Table of Contents

In [1]:
```python
import numpy as np
np.__version__
```

Out[1]: '1.22.4'

文档阅读说明：

- 🐧 表示 Tip
- ⚠️ 表示注意事项

本部分内容主要介绍与NumPy相关的高性能、分布式数值计算用法和工具。它们的安装都比较简单，参考文档即可。我们这里侧重介绍一下每个工具是干什么的，有什么特点，我们什么时候需要使用它们。

Numba

文档：Numba documentation — Numba 0.55.2+0.g2298ad618.dirty-py3.7-linux-x86_64.egg documentation

Numba是适用于Python的即时编译器，最适合用在使用NumPy数组和函数，以及循环的代码中。最常用的使用方法是通过装饰器。当调用一个Numba的装饰器时，它会被编译为「即时」的机器代码以供执行，全部或部分代码随后可以以机器代码的速度运行。

概括来说，这几种情况适合使用Numba：

- 很多数学计算
- 使用了很多Numpy
- 有很多循环

它的原理是，通过读取装饰函数的Python字节码，并将其与函数输入的参数类型信息相结合，分析和优化代码后，使用LLVM编译器根据CPU定制生成函数的机器代码版本。之后的调用都会使用该编译后的版本。

In [2]:
```python
from numba import jit
```

In [14]:
```python
def func_normal(a):
    x = np.median(a)
    y = np.max(a)
    t = x / y;
    z = x * np.sqrt(1 + t * t)
    m = 0.0
    for i in range(a.shape[0]):
        m += np.tanh(a[i, i])
        m /= z
    return a + m
```

In [6]:
```python
a = np.arange(100, dtype=np.int32).reshape(10, 10)
```

In [15]:
```python
%timeit func_normal(a)
```

```
68.2 µs ± 2.32 µs per loop (mean ± std. dev. of 7 runs, 10000 loops each)
```

In [16]:
```
@jit(nopython=True)
def func_numba(a):
    x = np.median(a)
    y = np.max(a)
    t = x / y;
    z = x * np.sqrt(1 + t * t)
    m = 0.0
    for i in range(a.shape[0]):
        m += np.tanh(a[i, i])
        m /= z
    return a + m
```

In [19]:
```
prebuild = func_numba(a)
```

In [20]:
```
%timeit func_numba(a)
```

```
1.68 µs ± 33.8 ns per loop (mean ± std. dev. of 7 runs, 1000000 loops each)
```

可以很明显看出性能的提升。

jit与njit

`Numba` 有两种模式：

- `nopython` 模式：用 `@jit(nopython=True)` 或 `@njit` 装饰器装饰。这种模式下，函数将完全在编译模式下运行，不需要Python解释器参与。这也是 `Numba` 推荐的使用方式。
- `object` 模式：直接用 `@jit` 装饰时，如果 `nopython` 模式失败，则会使用 `object` 模式进行编译，此时一部分可「Numba」的代码会使用机器代码执行，剩下的则使用Python编译器执行。

In [3]:
```
from numba import njit
import pandas as pd
```

In [4]:
```
@njit
def jit_fail(x):
    df = pd.DataFrame(x)
    df += 1
    cov = df.cov()
    return cov
```

In [5]:
```
x = {'a': [1, 2, 3], 'b': [20, 30, 40]}
```

In [6]:
```
jit_fail(x)
```

```
---------------------------------------------------------------------------
TypingError                               Traceback (most recent call last)
<ipython-input-6-1a477a3676a1> in <module>
----> 1 jit_fail(x)

/usr/local/lib/python3.8/site-packages/numba/core/dispatcher.py in _compile_for_a
rgs(self, *args, **kws)
    399                 e.patch_message(msg)
    400
--> 401             error_rewrite(e, 'typing')
    402         except errors.UnsupportedError as e:
    403             # Something unsupported is present in the user code, add help
info

/usr/local/lib/python3.8/site-packages/numba/core/dispatcher.py in error_rewrite
(e, issue_type)
    342                 raise e
    343             else:
--> 344                 reraise(type(e), e, None)
    345
    346         argtypes = []

/usr/local/lib/python3.8/site-packages/numba/core/utils.py in reraise(tp, value,
tb)
     78         value = tp()
     79     if value.__traceback__ is not tb:
---> 80         raise value.with_traceback(tb)
     81     raise value
     82

TypingError: Failed in nopython mode pipeline (step: nopython frontend)
non-precise type pyobject
[1] During: typing of argument at <ipython-input-4-481c7b069f0d> (3)

File "<ipython-input-4-481c7b069f0d>", line 3:
def jit_fail(x):
    df = pd.DataFrame(x)
    ^

This error may have been caused by the following argument(s):
- argument 0: cannot determine Numba type of <class 'dict'>
```

In [7]:

```
@jit
def jit_succ(x):
    df = pd.DataFrame(x)
    df += 1
    cov = df.cov()
    return cov
```

In [8]:

```
# 会有警告
cov = jit_succ(x)
```

```
<ipython-input-7-cb5f8409f203>:1: NumbaWarning:
Compilation is falling back to object mode WITH looplifting enabled because Funct
ion "jit_succ" failed type inference due to: non-precise type pyobject
[1] During: typing of argument at <ipython-input-7-cb5f8409f203> (3)

File "<ipython-input-7-cb5f8409f203>", line 3:
def jit_succ(x):
    df = pd.DataFrame(x)
    ^

  @jit
/usr/local/lib/python3.8/site-packages/numba/core/object_mode_passes.py:177: Numb
aWarning: Function "jit_succ" was compiled in object mode without forceobj=True.

File "<ipython-input-7-cb5f8409f203>", line 2:
@jit
def jit_succ(x):
^

  warnings.warn(errors.NumbaWarning(warn_msg,
/usr/local/lib/python3.8/site-packages/numba/core/object_mode_passes.py:187: Numb
aDeprecationWarning:
Fall-back from the nopython compilation path to the object mode compilation path
has been detected, this is deprecated behaviour.

For more information visit http://numba.pydata.org/numba-doc/latest/reference/dep
recation.html#deprecation-of-object-mode-fall-back-behaviour-when-using-jit

File "<ipython-input-7-cb5f8409f203>", line 2:
@jit
def jit_succ(x):
^

  warnings.warn(errors.NumbaDeprecationWarning(msg,
```

In [13]:
```
%timeit jit_succ(x)
```

```
559 µs ± 16 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
```

In [10]:
```
def func(x):
    df = pd.DataFrame(x)
    df += 1
    cov = df.cov()
    return cov
```

In [14]:
```
%timeit func(x)
```

```
514 µs ± 29.8 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
```

此时性能差不多，`Numba` 反而会慢一些，因为它还要判断是不是可以编译优化。

官方文档还有其他一些特性，不过我们主要关注和性能相关的几个。

Loops

`Numba` 对循环可以进行优化：

In [116…
```python
def get_primes(x):
    res = []
    for v in range(x+1):
        if v < 2:
            continue
        flag = True
        for i in range(2, int(np.sqrt(v)) + 1):
            if v % i == 0:
                flag = False
        if flag:
            res.append(v)
    return res
```

In [117…
```python
is_prime(10)
```

Out[117…
```
[2, 3, 5, 7]
```

In [118…
```python
x = 100000
```

In [119…
```python
%timeit get_primes(x)
```

```
1.28 s ± 48 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

In [120…
```python
@njit
def jit_get_primes(x):
    res = []
    for v in range(x+1):
        if v < 2:
            continue
        flag = True
        for i in range(2, int(np.sqrt(v)) + 1):
            if v % i == 0:
                flag = False
        if flag:
            res.append(v)
    return res
```

In [121…
```python
prebuild = jit_get_primes(x)
```

In [122…
```python
%timeit jit_get_primes(x)
```

```
77.7 ms ± 2.16 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

可以看出效果还是很明显的，不过我们在使用时尽量做一下性能对比，以做到心中有数。

FastMath

在某些情况下，可以通过放松一些严格的（IEEE754）数值获得额外的性能提升。

> IEEE 二进制浮点数算术标准（ IEEE 754 ）是 20 世纪 80 年代以来最广泛使用的浮点数运算标准，为许多 CPU 与 浮点运算器所采用。这个标准定义了表示浮点数的格式（包括负零 -0）与反常值（denormal number），一些特殊数值（（无穷（Inf）与非数值（NaN）），以及这些数值的 "浮点数运算符"；它也指明了四种数值舍入规则和五种例外状况（包括例外发生的时机与处理方式）。——维基百科

以官方文档例子来说明：

In [205…
```
@njit(fastmath=False)
def do_sum(A):
    acc = 0.
    # without fastmath, this loop must accumulate in strict order
    for x in A:
        acc += np.sqrt(x)
    return acc

@njit(fastmath=True)
def do_sum_fast(A):
    acc = 0.
    # with fastmath, the reduction can be vectorized as floating point
    # reassociation is permitted.
    for x in A:
        acc += np.sqrt(x)
    return acc
```

In [206…
```
a = np.arange(40000)
```

In [207…
```
prebuild1 = do_sum(a)
prebuild2 = do_sum_fast(a)
```

In [208…
```
prebuild1, prebuild2
```

Out[208…
```
(5333233.1256554425, 5333233.1256554425)
```

In [209…
```
%timeit do_sum(a)
```

```
70 µs ± 678 ns per loop (mean ± std. dev. of 7 runs, 10000 loops each)
```

In [210…
```
%timeit do_sum_fast(a)
```

```
53.1 µs ± 1.58 µs per loop (mean ± std. dev. of 7 runs, 10000 loops each)
```

默认情况下，编译器在浮点优化方面收到严格限制（如重新关联浮点表达式），因为这样的优化可能导致结果改变。比如：

- (10000001.0f * 10000001.0f) / 10000001.0f == 10000000.0f
- 10000001.0f * (10000001.0f / 10000001.0f) == 10000001.0f

第一个表达式括号里的会超出32位精度，会舍入。

更多关于这方面的知识可以参考：

- SIMD vectorization
- Floating Point Optimization

Parallel

In [199…
```
from numba import prange
```

In [211…
```
@njit(parallel=True)
def do_sum_parallel(A):
```

```
    # each thread can accumulate its own partial sum,
    # and then a cross
    # thread reduction is performed to obtain the result to return
    n = len(A)
    acc = 0.
    for i in prange(n):
        acc += np.sqrt(A[i])
    return acc

@njit(parallel=True, fastmath=True)
def do_sum_parallel_fast(A):
    n = len(A)
    acc = 0.
    for i in prange(n):
        acc += np.sqrt(A[i])
    return acc
```

In [212…

```
prebuild1 = do_sum_parallel(a)
prebuild2 = do_sum_parallel_fast(a)
prebuild1, prebuild2
```

Out[212…

```
(5333233.125655441, 5333233.125655442)
```

In [213…

```
%timeit do_sum_parallel(a)
```

```
108 µs ± 1.3 µs per loop (mean ± std. dev. of 7 runs, 10000 loops each)
```

In [214…

```
%timeit do_sum_parallel_fast(a)
```

```
95.5 µs ± 3.72 µs per loop (mean ± std. dev. of 7 runs, 10000 loops each)
```

JAX

文档：JAX Quickstart — JAX documentation

JAX是运行在CPU、GPU和TPU上的NumPy，两者关系：

- JAX提供了一个方便的受NumPy启发的接口。
- 通过鸭子类型，JAX数组通常可以直接替代NumPy数组。
- 与NumPy数组不同，JAX数组是不可变的。

替换NumPy

In [215…

```
import jax.numpy as jnp
```

In [216…

```
jnp.arange(10)
```

```
WARNING:absl:No GPU/TPU found, falling back to CPU. (Set TF_CPP_MIN_LOG_LEVEL=0 a
nd rerun for more info.)
```

Out[216…

```
DeviceArray([0, 1, 2, 3, 4, 5, 6, 7, 8, 9], dtype=int32)
```

In [217…

```
list(_)
```

Out[217…

```
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
```

In [218…
```
from jax import random
```

In [221…
```
key = random.PRNGKey(42)
```

In [223…
```
a = random.normal(key, (2, 3))
a
```

Out[223…
```
DeviceArray([[ 0.61226517,  1.1225883 ,  1.1373315 ],
             [-0.81273264, -0.8904051 ,  0.12623137]], dtype=float32)
```

In [224…
```
b = random.normal(key, (3, 2))
b
```

Out[224…
```
DeviceArray([[ 0.61226517,  1.1225882 ],
             [ 1.1373315 , -0.8127326 ],
             [-0.8904051 ,  0.12623137]], dtype=float32)
```

In [225…
```
jnp.dot(a, b)
```

Out[225…
```
DeviceArray([[ 0.63893783, -0.08147554],
             [-1.6226908 , -0.1727684 ]], dtype=float32)
```

In [226…
```
np.dot(a, b)
```

Out[226…
```
array([[ 0.63893783, -0.08147555],
       [-1.6226908 , -0.1727684 ]], dtype=float32)
```

jit

`jit` 主要用来加速。

In [227…
```
from jax import jit
```

In [232…
```
def func_normal(a):
    x = jnp.median(a)
    y = jnp.max(a)
    t = x / y;
    z = x * jnp.sqrt(1 + t * t)
    m = 0.0
    for i in range(a.shape[0]):
        m += jnp.tanh(a[i, i])
        m /= z
    return a + m
```

In [233…
```
a = np.arange(100, dtype=np.int32).reshape(10, 10)
```

In [235…
```
pre = jit(func_normal)(a)
```

In [238…
```
%timeit func_normal(a)
```

```
5.83 ms ± 57.9 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
```

In [236…
```
%timeit jit(func_normal)(a)
```

```
42.5 µs ± 2.45 µs per loop (mean ± std. dev. of 7 runs, 10000 loops each)
```

grad

`grad` 用来计算导数。

In [240…
```
from jax import grad
```

以Sigmoid函数为例：

$$f(x) = \frac{1}{1+e^{-x}}$$

它的导数为： `f(x) * (1-f(x))` 。

In [245…
```
def sigmoid(x):
    return 1.0 / (1.0 + jnp.exp(-x))
```

In [253…
```
def dsigmoid(x):
    x = sigmoid(x)
    return x * (1-x)
```

In [254…
```
dersigmoid = grad(sigmoid)
```

In [255…
```
dersigmoid(2.)
```

Out[255…
```
DeviceArray(0.10499357, dtype=float32)
```

In [256…
```
dsigmoid(2.)
```

Out[256…
```
DeviceArray(0.10499363, dtype=float32)
```

vmap

`vmap` 用于自动向量化或批量化。以官方文档为例：

In [258…
```
mat = random.normal(key, (150, 100))
```

In [259…
```
batched_x = random.normal(key, (10, 100))
```

首先看简单循环版：

In [260…
```
def apply_matrix(v):
    return jnp.dot(mat, v)
```

In [261…
```
def naive_batched(v_batched):
    return jnp.stack([apply_matrix(v) for v in v_batched])
```

In [265…
```
naive_batched(batched_x).shape
```

Out[265…
```
(10, 150)
```

In [275…
```
%timeit naive_batched(batched_x).block_until_ready()
```

```
3.78 ms ± 168 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
```

接下来是矩阵乘法（手动Batch）版：

In [276…
```
def batched_apply_matrix(v_batched):
    return jnp.dot(v_batched, mat.T)
```

In [277…
```
%timeit batched_apply_matrix(batched_x).block_until_ready()
```

```
226 µs ± 24.7 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
```

最后是 `vmap`：

In [278…
```
from jax import vmap, jit
```

In [281…
```
@jit
def vmap_apply_matrix(v_batched):
    return vmap(apply_matrix)(v_batched)
```

In [282…
```
%timeit vmap_apply_matrix(batched_x).block_until_ready()
```

```
18.9 µs ± 545 ns per loop (mean ± std. dev. of 7 runs, 100000 loops each)
```

这在没法使用矩阵乘法的时候非常有用。

最后值得一提的是，三个方法乃至 `jnp` 既可以单独使用，也可以联合起来使用。实际使用时可以根据自己的需要灵活组合。

这里我们简单介绍一下，更多内容可以进一步阅读文档。

Cython

[Welcome to Cython's Documentation — Cython 3.0.0a10 documentation]

Cython在本章中都比较特别，它是一种编程语言，使得编写C扩展像Python一样容易。它旨在成为Python的超集，赋予它高级、面向对象和动态编程。Cython代码会被翻译成优化的C/C++代码并编译为Python扩展模块。不仅使得程序执行与C语言紧密集成，同时保持Python的易开发性。

看个最简单的例子：

In [5]:
```
# 加载扩展
%load_ext Cython
```

In [47]:
```
%%cython

cdef int a = 0
for i in range(10):
    a += i
print(a)
```

```
45
```

annotate

可以使用 `annotate` 选项查看代码分析：

In [48]:
```
%%cython --annotate

cdef int a = 0
for i in range(10):
    a += i
print(a)
```

45

Out[48]: Generated by Cython 0.29.30

Yellow lines hint at Python interaction.
Click on a line that starts with a " + " to see the C code that Cython generated for it.

```
 1:
+2: cdef int a = 0
+3: for i in range(10):
+4:     a += i
+5: print(a)
```

下面显示的是纯Python版，不过这种情况下需要类型标记。

In [49]:
```
%%cython --annotate

a: cython.int = 0
for i in range(10):
    a += i
print(a)
```

45

Out[49]: Generated by Cython 0.29.30

Yellow lines hint at Python interaction.
Click on a line that starts with a " + " to see the C code that Cython generated for it.

```
 1:
+2: a: cython.int = 0
+3: for i in range(10):
+4:     a += i
+5: print(a)
```

当然，即便是纯Python代码，也可以使用Cython先编译，获得性能提升。不过对于性能关键的代码，添加静态类型声明通常很有用。

In [50]:
```
%%cython --annotate

a = 0
for i in range(10):
    a += i
print(a)
```

45

Out[50]: Generated by Cython 0.29.30

Yellow lines hint at Python interaction.
Click on a line that starts with a " + " to see the C code that Cython generated for it.

```
 1: 
+2: a = 0
+3: for i in range(10):
+4:     a += i
+5: print(a)
```

cfunc/cdef

Python函数调用可能很耗时——在Cython中可能是双重的，因为可能需要在Python对象之间进行转换才能调用。因此Cython提供了声明C样式函数的方法，Cython特定的 `cdef` 语句，以及 `@cfunc` 装饰器用以在Python语法中声明C样式函数。两种方法会生成相同的C代码。

In [2]:
```
import cython
```

In [3]:
```
@cython.cfunc
@cython.exceptval(-2, check=True)
def f(x: cython.double) -> cython.double:
    return x ** 2 - x
```

In [6]:
```
%%cython

cdef double f(double x) except? -2:
    return x ** 2 - x
```

性能对比

接下来，我们用实际例子来对比性能。

In [24]:
```
# 标准Python版
def get_primes(num):
    res = [0] * 1000
    v = 2
    len_res = 0
    while len_res < num:
        flag = True
        for i in range(2, int(np.sqrt(v)) + 1):
            if v % i == 0:
                flag = False
        if flag:
            res[len_res] = v
            len_res += 1
        v += 1
    return res
```

In [7]:
```
%%cython

cdef extern from "math.h":
    double sqrt(double x)

def cython_get_primes(int num):
    cdef int i, n, v=2, len_res=0
    cdef flag
    cdef int res[1000]

    while len_res < num:
        flag = True
        n = int(sqrt(v)) + 1
        for i in range(2, n):
            if v % i == 0:
                flag = False
        if flag:
            res[len_res] = v
            len_res += 1
        v += 1
    return res
```

In [30]:
```
%timeit ps1 = cython_get_primes(1000)
```

```
2.12 ms ± 157 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
```

In [31]:
```
%timeit ps2 = get_primes(1000)
```

```
37.4 ms ± 471 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

In [32]:
```
ps1 == ps2
```

Out[32]:
```
True
```

我们再对比一下直接编译后的Python代码，在code目录下执行：

`python3 python setup.py build_ext --inplace`

In [37]:
```
# 导入
%cd code
```

```
/Users/Yam/Yam/powerful-numpy/src/skilled/code
```

In [38]:
```
import primes
```

In [44]:
```
ps3 = primes.get_primes(1000)
```

In [45]:
```
ps3 ==  ps2
```

Out[45]:
```
True
```

In [46]:
```
%timeit primes.get_primes(1000)
```

```
23.1 ms ± 1.14 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

CuPy

文档：CuPy – NumPy & SciPy for GPU — CuPy 10.5.0 documentation

Cupy是一个兼容NumPy/SciPy的数组库，用于使用Python进行GPU加速计算。CuPy充当在NVIDIA CUDA或AMD ROCm平台上运行现有NumPy/SciPy代码的替代品。其主要目标是为Python用户提供GPU加速能力，无需深入了解底层GPU技术。

⚠️注意，本节内容需要cuda环境。

In [2]:
```python
import cupy as cp
cp.__version__
```

Out[2]:
```
'10.5.0'
```

cupy.ndarray

In [3]:
```python
x_gpu = cp.array([1,2,3])
```

In [4]:
```python
x_gpu
```

Out[4]:
```
array([1, 2, 3])
```

In [5]:
```python
type(x_gpu)
```

Out[5]:
```
cupy._core.core.ndarray
```

`cuda.ndarray` 与 `np.ndarray` 的主要区别在于CuPy会把数组分配在当前设备（某一张GPU卡）上。其他的API都是和NumPy几乎没有区别的。如果熟悉NumPy，等于熟悉了CuPy。

In [6]:
```python
rng = cp.random.default_rng(42)
```

In [7]:
```python
rng.integers(0, 10, (2,3))
```

Out[7]:
```
array([[5, 4, 0],
       [7, 2, 3]])
```

Device

这是CuPy比较重要的一个概念——「当前设备」，这是默认的GPU设备，数组的分配、操作和计算都在它上面运行。

In [8]:
```python
x_gpu0 = cp.array([1,2,3])
```

In [9]:
```python
x_gpu0.device
```

Out[9]:
```
<CUDA Device 0>
```

In [10]:
```python
with cp.cuda.Device(1):
    x_gpu1 = cp.array([1,2,3])
```

In [11]:
```python
x_gpu1.device
```

Out[11]:
```
<CUDA Device 1>
```

注意，这里你得有两张（或以上）的卡才行。比如我们再来一张不存在的卡：

In [12]:
```
with cp.cuda.Device(2):
    x_gpu2 = cp.array([1,2,3])
```

```
---------------------------------------------------------------------------
CUDARuntimeError                          Traceback (most recent call last)
Input In [12], in <cell line: 1>()
----> 1 with cp.cuda.Device(2):
      2     x_gpu2 = cp.array([1,2,3])

File cupy/cuda/device.pyx:184, in cupy.cuda.device.Device.__enter__()

File cupy_backends/cuda/api/runtime.pyx:365, in cupy_backends.cuda.api.runtime.se
tDevice()

File cupy_backends/cuda/api/runtime.pyx:142, in cupy_backends.cuda.api.runtime.ch
eck_status()

CUDARuntimeError: cudaErrorInvalidDevice: invalid device ordinal
```

Data Transfer

主要指GPU卡和host（挂载卡的主机）之间的传输。

In [16]:
```
x_cpu = np.array([1,2,3])
```

In [18]:
```
type(x_cpu)
```

Out[18]:
```
numpy.ndarray
```

In [19]:
```
# 移动到GPU上
x_gpu = cp.asarray(x_cpu)
```

In [21]:
```
type(x_gpu)
```

Out[21]:
```
cupy._core.core.ndarray
```

`cp.asarray` 也可以在GPU卡之间互相移动。

In [22]:
```
with cp.cuda.Device(1):
    x_gpu2 = cp.asarray(x_gpu)
```

In [24]:
```
x_gpu2.device
```

Out[24]:
```
<CUDA Device 1>
```

注意，`cp.asarray` 不会复制数据，如果需要复制，可以使用 `cp.array(arr, dtype, copy=True)` 。它实际上等价于 `cp.array(a, dtype, copy=False)` 。

`copy=True` 会返回一个新数组，否则会返回对象。

In [40]:
```
arr = cp.array([1,2,3])
cp.asarray(arr) is arr
```

Out[40]: True

In [41]:
```
# 从GPU到Host
x_cpu2 = cp.asnumpy(x_gpu2)
x_cpu2
```

Out[41]: array([1, 2, 3])

In [42]:
```
type(x_cpu2)
```

Out[42]: numpy.ndarray

In [43]:
```
# 或者使用`get`方法
x_gpu2.get()
```

Out[43]: array([1, 2, 3])

In [44]:
```
type(_)
```

Out[44]: numpy.ndarray

`cp.asnumpy` 返回NumPy数组（在Host上），`cp.asarray` 返回一个CuPy数组（在当前卡上）。两个方法都可以接受任意的输入（cp或np的数组）。

Memory

在GPU编程中，内存管理是个比较重要的环节。CuPy使用内存池管理内存，包括两种：

- Device内存池（GPU Memory），分配GPU内存时使用
- Pinned内存池（非交换CPU Memory），CPU到GPU数据传输时使用

In [3]:
```
mempool = cp.get_default_memory_pool()
pinpool = cp.get_default_pinned_memory_pool()
```

In [4]:
```
# 400bytes CPU内存
a_cpu = np.arange(100, dtype=np.float32)
```

In [5]:
```
a_cpu.nbytes
```

Out[5]: 400

In [6]:
```
mempool.used_bytes()
```

Out[6]: 0

In [7]:
```
mempool.total_bytes()
```

Out[7]: 0

In [8]:
```
pinpool.n_free_blocks()
```

Out[8]: 0

从CPU到GPU，一旦传输完成，pinned memory会被释放。

注意，实际分配的大小可能会四舍五入到大于请求大小的值。

In [9]:
```
a = cp.array(a_cpu)
```

In [10]:
```
a.nbytes
```

Out[10]: 400

In [11]:
```
mempool.used_bytes()
```

Out[11]: 512

In [12]:
```
mempool.total_bytes()
```

Out[12]: 512

In [13]:
```
pinpool.n_free_blocks()
```

Out[13]: 1

如果数组超出所在域，GPU内存会被释放。

In [14]:
```
a = None
```

In [15]:
```
mempool.used_bytes()
```

Out[15]: 0

In [16]:
```
mempool.total_bytes()
```

Out[16]: 512

In [17]:
```
pinpool.n_free_blocks()
```

Out[17]: 1

使用 `free_all_blocks` 来清理内存池。

In [22]:
```
mempool.free_all_blocks()
```

In [23]:
```
mempool.used_bytes()
```

Out[23]: 0

In [24]:
```
mempool.total_bytes()
```

Out[24]: 0

In [26]:
```
pinpool.free_all_blocks()
```

In [27]:
```
pinpool.n_free_blocks()
```

Out[27]: 0

CUDA编程中 `threads` ， `blocks` 和 `grids` 是三个重要的概念：

- thread：一个thread是运行在单个GPU核上的一系列指令
- block：多个threads在GPU上以block的抽象单元执行
- grid：block的block又被称为grid

也可以对GPU的内存进行硬限制：

```
export CUPY_GPU_MEMORY_LIMIT="1073741824"

# or

export CUPY_GPU_MEMORY_LIMIT="50%"
```

或使用内置的方法：

In [55]:
```python
mempool = cp.get_default_memory_pool()
```

In [56]:
```python
with cp.cuda.Device(0):
    mempool.set_limit(size=1024**3)
```

In [57]:
```python
cp.get_default_memory_pool().get_limit()
```

Out[57]: 1073741824

也可以通过API对内存池自定义或修改，具体参见文档：

Memory Management — CuPy 10.5.0 documentation

CuPy和NumPy在某些行为上会有一些细微的不同，包括：

- 浮点数转整数
- 随机方法
- 越界索引
- 重复索引处理
- 0维数组
- Matrix类型
- 数据类型
- UFUNC
- 随机种子
- NaN处理

具体可参见文档：Differences between CuPy and NumPy — CuPy 10.5.0 documentation

In [ ]:
```python

```

CuPy可以和很多其他库结合使用，比如NumPy，Numba，PyTorch等，具体可参考文档：

Interoperability — CuPy 10.5.0 documentation

这部分内容涉及到了cuda编程，我们可能需要更灵活的控制，可以考虑使用PyCuda。

Sparse

文档：Sparse — sparse 0.13.0+0.g0b7dfeb.dirty documentation

`Sparse` 在NumPy和scipy.sparse上实现了任意维度的「稀疏数组」。

主要的数据结构参照遵循稀疏矩阵的Coordinate List（COO）布局，并将其扩展到多个维度。

dmi1	dim2	dim3	...	data
0	0	0	.	10
0	0	3	.	13
0	2	2	.	9
3	1	4	.	21

除了存储，所有数组相关的操作（转置、reshape、切片、乘法等）都需要重新实现。

此外，本仓库还包括其他几个数据结构，比如Dictionary of Keys（DOK）格式，它可以很好地推广到任意数量的维度。DOK适合编写和操作，但其他操作并不支持。常用的最佳实践是使用DOK编写一个数组，然后转为另一种格式执行其他操作。

也支持Compressed Sparse Row/Column（CSR/CSC）格式。

创建

In [4]:
```
import sparse as se
se.__version__
```

Out[4]: '0.13.0'

In [34]:
```
rng = np.random.default_rng(42)
a = rng.random((100, 100, 100))
```

In [35]:
```
# 构造一个稀疏矩阵，90%为0
a[a<0.9] = 0
```

In [36]:
```
s = se.COO(a)
```

In [37]:
```
s.nbytes
```

Out[37]: 3205760

In [38]:
```
a.nbytes
```

Out[38]: 8000000

In [39]:
```
s
```

Out[39]:

Format	coo
Data Type	float64
Shape	(100, 100, 100)
nnz	100180
Density	0.10018
Read-only	True
Size	3.1M
Storage ratio	0.4

In [40]:
```
s.data
```

Out[40]:
```
array([0.97562235, 0.92676499, 0.97069802, ..., 0.98212211, 0.95084277,
       0.98694171])
```

In [41]:
```
s.coords
```

Out[41]:
```
array([[ 0,  0,  0, ..., 99, 99, 99],
       [ 0,  0,  0, ..., 99, 99, 99],
       [ 5, 11, 22, ..., 94, 95, 98]])
```

也可以直接通过坐标和值创建：

In [15]:
```
coords = [[0, 1, 2, 3, 4],
          [0, 1, 2, 3, 4]]
data = [10, 20, 30, 40, 50]
s = se.COO(coords, data, shape=(5, 5))
```

In [16]:
```
s
```

Out[16]:

Format	coo
Data Type	int64
Shape	(5, 5)
nnz	5
Density	0.2
Read-only	True
Size	120
Storage ratio	0.6

In [17]:
```
s.todense()
```

Out[17]:
```
array([[10,  0,  0,  0,  0],
       [ 0, 20,  0,  0,  0],
       [ 0,  0, 30,  0,  0],
       [ 0,  0,  0, 40,  0],
       [ 0,  0,  0,  0, 50]])
```

维度也可以比较随意：

In [23]:
```
coords = [[0, 3, 2, 1], [4, 1, 2, 0]]
data = [1, 4, 2, 1]
s = se.COO(coords, data, shape=(6, 5))
s.todense()
```

Out[23]:
```
array([[0, 0, 0, 0, 1],
       [1, 0, 0, 0, 0],
       [0, 0, 2, 0, 0],
       [0, 4, 0, 0, 0],
       [0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0]])
```

In [24]:
```
# 指定填充值
s = se.COO(coords, data, shape=(5,5), fill_value=-1)
s.todense()
```

Out[24]:
```
array([[-1, -1, -1, -1,  1],
       [ 1, -1, -1, -1, -1],
       [-1, -1,  2, -1, -1],
       [-1,  4, -1, -1, -1],
       [-1, -1, -1, -1, -1]])
```

从SciPy的稀疏矩阵、从NumPy的数组生成：

- `se.COO.from_scipy_sparse(x)`
- `se.COO.from_numpy(x)`

也支持随机：

In [28]:
```
s = se.random((5, 5), density=0.1)
s
```

Out[28]:

Format	coo
Data Type	float64
Shape	(5, 5)
nnz	2
Density	0.08
Read-only	True
Size	20
Storage ratio	0.1

In [29]:
```
s.todense()
```

Out[29]:
```
array([[0.        , 0.        , 0.1182219 , 0.        , 0.        ],
       [0.        , 0.        , 0.        , 0.        , 0.        ],
       [0.        , 0.        , 0.        , 0.        , 0.        ],
       [0.        , 0.        , 0.        , 0.        , 0.        ],
       [0.        , 0.        , 0.        , 0.        , 0.65295601]])
```

In [32]:
```
s.data
```

Out[32]:
```
array([0.1182219 , 0.65295601])
```

In [33]:
```
s.coords
```

Out[33]:
```
array([[0, 4],
       [2, 4]], dtype=uint8)
```

或者通过传入字典创建：

In [42]:
```
d = {(0, 0, 0): 1, (1, 2, 3): 2, (1, 1, 0): 3}
s = se.COO(d)
```

In [44]:
```
s.shape
```

Out[44]:
```
(2, 3, 4)
```

In [45]:
```
s
```

Out[45]:

Format	coo
Data Type	int64
Shape	(2, 3, 4)
nnz	3
Density	0.125
Read-only	True
Size	96
Storage ratio	0.5

也可以通过数组：

In [48]:
```
L = [((0, 0), 1),
     ((1, 1), 2),
     ((0, 0), 3)]
```

In [50]:
```
s = se.COO(L)
s.todense()
```

Out[50]:
```
array([[4, 0],
       [0, 2]])
```

或者从DOK转换过来：

In [46]:
```
s1 = se.DOK((5, 5))
s1
```

Out[46]:

Format	dok
Data Type	float64
Shape	(5, 5)
nnz	0
Density	0.0
Read-only	False
Size	0
Storage ratio	0.0

In [51]:
```
s1[1:3, 1:3] = [[4,5],[6,7]]
```

In [52]:
```
s1.todense()
```

Out[52]:
```
array([[0., 0., 0., 0., 0.],
       [0., 4., 5., 0., 0.],
       [0., 6., 7., 0., 0.],
       [0., 0., 0., 0., 0.],
       [0., 0., 0., 0., 0.]])
```

In [59]:
```
s1.coords
```

```
---------------------------------------------------------------------------
AttributeError                            Traceback (most recent call last)
Input In [59], in <cell line: 1>()
----> 1 s1.coords

AttributeError: 'DOK' object has no attribute 'coords'
```

In [56]:
```
s1.data
```

Out[56]:
```
{(1, 1): 4.0, (1, 2): 5.0, (2, 1): 6.0, (2, 2): 7.0}
```

In [53]:
```
s2 = s1.asformat("coo")
```

In [54]:
```
s2.todense()
```

Out[54]:
```
array([[0., 0., 0., 0., 0.],
       [0., 4., 5., 0., 0.],
       [0., 6., 7., 0., 0.],
       [0., 0., 0., 0., 0.],
       [0., 0., 0., 0., 0.]])
```

In [58]:
```
s2.coords
```

Out[58]:
```
array([[1, 1, 2, 2],
       [1, 2, 1, 2]])
```

In [57]:
```
s2.data
```

Out[57]:
```
array([4., 5., 6., 7.])
```

In [61]:
```
# 这样也可以转换
s3 = se.COO(s1)
```

```
s3.todense()
```

Out[61]:

```
array([[0., 0., 0., 0., 0.],
       [0., 4., 5., 0., 0.],
       [0., 6., 7., 0., 0.],
       [0., 0., 0., 0., 0.],
       [0., 0., 0., 0., 0.]])
```

转换

`COO` 对象可以转换成其他格式，包括：

- `COO.todense` ：转成NumPy数组
- `COO.mayhbe_densify` ：基于某些条件转为NumPy数组
- `COO.to_scipy_sparse` ：如果数组是二维，则转成 `spicy.sparse.coo_matrix`
- `COO.tocsr` ：如果数组是二维，转成 `scipy.sparse.csr_matrix`
- `COO.tocsc` ：如果数组是二维，转成 `scipy.sparse.csc_matrix`

着重说一下第二个API，它接受两个参数：max_size（输出的最大元素数，默认1000）和min_density（输出的最小密度，默认0.25），当一个稀疏数组两个条件都不满足时，会抛出异常。

In [128…

```
x = np.zeros((5, 5), dtype=np.uint8)
x[2, :] = 1
s = se.COO.from_numpy(x)
```

In [129…

```
x
```

Out[129…

```
array([[0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0],
       [1, 1, 1, 1, 1],
       [0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0]], dtype=uint8)
```

In [146…

```
# 25满足，0.9不满足
s.maybe_densify(max_size=25, min_density=0.21)
```

Out[146…

```
array([[0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0],
       [1, 1, 1, 1, 1],
       [0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0]], dtype=uint8)
```

In [147…

```
# 24不满足，0.1满足
s.maybe_densify(max_size=24, min_density=0.1)
```

Out[147…

```
array([[0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0],
       [1, 1, 1, 1, 1],
       [0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0]], dtype=uint8)
```

In [148…

```
# 都满足
s.maybe_densify(max_size=25, min_density=0.1)
```

```
Out[148…  array([[0, 0, 0, 0, 0],
                 [0, 0, 0, 0, 0],
                 [1, 1, 1, 1, 1],
                 [0, 0, 0, 0, 0],
                 [0, 0, 0, 0, 0]], dtype=uint8)
```

```
In [149…  # 都不满足
          s.maybe_densify(max_size=24, min_density=0.21)
```

```
---------------------------------------------------------------------------
ValueError                                Traceback (most recent call last)
Input In [149], in <cell line: 2>()
      1 # 都不满足
----> 2 s.maybe_densify(max_size=24, min_density=0.21)

File /home/env/anaconda3/envs/tf29/lib/python3.8/site-packages/sparse/_coo/core.p
y:1379, in COO.maybe_densify(self, max_size, min_density)
   1377     return self.todense()
   1378 else:
-> 1379     raise ValueError(
   1380         "Operation would require converting " "large sparse array to dens
e"
   1381     )

ValueError: Operation would require converting large sparse array to dense
```

计算

```
In [162…  s = se.random((3, 3, 3), density=0.1)
          s.todense()
```

```
Out[162…  array([[[0.        , 0.        , 0.        ],
                  [0.        , 0.        , 0.        ],
                  [0.        , 0.        , 0.        ]],

                 [[0.        , 0.        , 0.        ],
                  [0.82191339, 0.        , 0.        ],
                  [0.        , 0.        , 0.        ]],

                 [[0.        , 0.        , 0.        ],
                  [0.        , 0.        , 0.        ],
                  [0.        , 0.312388  , 0.        ]]])
```

```
In [163…  y = np.sin(s) + s.T * 1
          y
```

Out[163...

Format	coo
Data Type	float64
Shape	(3, 3, 3)
nnz	4
Density	0.14814814814814814
Read-only	True
Size	44
Storage ratio	0.2

In [164...

```
y.todense()
```

Out[164...

```
array([[[0.        , 0.        , 0.        ],
        [0.        , 0.82191339, 0.        ],
        [0.        , 0.        , 0.        ]],

       [[0.        , 0.        , 0.        ],
        [0.73244985, 0.        , 0.        ],
        [0.        , 0.        , 0.312388  ]],

       [[0.        , 0.        , 0.        ],
        [0.        , 0.        , 0.        ],
        [0.        , 0.30733194, 0.        ]]])
```

更多内容可参考：

Operations on COO and GCXS arrays — sparse 0.13.0+0.g0b7dfeb.dirty documentation

Dask

文档：Dask — Dask documentation

Dask主要用于并行计算。包括两部分：

- 针对计算优化的动态任务调度，类似于Airflow，Luigi，Celery或Make，但针对交互式计算工作负载进行了优化。
- 大数据集合，如并行数组，DataFrame，列表等，将NumPy，Pandas或Python迭代器等常见接口扩展到大于内存或分布式环境。这些并行集合在动态任务调度程序上运行。

整体架构如下：

Dask可以处理很多数据集合，我们这里以数组（Array）为例。关于Dask，我们在第一节《数组对象》也略有提及。

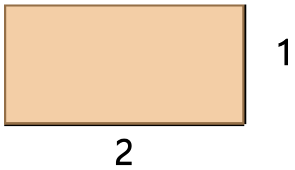
In [15]:

```
import dask.array as da
```

In [4]:
```python
a = np.array([2,3], like=da.array([1,1]))
a
```

Out[4]:

	Array	Chunk
Bytes	16 B	16 B
Shape	(2,)	(2,)
Count	1 Tasks	1 Chunks
Type	int64	numpy.ndarray



In [5]:
```python
a.compute()
```

Out[5]:
```
array([2, 3])
```

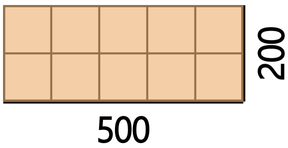
创建

In [6]:
```python
data = np.arange(100_000).reshape(200, 500)
```

In [7]:
```python
a = da.from_array(data, chunks=(100, 100))
a
```

Out[7]:

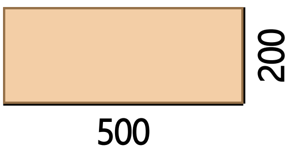
	Array	Chunk
Bytes	781.25 kiB	78.12 kiB
Shape	(200, 500)	(100, 100)
Count	10 Tasks	10 Chunks
Type	int64	numpy.ndarray



In [8]:
```python
# 自动chunk
b = da.from_array(data)
b
```

Out[8]:

	Array	Chunk
Bytes	781.25 kiB	781.25 kiB
Shape	(200, 500)	(200, 500)
Count	1 Tasks	1 Chunks
Type	int64	numpy.ndarray

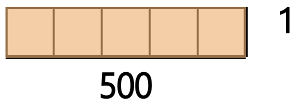


索引

In [9]:
```python
a[0]
```

Out[9]:

	Array	Chunk
Bytes	3.91 kiB	800 B
Shape	(500,)	(100,)
Count	15 Tasks	5 Chunks
Type	int64	numpy.ndarray

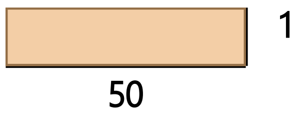


In [10]:

```
a[:50, 200]
```

Out[10]:

	Array	Chunk
Bytes	400 B	400 B
Shape	(50,)	(50,)
Count	11 Tasks	1 Chunks
Type	int64	numpy.ndarray



计算

Dask是惰性估计的，会生成一个用于计算的Dask任务图，请求结果时才会计算。计算和NumPy类似，也可以结合NumPy。

In [11]:

```
a.compute()
```

Out[11]:

```
array([[    0,     1,     2, ...,   497,   498,   499],
       [  500,   501,   502, ...,   997,   998,   999],
       [ 1000,  1001,  1002, ...,  1497,  1498,  1499],
       ...,
       [98500, 98501, 98502, ..., 98997, 98998, 98999],
       [99000, 99001, 99002, ..., 99497, 99498, 99499],
       [99500, 99501, 99502, ..., 99997, 99998, 99999]])
```

In [12]:

```
a.mean()
```

Out[12]:

	Array	Chunk
Bytes	8 B	8.0 B
Shape	()	()
Count	26 Tasks	1 Chunks
Type	float64	numpy.ndarray

In [13]:

```
a.mean().compute()
```

Out[13]:

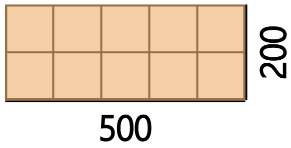
```
49999.5
```

In [14]:

```
np.sin(a)
```

Out[14]:

	Array	Chunk
Bytes	781.25 kiB	78.12 kiB
Shape	(200, 500)	(100, 100)
Count	20 Tasks	10 Chunks
Type	float64	numpy.ndarray



In [15]:

```
_.compute()
```

Out[15]:

```
array([[ 0.        ,  0.84147098,  0.90929743, ...,  0.58781939,
         0.99834363,  0.49099533],
       [-0.46777181, -0.9964717 , -0.60902011, ..., -0.89796748,
        -0.85547315, -0.02646075],
       [ 0.82687954,  0.9199906 ,  0.16726654, ...,  0.99951642,
         0.51387502, -0.4442207 ],
       ...,
       [-0.99720859, -0.47596473,  0.48287891, ..., -0.76284376,
         0.13191447,  0.90539115],
       [ 0.84645538,  0.00929244, -0.83641393, ...,  0.37178568,
        -0.5802765 , -0.99883514],
       [-0.49906936,  0.45953849,  0.99564877, ...,  0.10563876,
         0.89383946,  0.86024828]])
```

任务图

In [20]:

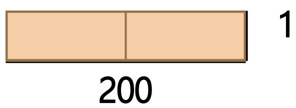
```
c = a.max(axis=1)[::-1] + 10
```

In [21]:

```
c
```

Out[21]:

	Array	Chunk
Bytes	1.56 kiB	800 B
Shape	(200,)	(100,)
Count	30 Tasks	2 Chunks
Type	int64	numpy.ndarray



In [23]:

```
c.dask
```

Out[23]:

HighLevelGraph

HighLevelGraph with 6 layers and 30 keys from all layers.

▶ Layer1: array

▶ Layer2: amax

▶ Layer3: amax-partial

▶ Layer4: amax-aggregate

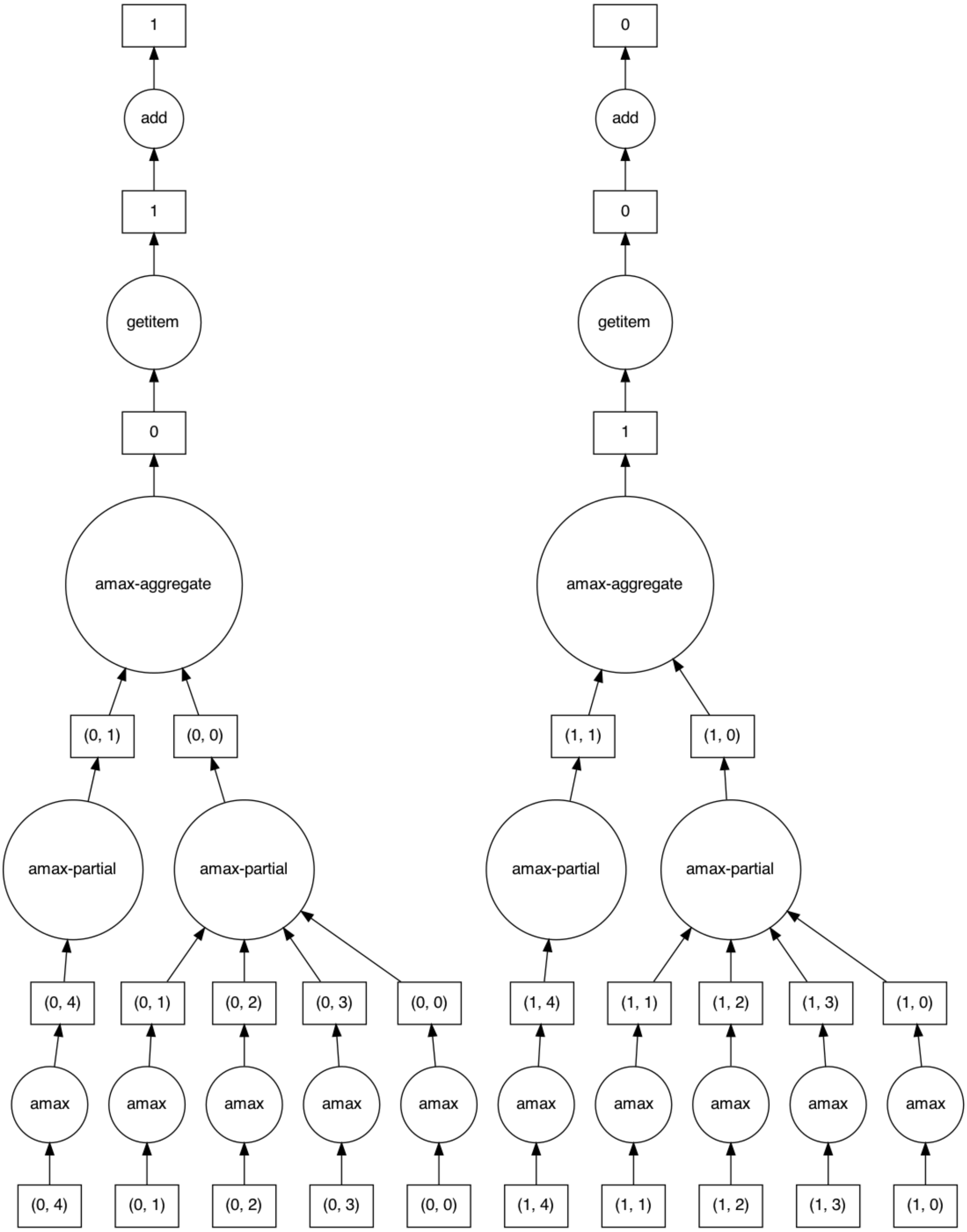
▶ Layer5: getitem

▶ Layer6: add

In [24]:

```
c.visualize()
```

Out[24]:



底层API

使用 `delayed` 装饰器将函数调用包装到一个延迟构造的任务图中:

In [1]:

```python
import dask
```

In [6]:

```python
@dask.delayed
def inc(x):
    return x+1
@dask.delayed
def add(x, y):
    return x+y
```

In [10]:
```python
a = inc(1)
b = inc(2)
c = add(a, b)
```

In [12]:
```python
a, b, c
```

Out[12]:
```
(Delayed('inc-171697d8-9c8e-42a6-b8f2-3a1c5ff36faa'),
 Delayed('inc-5a5d5200-1e59-4d9d-b0e5-049cad501cf4'),
 Delayed('add-3d37a606-f83d-401e-bacb-c16f9bec7c9a'))
```

In [13]:
```python
c = c.compute()
c
```

Out[13]:
```
5
```

调度

在生成任务图后，调度程序默认使用计算机线程池运行计算。

线程调度使用本地的 `concurrent.futures.ThreadPoolExecutor` 执行计算，是Dask Array，Dask DataFrame和Dask Delayed的默认选择。

由于Python的全局解释器锁 (GIL)，此调度程序仅在计算由非Python代码主导时提供并行性。主要是在NumPy数组、Pandas DataFrames中的数字数据上操作或使用任何生态系统中其他基于C/C++/Cython的项目。

In [3]:
```python
# 对scheduler进行配置
dask.config.set(scheduler="threads")
```

Out[3]:
```
<dask.config.set at 0x104bfdbe0>
```

In [5]:
```python
dask.config.get("scheduler")
```

Out[5]:
```
'threads'
```

进程调度使用本地的 `concurrent.futures.ProcessPoolExecutor` 执行计算，是Dask Bag的默认选择。

每个任务及其所有依赖项都被传送到本地进程执行，然后它们的结果被传送回主进程。可以绕过Python的GIL问题。但是将数据移动到进程可能会导致性能下降，尤其是在进程间传输大量数据时。当不涉及任务间数据传输，输出输入都很小时是一个很好的选择。

In [6]:
```python
dask.config.set(scheduler='processes')
```

Out[6]:
```
<dask.config.set at 0x1046037c0>
```

In [7]:
```python
dask.config.get("scheduler")
```

Out[7]:
```
'processes'
```

单线程同步调度器在一个本地线程中执行所有的计算，没有并行。一般用于调试或分析。比如Jupyter Notebook的魔法方法 `%debug` ， `%pdb` ， `%prun` 等在使用并行Dask调度时将无法正常工作。

In [8]:
```
dask.config.set(scheduler='synchronous')
```

Out[8]:
```
<dask.config.set at 0x104bfd9d0>
```

In [9]:
```
dask.config.get("scheduler")
```

Out[9]:
```
'synchronous'
```

Dask支持使用分布式调度器进行更多控制，它可以在单台或多台机器上工作，可将其视为「高级调度器」。这也是目前比较推荐的方式。

之所以在单台机器上也推荐使用，原因在于：

- 提供异步API访问，尤其是Futures
- 提供诊断仪表板，可以提供有关性能和进度的意见
- 以更复杂的方式处理数据的局部性，在需要多个进程的工作负载上比多处理器调度器更有效

In [10]:
```
from dask.distributed import Client
```

In [11]:
```
client = Client()
```

In [12]:
```
client
```

Out[12]:

Client

Client-81d68614-e4ad-11ec-9f7c-acde48001122

Connection method: Cluster object **Cluster type:** distributed.LocalCluster

Dashboard: http://127.0.0.1:8787/status

▸ Cluster Info

In [13]:
```
dask.config.get("scheduler")
```

Out[13]:
```
'dask.distributed'
```

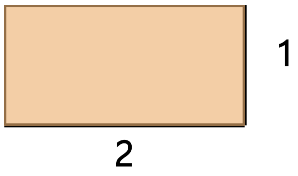
请注意上面 `Dashboard` 的地址，可以直接访问。

当然了，除了上面的这种全局配置方法，也可以使用上下文管理器，或执行 `compute` 时通过参数传入。

In [18]:
```
x = da.array([1,2])
x
```

Out[18]:

	Array	Chunk
Bytes	16 B	16 B
Shape	(2,)	(2,)
Count	1 Tasks	1 Chunks
Type	int64	numpy.ndarray



In [21]:
```
with dask.config.set(scheduler="threads"):
    xo = x.compute()
```

In [22]:
```
xo
```

Out[22]:
```
array([1, 2])
```

In [23]:
```
dask.config.get("scheduler")
```

Out[23]:
```
'dask.distributed'
```

In [25]:
```
x.compute(sheduler="threads")
```

Out[25]:
```
array([1, 2])
```

更多关于分布式调度器的使用可参阅文档:

[Deploy Dask Clusters — Dask documentation]

性能对比

In [7]:
```
%%time
rng = np.random.default_rng(42)
x = rng.normal(10, 0.1, size=(20000, 20000))
y = x.mean(axis=0)[::100]
```

```
CPU times: user 8.14 s, sys: 894 ms, total: 9.03 s
Wall time: 9.48 s
```

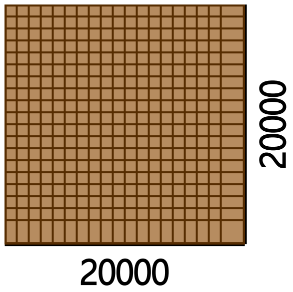
In [8]:
```
%%time
x = da.random.normal(
    10, 0.1, size=(20000, 20000), chunks=(1000, 1000)
)
y = x.mean(axis=0)[::100]
o = y.compute()
```

```
CPU times: user 26.1 s, sys: 596 ms, total: 26.7 s
Wall time: 8.75 s
```

In [9]:
```
x
```

Out[9]:

	Array	Chunk
Bytes	2.98 GiB	7.63 MiB
Shape	(20000, 20000)	(1000, 1000)
Count	400 Tasks	400 Chunks
Type	float64	numpy.ndarray



Dask完成的更快，但使用了更多的总CPU时间。

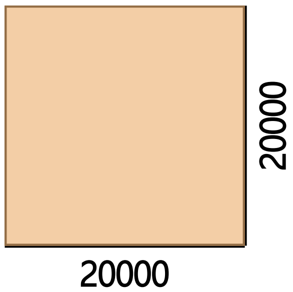
In [43]:
```
%%time
x = da.random.normal(
    10, 0.1, size=(20000, 20000), chunks=(20000, 20000)
)
y = x.mean(axis=0)[::100]
o = y.compute()
```

```
CPU times: user 39.3 s, sys: 8.38 s, total: 47.7 s
Wall time: 59.3 s
```

In [44]:
```
x
```

Out[44]:

	Array	Chunk
Bytes	2.98 GiB	2.98 GiB
Shape	(20000, 20000)	(20000, 20000)
Count	1 Tasks	1 Chunks
Type	float64	numpy.ndarray



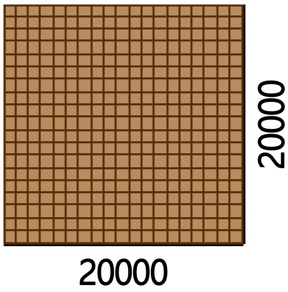
In [41]:
```
%%time
x = da.random.normal(
    10, 0.1, size=(20000, 20000), chunks=(25, 25)
)
y = x.mean(axis=0)[::100]
o = y.compute()
```

```
CPU times: user 3min 30s, sys: 36.4 s, total: 4min 7s
Wall time: 4min 16s
```

In [39]:
```
x
```

Out[39]:

	Array	Chunk
Bytes	2.98 GiB	4.88 kiB
Shape	(20000, 20000)	(25, 25)
Count	640000 Tasks	640000 Chunks
Type	float64	numpy.ndarray



Xarray

文档：xarray: N-D labeled arrays and datasets in Python

xarray在原始的类NumPy数组之上以维度、坐标和属性的形式引入标签，从而提供更直观、更简洁且不易出错的开发体验。

与之相关的工具包可参见：

Installation

xarray有两个核心的数据结构，它们构建在NumPy和Pandas之上，并进行了扩展，都是多维的：

- DataArray：有标签的N维数组
- Dataset：多维内存数组数据库

In [2]:
```
import xarray as xr
xr.__version__
```

Out[2]:
```
'2022.3.0'
```

创建

In [106…
```
rng = np.random.default_rng(42)
a = rng.normal(size=(2,3))
a
```

Out[106…
```
array([[ 0.30471708, -1.03998411,  0.7504512 ],
       [ 0.94056472, -1.95103519, -1.30217951]])
```

In [107…
```
data = xr.DataArray(a, dims=("x", "y"), coords={"x": [10, 20]})
```

In [108…
```
data
```

Out[108… xarray.DataArray (**x**: 2, y: 3)

array([[0.30471708, -1.03998411, 0.7504512],
       [0.94056472, -1.95103519, -1.30217951]])

▼ Coordinates:

x	(x)	int64	10 20

► Attributes: (0)

In [109…
```
data.x
```

Out[109… xarray.DataArray 'x' (**x**: 2)

array([10, 20])

▼ Coordinates:

x	(x)	int64	10 20

► Attributes: (0)

In [110…
```
data.y
```

Out[110… xarray.DataArray 'y' (y: 3)

array([0, 1, 2])

► Coordinates: (0)

► Attributes: (0)

In [111…
```
data.values
```

Out[111…
```
array([[ 0.30471708, -1.03998411,  0.7504512 ],
       [ 0.94056472, -1.95103519, -1.30217951]])
```

In [112…
```
data.dims
```

Out[112…
```
('x', 'y')
```

In [113…
```
data.coords
```

Out[113…
```
Coordinates:
  * x        (x) int64 10 20
```

In [114…
```
data.attrs
```

Out[114…
```
{}
```

In [115…
```
data.x.values
```

Out[115…
```
array([10, 20])
```

In [116…
```
data.y.values
```

Out[116… array([0, 1, 2])

索引

In [60]:
```
data[0,:]
```

Out[60]: xarray.DataArray (y: 3)

array([0.30471708, -1.03998411, 0.7504512])

▼ Coordinates:

x	()	int64	10

► Attributes: (0)

In [63]:
```
data.loc[10]
```

Out[63]: xarray.DataArray (y: 3)

array([0.30471708, -1.03998411, 0.7504512])

▼ Coordinates:

x	()	int64	10

► Attributes: (0)

In [68]:
```
data.loc[0]
```

```
---------------------------------------------------------------------------
KeyError                                  Traceback (most recent call last)
/usr/local/lib/python3.8/site-packages/pandas/core/indexes/base.py in get_loc(sel
f, key, method, tolerance)
   3620             try:
-> 3621                 return self._engine.get_loc(casted_key)
   3622             except KeyError as err:

/usr/local/lib/python3.8/site-packages/pandas/_libs/index.pyx in pandas._libs.ind
ex.IndexEngine.get_loc()

/usr/local/lib/python3.8/site-packages/pandas/_libs/index.pyx in pandas._libs.ind
ex.IndexEngine.get_loc()

pandas/_libs/hashtable_class_helper.pxi in pandas._libs.hashtable.Int64HashTable.
get_item()

pandas/_libs/hashtable_class_helper.pxi in pandas._libs.hashtable.Int64HashTable.
get_item()

KeyError: 0

The above exception was the direct cause of the following exception:

KeyError                                  Traceback (most recent call last)
<ipython-input-68-0dc99c936dd2> in <module>
----> 1 data.loc[0]

/usr/local/lib/python3.8/site-packages/xarray/core/dataarray.py in __getitem__(se
lf, key)
    197             labels = indexing.expanded_indexer(key, self.data_array.ndim)
    198             key = dict(zip(self.data_array.dims, labels))
--> 199         return self.data_array.sel(key)
    200 
    201     def __setitem__(self, key, value) -> None:

/usr/local/lib/python3.8/site-packages/xarray/core/dataarray.py in sel(self, inde
xers, method, tolerance, drop, **indexers_kwargs)
   1327         Dimensions without coordinates: points
   1328         """
-> 1329         ds = self._to_temp_dataset().sel(
   1330             indexers=indexers,
   1331             drop=drop,

/usr/local/lib/python3.8/site-packages/xarray/core/dataset.py in sel(self, indexe
rs, method, tolerance, drop, **indexers_kwargs)
   2499         """
   2500         indexers = either_dict_or_kwargs(indexers, indexers_kwargs, "se
l")
-> 2501         pos_indexers, new_indexes = remap_label_indexers(
   2502             self, indexers=indexers, method=method, tolerance=tolerance
   2503         )

/usr/local/lib/python3.8/site-packages/xarray/core/coordinates.py in remap_label_
indexers(obj, indexers, method, tolerance, **indexers_kwargs)
    419     }
    420 
--> 421     pos_indexers, new_indexes = indexing.remap_label_indexers(
    422         obj, v_indexers, method=method, tolerance=tolerance
    423     )
```

```
/usr/local/lib/python3.8/site-packages/xarray/core/indexing.py in remap_label_ind
exers(data_obj, indexers, method, tolerance)
    119     for dim, index in indexes.items():
    120         labels = grouped_indexers[dim]
--> 121         idxr, new_idx = index.query(labels, method=method, tolerance=tole
rance)
    122         pos_indexers[dim] = idxr
    123         if new_idx is not None:

/usr/local/lib/python3.8/site-packages/xarray/core/indexes.py in query(self, labe
ls, method, tolerance)
    239                             )
    240                         else:
--> 241                             indexer = self.index.get_loc(label_value)
    242                 elif label.dtype.kind == "b":
    243                     indexer = label

/usr/local/lib/python3.8/site-packages/pandas/core/indexes/base.py in get_loc(sel
f, key, method, tolerance)
   3621                     return self._engine.get_loc(casted_key)
   3622                 except KeyError as err:
-> 3623                     raise KeyError(key) from err
   3624                 except TypeError:
   3625                     # If we have a listlike key, _check_indexing_error will r
aise

KeyError: 0
```

In [70]:
```
# integer select
data.isel(x=0)
```

Out[70]: xarray.DataArray (y: 3)

array([0.30471708, -1.03998411, 0.7504512])

▼ Coordinates:

x	()	int64	10

► Attributes: (0)

In [71]:
```
data.isel(y=0)
```

Out[71]: xarray.DataArray (**x**: 2)

array([0.30471708, 0.94056472])

▼ Coordinates:

x	(x)	int64	10 20

► Attributes: (0)

In [73]:
```
# 直接select
data.sel(x=10)
```

Out[73]: xarray.DataArray (y: 3)

array([0.30471708, -1.03998411, 0.7504512])

▼ Coordinates:

x	()	int64	10

► Attributes: (0)

更多介绍可参阅：

Indexing and selecting data

属性

在设置DataArray时，设置元数据属性通常是个不错的实践。常见的属性包括 `long_name`， `units` 等。

In [117…
```
data.attrs["long_name"] = "random velocity"
data.attrs["units"] = "metres/sec"
data.attrs["description"] = "A random variable created as an example."
```

In [118…
```
data
```

Out[118… xarray.DataArray (**x**: 2, y: 3)

```
array([[ 0.30471708, -1.03998411,  0.7504512 ],
       [ 0.94056472, -1.95103519, -1.30217951]])
```

▼ Coordinates:

x	(x)	int64	10 20

▼ Attributes:

long_name : random velocity
units : metres/sec
description : A random variable created as an example.

In [119…
```
data.attrs
```

Out[119…
```
{'long_name': 'random velocity',
 'units': 'metres/sec',
 'description': 'A random variable created as an example.'}
```

In [120…
```
# 给坐标设置属性
data.x.attrs["units"] = "x units"
```

In [121…
```
data.x
```

Out[121…] xarray.DataArray 'x' (**x**: 2)

array([10, 20])

▼ Coordinates:

x	(x)	int64	10 20

▼ Attributes:

units : x units

计算

In [94]:
```
data + 10
```

Out[94]: xarray.DataArray (**x**: 2, y: 3)

array([[10.30471708, 8.96001589, 10.7504512],
       [10.94056472, 8.04896481, 8.69782049]])

▼ Coordinates:

x	(x)	int64	10 20

► Attributes: (0)

In [95]:
```
np.sin(data)
```

Out[95]: xarray.DataArray (**x**: 2, y: 3)

array([[0.3000233 , -0.86239618, 0.68196883],
       [0.80789103, -0.92857601, -0.96413891]])

▼ Coordinates:

x	(x)	int64	10 20

▼ Attributes:

long_name : random velocity
units : metres/sec
description : A random variable created as an example.

In [96]:
```
data.T
```

Out[96]: xarray.DataArray (y: 3, **x**: 2)

array([[0.30471708, 0.94056472],
       [-1.03998411, -1.95103519],
       [0.7504512 , -1.30217951]])

▼Coordinates:

x	(x)	int64	10 20

▼Attributes:

long_name : random velocity
units : metres/sec
description : A random variable created as an example.

In [97]:
```
data.sum()
```

Out[97]: xarray.DataArray

array(-2.29746581)

► Coordinates: (0)

► Attributes: (0)

In [98]:
```
data.mean(dim="x")
```

Out[98]: xarray.DataArray (y: 3)

array([0.6226409 , -1.49550965, -0.27586416])

► Coordinates: (0)

► Attributes: (0)

与NumPy对比一下:

In [100…
```
data.mean(axis=0)
```

Out[100…: xarray.DataArray (y: 3)

array([0.6226409 , -1.49550965, -0.27586416])

► Coordinates: (0)

► Attributes: (0)

In [99]:
```
data.mean(dim="y")
```

Out[99]: xarray.DataArray (**x**: 2)

array([0.00506139, -0.77088333])

▼ Coordinates:

x	(x)	int64	10 20

► Attributes: (0)

基于维度名称的广播（不需要插入虚拟尺寸进行对齐）：

In [15]:
```
[data.coords["y"]]
```

Out[15]:
```
[<xarray.DataArray 'y' (y: 3)>
 array([0, 1, 2])
 Dimensions without coordinates: y]
```

In [28]:
```
rng = np.random.default_rng(42)
a = xr.DataArray(rng.integers(0, 10, 3), [data.coords["y"]])
b = xr.DataArray(rng.integers(0, 10, 4), dims="z")
```

In [29]:
```
a
```

Out[29]: xarray.DataArray (**y**: 3)

array([0, 7, 6])

▼ Coordinates:

y	(y)	int64	0 1 2

► Attributes: (0)

In [30]:
```
b
```

Out[30]: xarray.DataArray (z: 4)

array([4, 4, 8, 0])

► Coordinates: (0)

► Attributes: (0)

In [31]:
```
a + b
```

Out[31]: xarray.DataArray (**y**: 3, z: 4)

```
array([[ 4,  4,  8,  0],
       [11, 11, 15,  7],
       [10, 10, 14,  6]])
```

▼ Coordinates:

y	(y)	int64	0 1 2

► Attributes: (0)

In [32]:
```
a.values + b.values
```

```
---------------------------------------------------------------------------
ValueError                                Traceback (most recent call last)
<ipython-input-32-db9ccfe54ec4> in <module>
----> 1 a.values + b.values

ValueError: operands could not be broadcast together with shapes (3,) (4,)
```

意味着大多数情况下不需要担心维度顺序：

In [13]:
```
data.shape
```

Out[13]:
```
(2, 3)
```

In [12]:
```
data - data.T
```

Out[12]: xarray.DataArray (**x**: 2, y: 3)

```
array([[0., 0., 0.],
       [0., 0., 0.]])
```

▼ Coordinates:

x	(x)	int64	10 20

► Attributes: (0)

更多可参阅：

Computation

GroupBy

In [82]:
```
rng = np.random.default_rng(42)
a = xr.DataArray(rng.integers(1, 10, (2, 3)), dims=("x", "y"))
a
```

Out[82]: xarray.DataArray (x: 2, y: 3)

```
array([[1, 7, 6],
       [4, 4, 8]])
```

► Coordinates: (0)

► Attributes: (0)

In [83]:
```python
labels = xr.DataArray(["E", "F", "E"], dims="y", name="labels")
labels
```

Out[83]: xarray.DataArray 'labels' (y: 3)

```
array(['E', 'F', 'E'], dtype='<U1')
```

► Coordinates: (0)

► Attributes: (0)

In [85]:
```python
a.groupby(labels).mean("y")
```

Out[85]: xarray.DataArray (x: 2, **labels**: 2)

```
array([[3.5, 7. ],
       [6. , 4. ]])
```

▼ Coordinates:

labels	(labels)	object	'E' 'F'

► Attributes: (0)

In [86]:
```python
a.groupby(labels).mean("x")
```

Out[86]: xarray.DataArray (y: 3)

```
array([2.5, 5.5, 7. ])
```

► Coordinates: (0)

► Attributes: (0)

In [87]:
```python
# 1 4 6 8 一组
# 7 4 一组
a.groupby(labels).map(lambda x: x - x.min())
```

Out[87]: xarray.DataArray (x: 2, y: 3)

array([[0, 3, 5],
       [3, 0, 7]])

► Coordinates: (0)

► Attributes: (0)

可视化

In [125…
```
rng = np.random.default_rng(42)
a = xr.DataArray(
    rng.integers(1, 10, (2, 3)),
    dims=("x", "y"),
    coords={"x": [10, 20], "y": [10, 20, 30]},
    attrs={
        "long_name": "random integers",
        "units": "null",
        "description": "demo random"
    }
)
```

In [126…
```
a.x.attrs["units"] = "x 10-20"
```

In [127…
```
a
```

Out[127… xarray.DataArray (**x**: 2, **y**: 3)

array([[1, 7, 6],
       [4, 4, 8]])

▼ Coordinates:

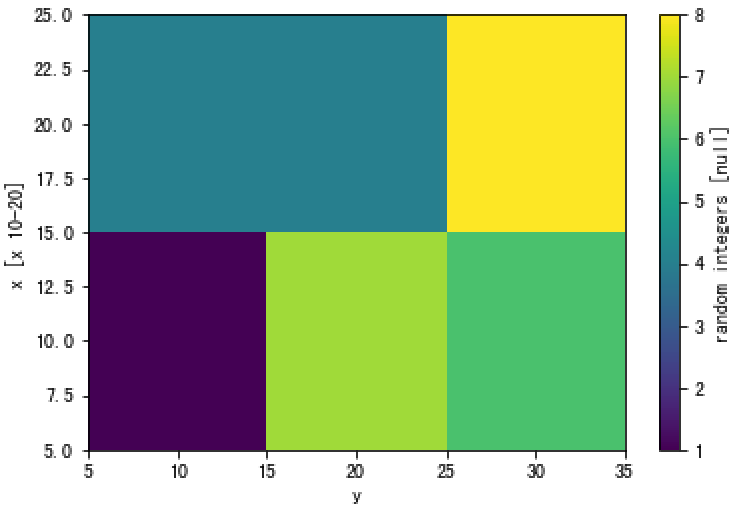
x	(x)	int64	10 20
y	(y)	int64	10 20 30

▼ Attributes:

long_name : random integers
units : null
description : demo random

In [128…
```
a.plot()
```

Out[128…
```
<matplotlib.collections.QuadMesh at 0x11b0604f0>
```



小结

In [ ]:

参考

- Beyond Numpy Arrays in Python

In [ ]: