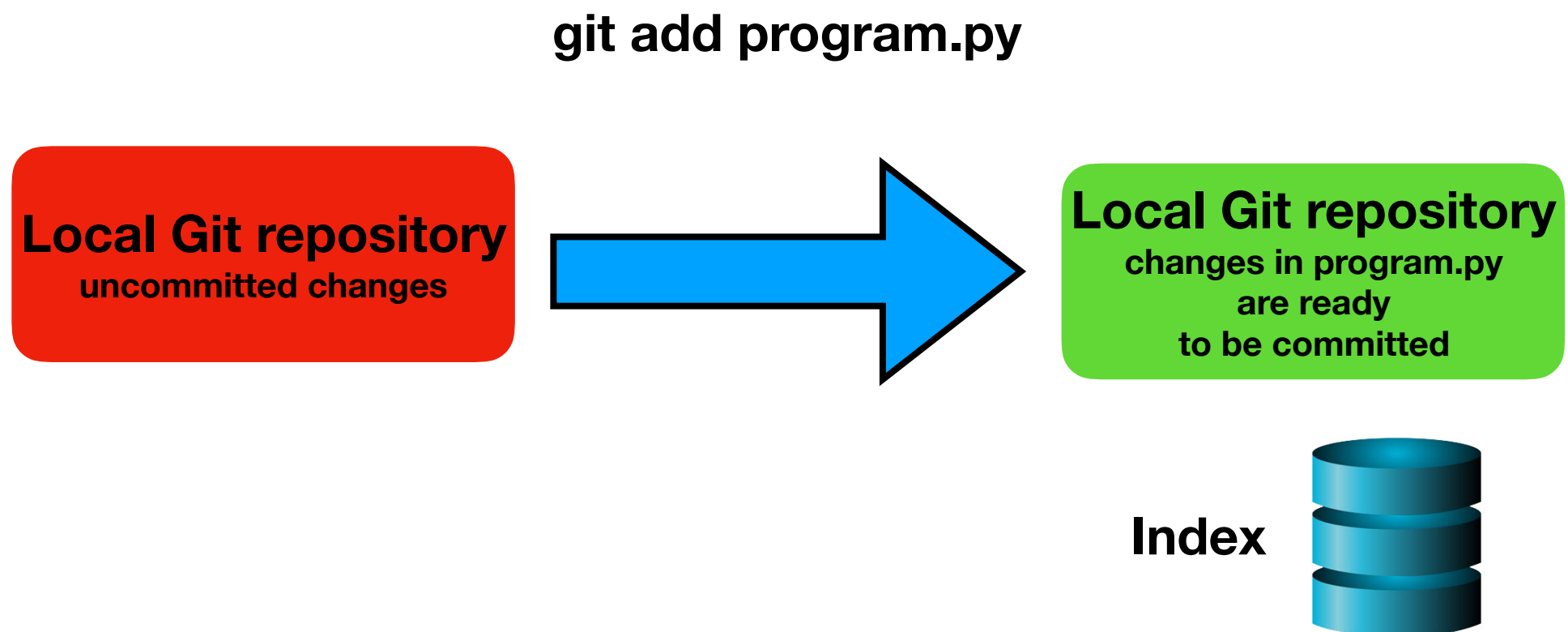
Git v2, Complexity, Floating-point arithmetic
Numerical stability

Git v2



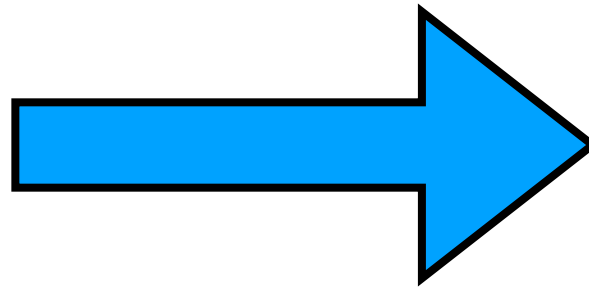
Create program.py consisting of K lines





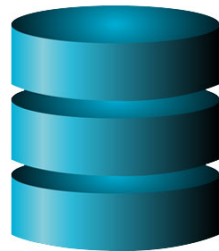
git commit -m “implemented program”

Local Git repository
changes in program.py
are ready
to be committed



Local Git repository

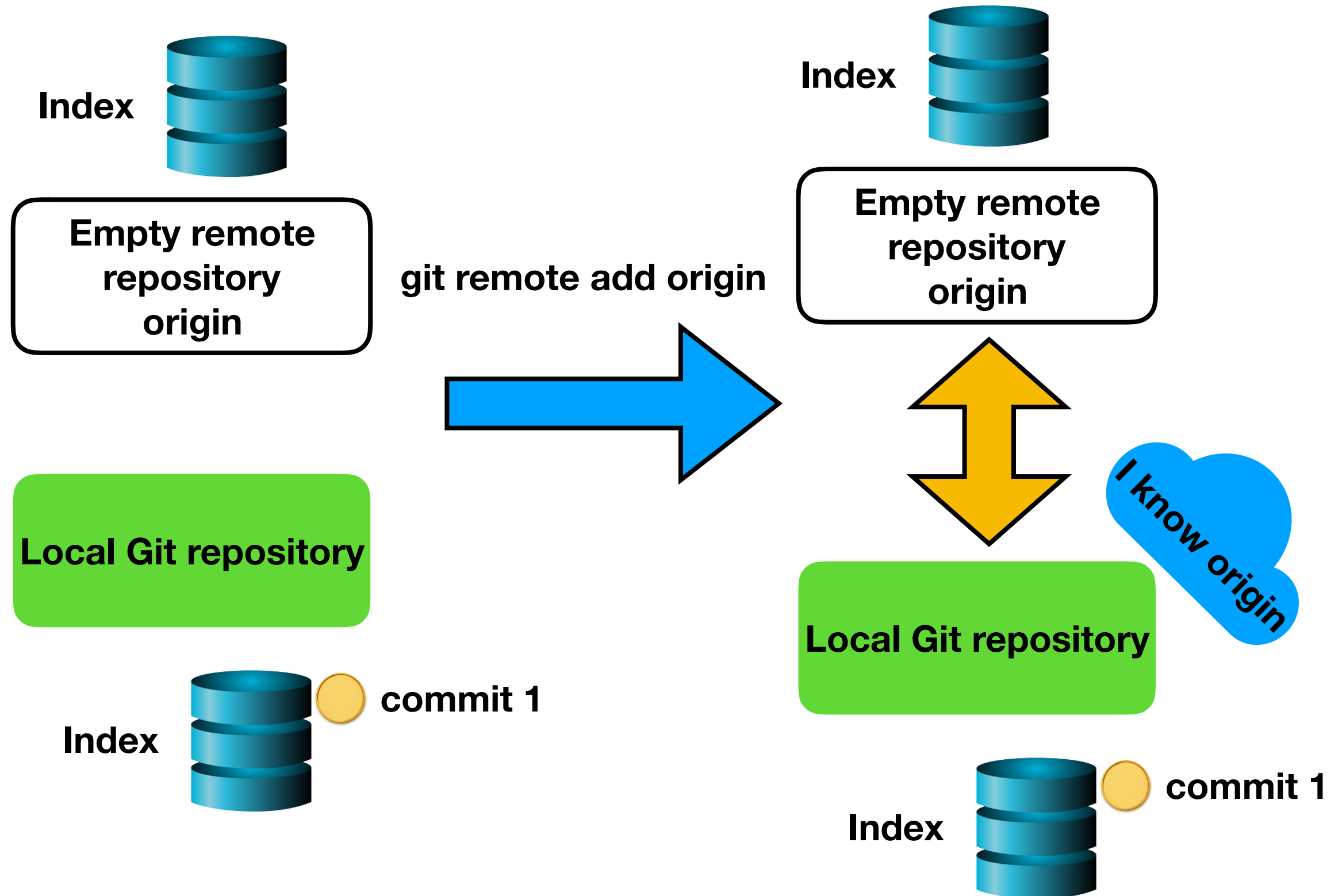
Index

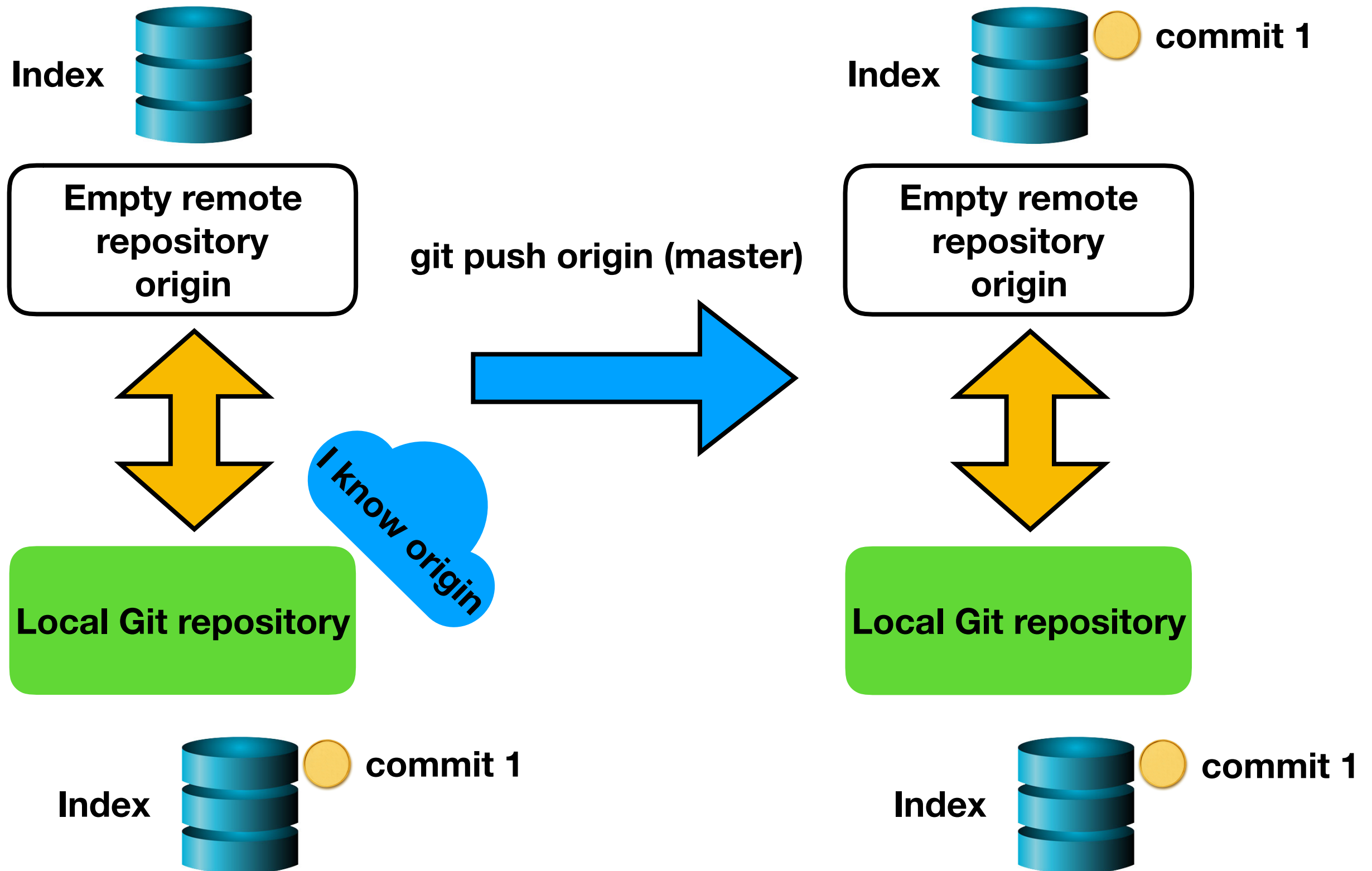


Index

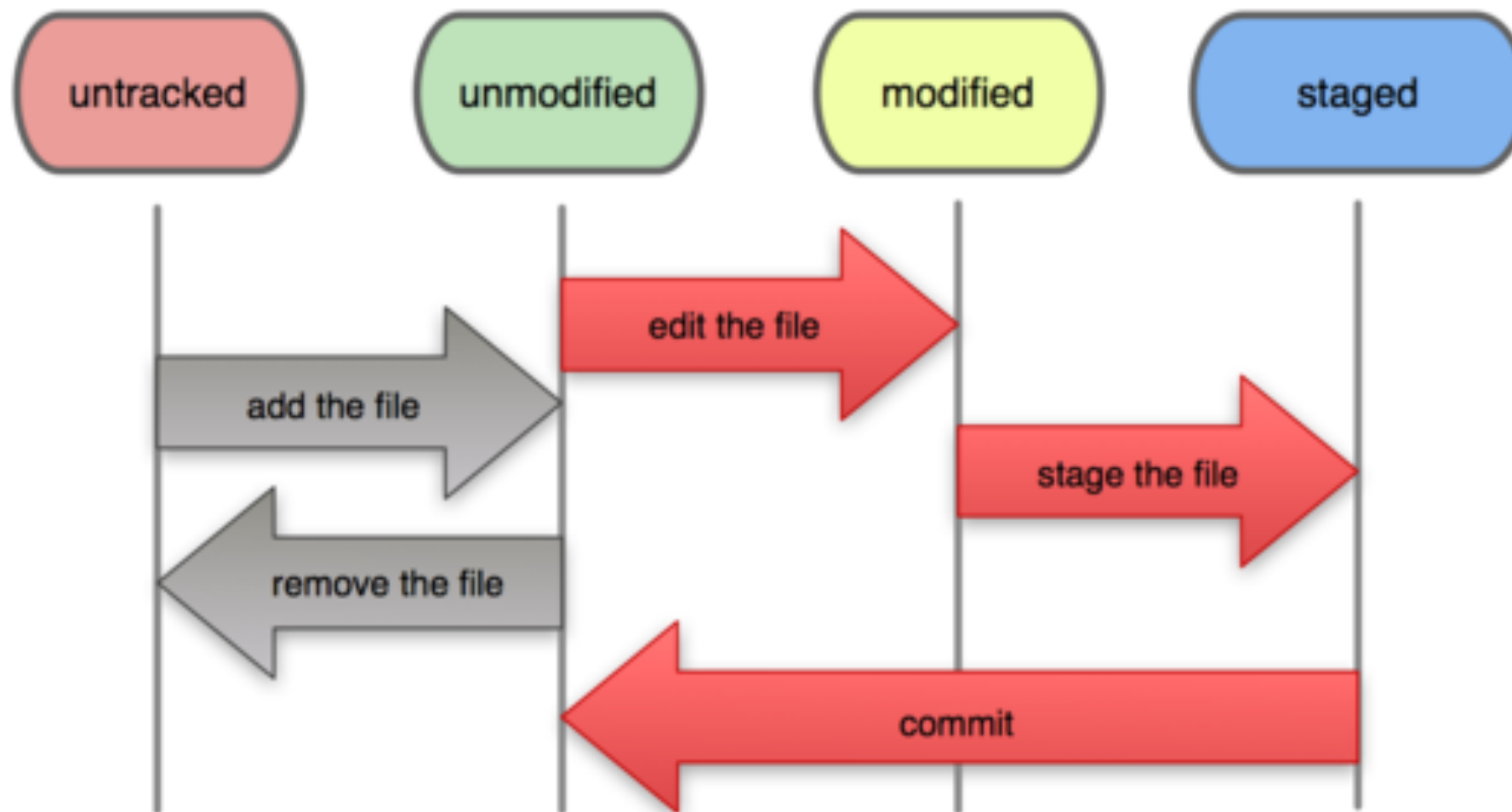


commit 1





File Status Lifecycle



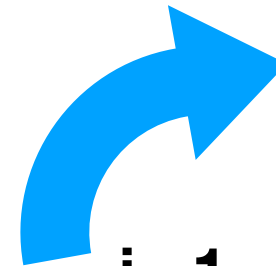


=

git checkout commit i

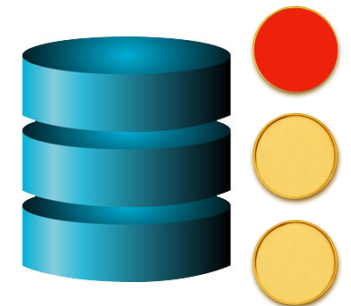
Local Git repository

Local Git repository



$i = 1$

Index



Index

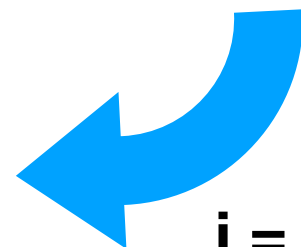


commit 1

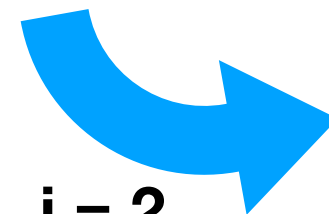
commit 2

commit N

Local Git repository



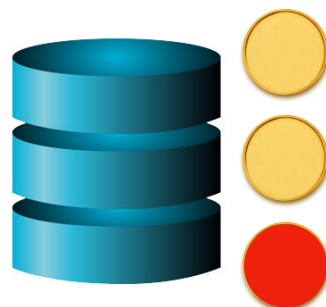
$i = N$



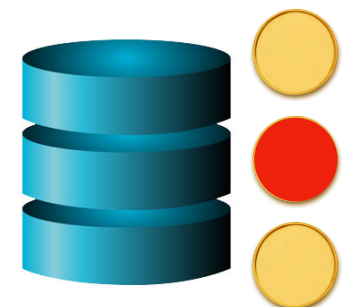
$i = 2$

Local Git repository

Index



Index



Check here for more examples:

<http://git-lectures.github.io>

Complexity

One of definitions: it is a measure of computational cost

In order to give a more formal definition quite a big formalism should be introduced (see recommended materials for this week).

We will operate with a concept.

Complexity

The notion of complexity is about how good or bad is the algorithm.
We want to think in an abstract way, independent of:

- implementation details (Python, C++, matlab)
- hardware (stm32, intel Pentium D, Intel Core i7-8700K)
- etc and whatnot

Complexity

Let us use constant time operation (elementary operations).

E.g. + and *

Remember: real runtime doesn't matter (does it ?)

$$3 + 5 = \begin{array}{r} 0011 \\ + 0101 \\ \hline 1000 \end{array}$$

Complexity

Let us use constant time operation (elementary operations).

E.g. + and *

Remember: real runtime doesn't matter (does it ?)

$$3 + 5 = \begin{array}{r} 0011 \\ + 0101 \\ \hline 1000 \end{array}$$

$$T(n) = c \cdot n$$

c - is a cost for summation of one bits

Complexity

Let us use constant time operation (elementary operations).

E.g. + and *

Remember: real runtime doesn't matter (does it ?)

$$3 + 5 = \begin{array}{r} 0011 \\ + 0101 \\ \hline 1000 \end{array}$$

$$T(n) = c \cdot n$$

c - is a cost for summation of one bits

c_1 - for cpu1

c_2 - for cpu2

Complexity

In order to get rid of c we will use **Asymptotic complexity** with big-O notation.

Complexity

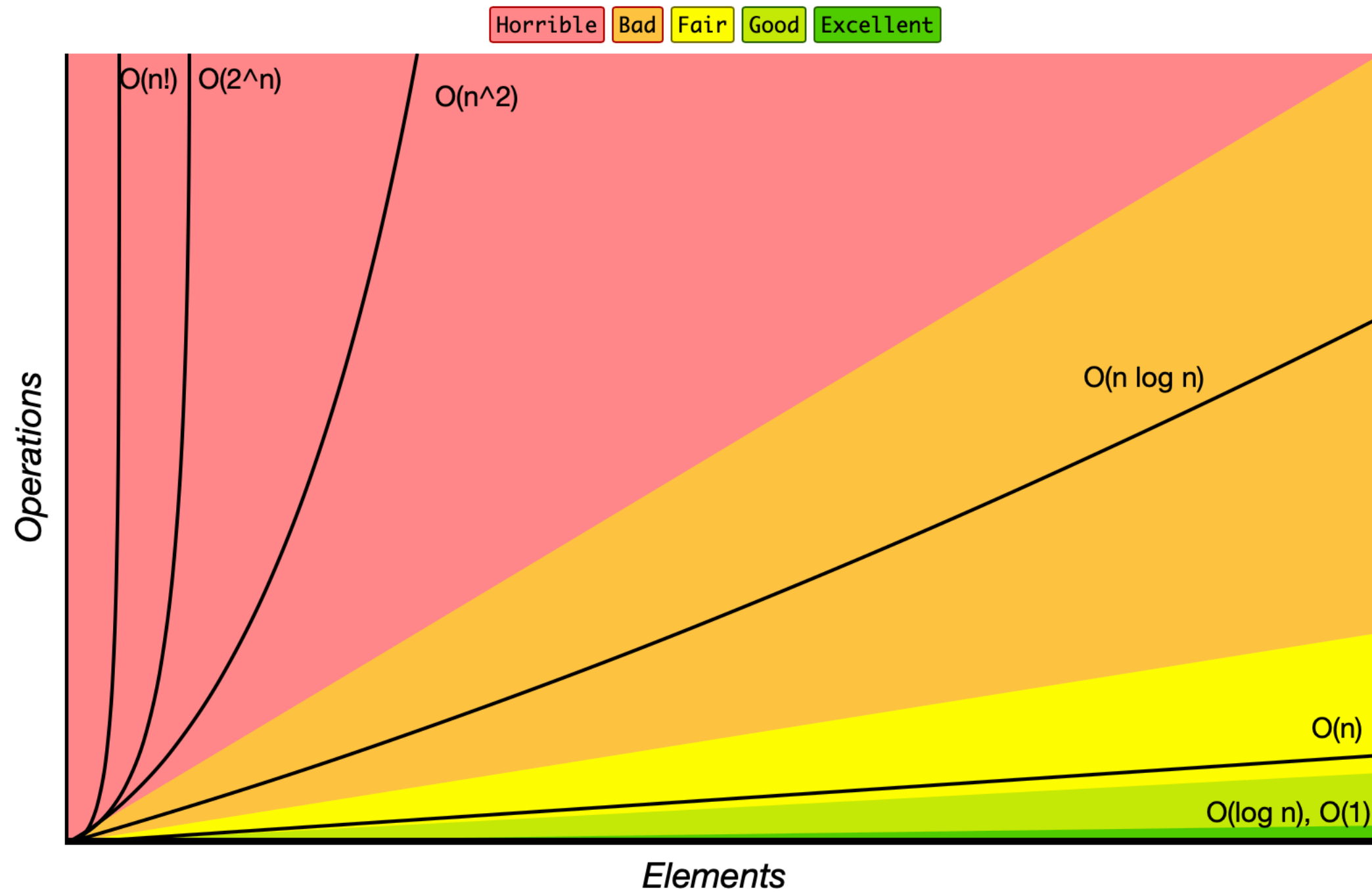
In order to get rid of c we will use **Asymptotic complexity** with big-O notation.

Definition: for any monotonic functions $f(n)$ and $g(n)$ from positive integers to the positive integers $f(n) = O(g(n))$ when there exists constants $c > 0$ and $n_0 > 0$ such that

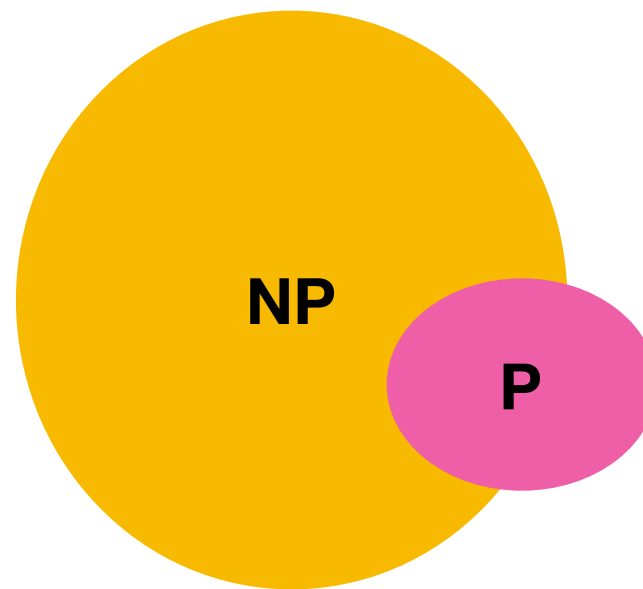
$$f(n) \leq c \cdot g(n), \text{ for all } n \geq n_0$$

Complexity

Big-O Complexity Chart



Complexity



???

Representation of numbers

Fixed point

The most straightforward format for the representation of real numbers is **fixed point** representation, a.k.a **Qm.n** format.

Qm.n number is in the range $[-2^m, 2^m - 2^{-n}]$ with the resolution 2^{-n}
requires $m + n + 1$ bits for storage.

Representation of numbers

Floating point

We are mostly interested in **floating point numbers** represented as e.g.

$$1.2345 = \underbrace{12345}_{\text{significand}} \times \underbrace{10}_{\text{base}} \overbrace{-4}^{\text{exponent}}$$

IEEE 754

Single and double precision

$$X = \pm 1.\overline{b_1 b_2 \dots b_K} \cdot 2^e$$

$$X \in [X - \Delta X, X + \Delta X],$$

Single

- S EEEEEEEE FFFFFFFFFFFFFFFFFFFFFFFF
- 0 1 8 9 31

Double

- S EEEEEEEEEEE FF
- 0 1 11 12 63

Absolute accuracy

$$\Delta X \leq \frac{1}{2} 2^{-K} * 2^e \leq |X| \cdot 2^{-K-1}$$

Relative accuracy

$$\frac{\Delta X}{X} \leq 2^{-K-1}$$

The **relative accuracy** of single precision is $10^{-7} - 10^{-8}$, while for double precision is $10^{-14} - 10^{-16}$.

A **float32** takes **4 bytes**, **float64**, or double precision, takes **8 bytes**.

These are the only two floating point-types supported in hardware.

You should use **double precision** in CSE and **single** on GPU/Data Science.

| Format | Total bits | Significand bits | Exponent bits | Smallest number | Largest number |
|------------------|------------|------------------|---------------|---------------------------|--------------------------|
| Single precision | 32 | 23 + 1 sign | 8 | ca. $1.2 \cdot 10^{-38}$ | ca. $3.4 \cdot 10^{38}$ |
| Double precision | 64 | 52 + 1 sign | 11 | ca. $5.0 \cdot 10^{-324}$ | ca. $1.8 \cdot 10^{308}$ |

Machine zero exists

```
import numpy as np
```

```
n = 1.0  
d = np.inf  
i = 0
```

```
while d > 0:  
    d = n - n / 2  
    n = n / 2  
    i += 1
```

```
(1 / 2)**(i - 2)
```

5e-324

```
import numpy as np
```

```
n = 1.0  
d = np.inf  
i = 0
```

```
while d > 0:  
    d = n - n / 2  
    n = n / 2  
    i += 1
```

```
(1 / 2)**(i - 1)
```

0.0

See code