

lecture4

May 7, 2019

1 Lecture 4

- Sampling
- Automatic gradient
- Parallel computing on GPUs
- Cython

```
In [2]: import numpy as np
import numpy.random as rnd
import matplotlib
import matplotlib.pyplot as plt
%matplotlib inline
```

1.1 Sampling

Draw random samples from a uniform distribution.

```
In [3]: rnd.uniform?
```

```
In [4]: U = rnd.uniform(-1,1, size = 500)
print(U.shape)
print("Mean: {:.03f} var: {:.02f}".format(U.mean(), U.var()))

(500,)
Mean: 0.006 var: 0.31
```

Draw random samples from a normal (Gaussian) distribution.

```
In [5]: rnd.normal?
```

```
In [6]: G = rnd.normal(loc = 1, scale = 10, size = [1000,2])
print(G.shape)
print("Mean: [{:.03f},{:.03f}].format(*np.mean(G,0)))

(1000, 2)
Mean: [0.950,0.889]
```

```
In [7]: num_bins = 30
```

```
nums,ranges = np.histogram(U, bins = num_bins)
```

```
print(nums)
```

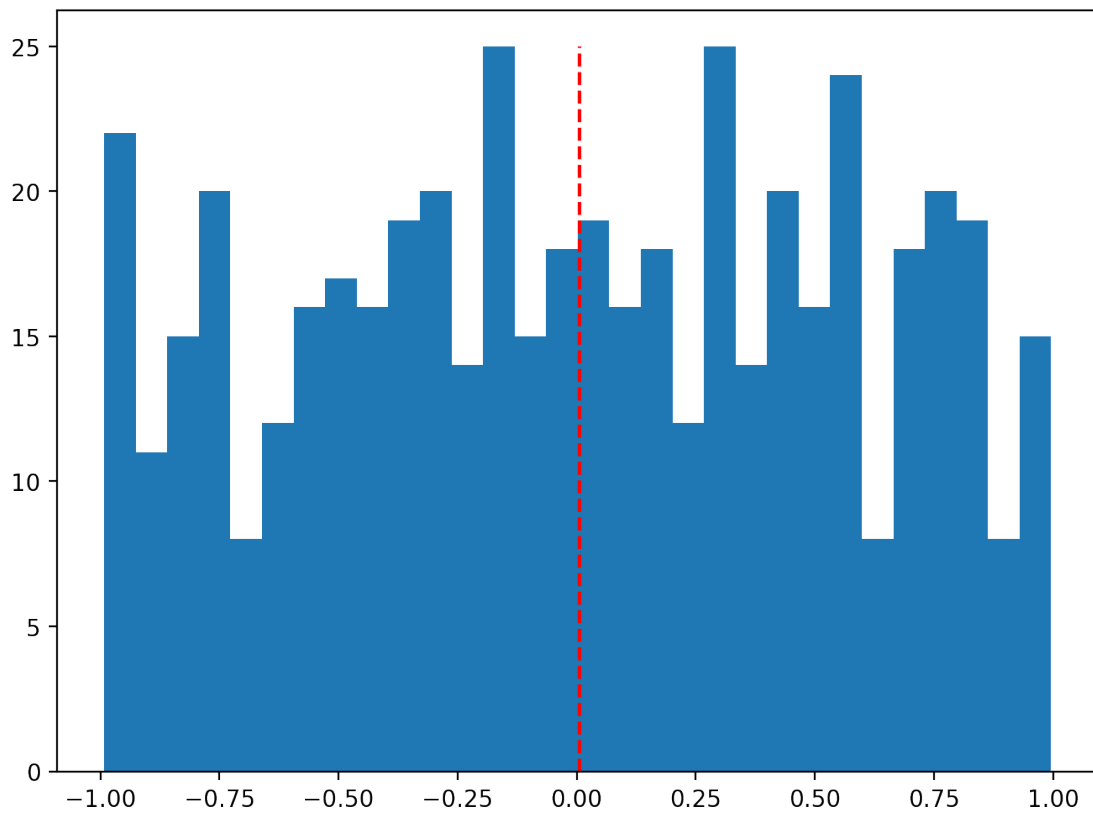
```
print(ranges)
```

```
plt.figure(figsize=(8,6), dpi=200)
```

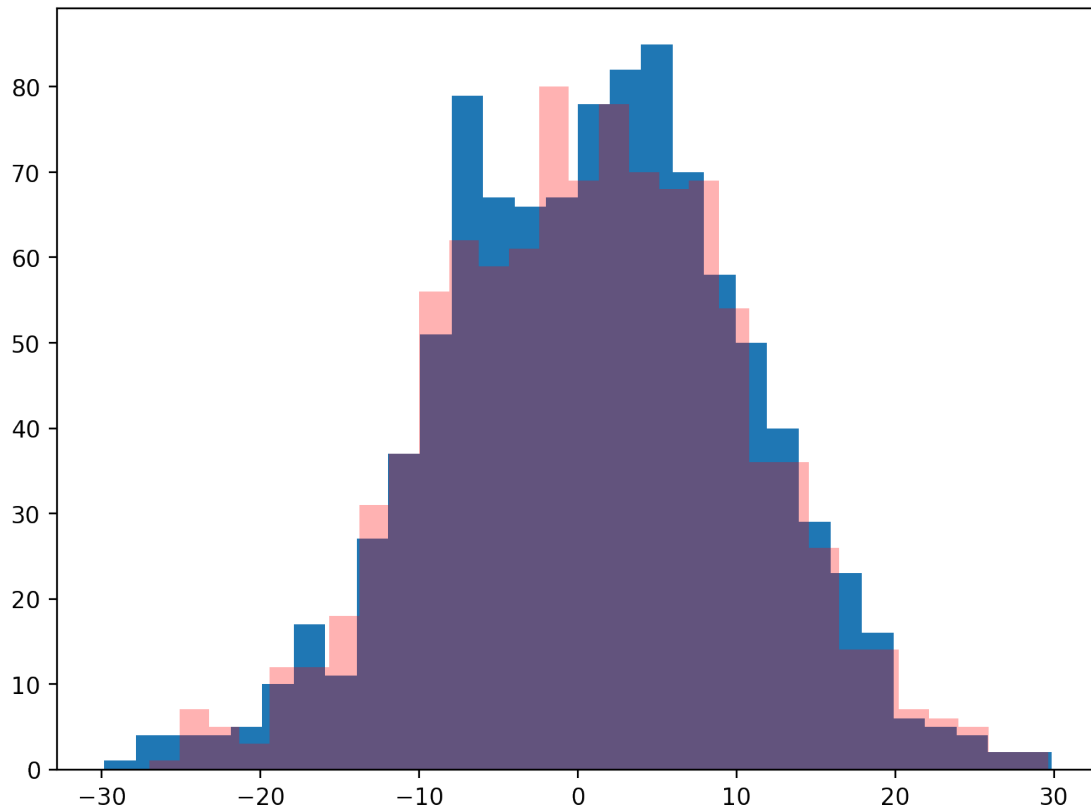
```
_ = plt.hist(U, bins=num_bins)
```

```
_ = plt.plot([U.mean()]*2,[0, np.max(nums)], '--', color='r') # plot dashed mean line
```

```
[22 11 15 20  8 12 16 17 16 19 20 14 25 15 18 19 16 18 12 25 14 20 16 24
 8 18 20 19  8 15]
[-0.99190391 -0.92563863 -0.85937334 -0.79310806 -0.72684277 -0.66057749
-0.5943122  -0.52804692 -0.46178164 -0.39551635 -0.32925107 -0.26298578
-0.1967205  -0.13045521 -0.06418993  0.00207535  0.06834064  0.13460592
 0.20087121  0.26713649  0.33340178  0.39966706  0.46593234  0.53219763
 0.59846291  0.6647282  0.73099348  0.79725877  0.86352405  0.92978934
 0.99605462]
```



```
In [8]: plt.figure(figsize=(8,6), dpi=200)
_ = plt.hist(G[:,0], bins=30)
_ = plt.hist(G[:,1], bins=30, alpha=0.3, color = 'r')
```



Let's draw some random samples from a multinomial distribution. We'll use our fruits from the first lecture.



```
In [9]: fruits = np.array([
    'watermelon',
    'apple',
    'grape',
    'grapefruit',
    'lemon',
    'banana',
    'cherry'
])

In [10]: n = 5 # number of samples
p = [1/len(fruits)]*len(fruits)
```

```

repeat = np.tile(fruits, (n,1)) # repeat multiple (5) times
print(repeat)

m1t = rnd.multinomial(1, p, size=(5)) # draw multinomial samples 5 times with an equal probability
print(m1t)

samples =repeat[m1t.astype(bool)] # show drawn samples
print(samples)

[['watermelon' 'apple' 'grape' 'grapefruit' 'lemon' 'banana' 'cherry']
 ['watermelon' 'apple' 'grape' 'grapefruit' 'lemon' 'banana' 'cherry']
 ['watermelon' 'apple' 'grape' 'grapefruit' 'lemon' 'banana' 'cherry']
 ['watermelon' 'apple' 'grape' 'grapefruit' 'lemon' 'banana' 'cherry']
 ['watermelon' 'apple' 'grape' 'grapefruit' 'lemon' 'banana' 'cherry']]
[[0 0 0 1 0 0]
 [0 0 0 0 1 0]
 [0 0 0 0 1 0]
 [0 0 1 0 0 0]
 [0 0 0 0 1 0]]
['lemon' 'banana' 'banana' 'grape' 'banana']

In [11]: p = [0.05, 0.70, 0.05, 0.05, 0.05, 0.05, 0.05] # adjust probabilities

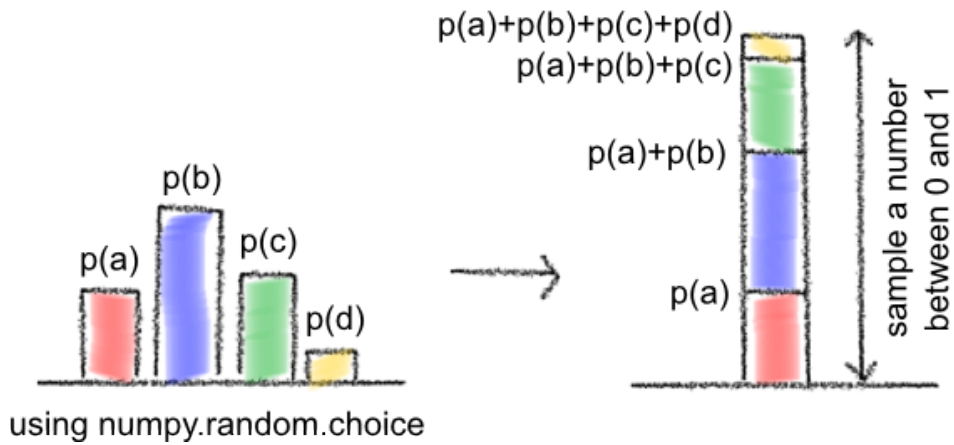
m2t = rnd.multinomial(1, p, size=(5)) # draw multinomial samples 5 times with given probabilities
print(m2t)

samples =repeat[m2t.astype(bool)] # show drawn samples
print(samples)

[[0 1 0 0 0 0 0]
 [0 1 0 0 0 0 0]
 [0 1 0 0 0 0 0]
 [0 1 0 0 0 0 0]
 [0 1 0 0 0 0 0]]
['apple' 'apple' 'apple' 'apple' 'apple']

```

1.1.1 Another way to make discrete choices



```
In [12]: p = [0.05, 0.70, 0.05, 0.05, 0.05, 0.05, 0.05]
```

```
# Cumulate them
l = np.cumsum([0] + p[:-1]) # lower-bounds
h = np.cumsum(p)             # upper-bounds
```

```
print(l)
print(h)
```

```
# Draw a number between 0 and 1
u = np.random.uniform(0, 1)
```

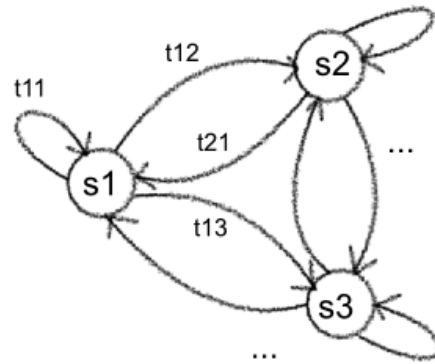
```
# Find which basket it belongs to
s = np.logical_and(u > l, u < h)
print(s)
```

```
# retrieve the label
fruits[np.argmax(s)]
```

```
[0.  0.05 0.75 0.8  0.85 0.9  0.95]
[0.05 0.75 0.8  0.85 0.9  0.95 1.  ]
[False True False False False False]
```

```
Out[12]: 'apple'
```

1.2 Markov Chain



A Markov chain transits between a set of states, where the transition between pairs of states is associated with a fixed probability. The set of probabilities can be stored in a transition matrix.

```
In [13]: # Transition matrix
```

```
T = np.array([
    [0.9,0.1,0.0], # transiting from state 1 to state 1,2,3
    [0.0,0.9,0.1], # transiting from state 2 to state 1,2,3
    [1.0,0.0,0.0], # transiting from state 3 to state 1,2,3
])
```

```
In [14]: # Add empty state to transition matrix
```

```
pad_shape = ((0, 0), (1, 0)) # ((before_1, after_1), (before_2, after_2))
P = np.pad(T, pad_shape, mode='constant')
print(P)
```

```
[[0.  0.9 0.1 0. ]
 [0.  0.  0.9 0.1]
 [0.  1.  0.  0. ]]
```

```
In [15]: def mcstep(X, P):
```

```
    Xp = np.dot(X, P)
    Xc = np.cumsum(Xp, axis=1)
    L,H = Xc[:, :-1], Xc[:, 1:]
    R = np.random.uniform(0, 1, (len(Xp), 1))
    states = np.logical_and((R > L), (R < H))
    #print(states.astype('int32'))
    return states.astype('int32')
```

```
In [17]: A = np.tile([1.0,0,0], (5,1))
```

```
# or
```

```
A = np.outer(np.ones([5]),[1.0,0,0]) # (5,1) x (1,3) -> (5,3)
```

```
num_steps = 10
```

```
for i in range(num_steps):
    A = mcstep(A, P)
```

```
A.mean(axis=0)
```

```
Out[17]: array([0.6, 0.4, 0. ])
```

1.3 Autograd

(<https://github.com/HIPS/autograd>)

```
In [21]: import autograd.numpy as ag_np
         from autograd import grad
         x = ag_np.ones(1)
         y = lambda x: 3 * x**2 + 2
         print(grad(y)(x))
```

```
float64
[6.]
```

```
In [22]: x1 = ag_np.ones(1)
         x2 = ag_np.ones(1)

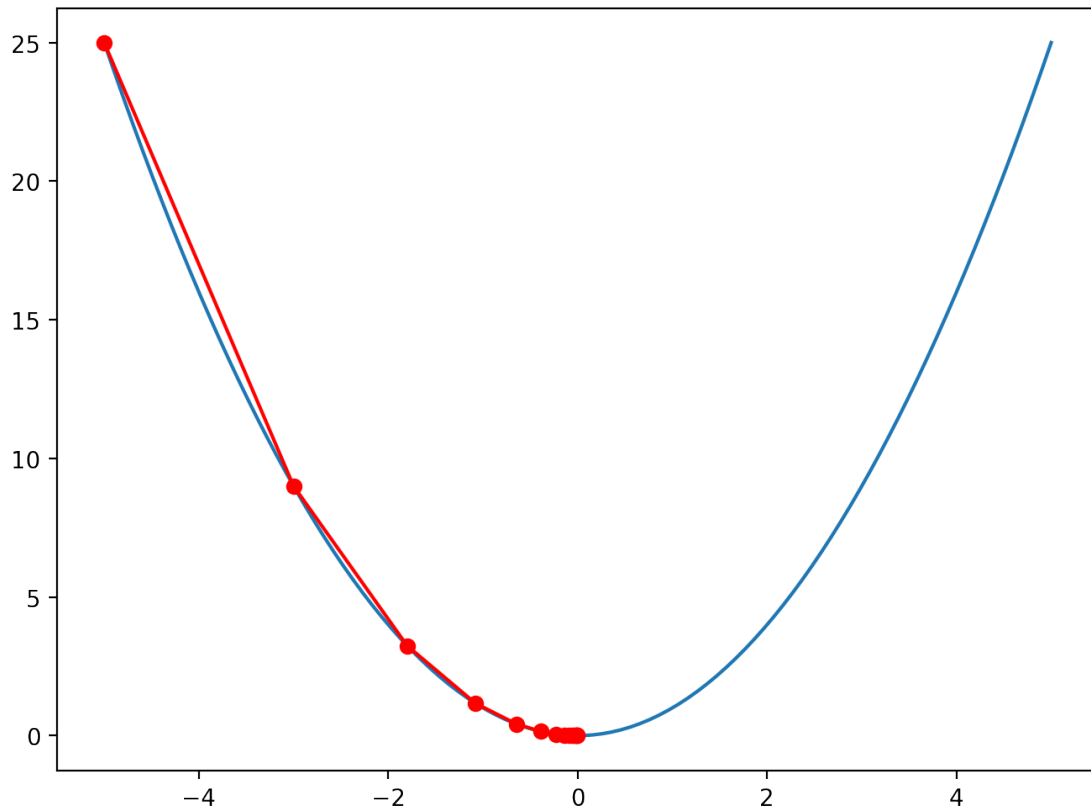
         y = lambda x1,x2 : 3*x1**3 + 4*2**x2

         print(grad(y,0)(x1,x2))
         print(grad(y,1)(x1,x2)) # 4*2**x2*ln(x2)

[9.]
[5.54517744]
```

```
In [26]: y = lambda x: x**2
         step_size = 0.2
         xs = np.array([-5.0])
         while abs(grad(y)(xs[-1])) > 1e-2:
             curr_val = xs[-1]
             next_val = curr_val - step_size*grad(y)(curr_val)
             xs = np.append(xs, next_val)
```

```
In [27]: x = np.linspace(-5, 5, 100)
         plt.figure(figsize=(8,6), dpi=200)
         _ = plt.plot(x,y(x))
         _ = plt.plot(xs, y(xs), "-o", c="r")
```



1.4 GPUs

(<https://github.com/cupy/cupy>)

```
In [36]: import numpy as np
         from time import time
         n = 1000
         X = np.random.normal(size = (n,n))
         Y = np.random.normal(size = (n,n))
         %timeit X.dot(Y)
```

5.64 ms ± 108 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)

```
In [37]: import cupy as cp
         X = cp.array(X)
         Y = cp.array(Y)
         %timeit X.dot(Y)
```

571 µs ± 346 ns per loop (mean ± std. dev. of 7 runs, 10000 loops each)

1.5 Cython

- Create new file *hello.pyx*. See the example file (*hello.pyx*) in the same Folder. The file contains a custom implementation of the matrix product with loops

Cython *hello.pyx* file `cimport cython import numpy as np cimport openmp from cython.parallel cimport prange`

```
@cython.boundscheck(False) @cython.wraparound(False)
cpdef dot(float[:, :] X, float[:, :] Y): cdef: int n,i,j,k float[:, :] Z n = X.shape[0] Z = np.zeros((n,n),
dtype = 'float') n = len(X) for i in prange(n, nogil = True): for j in range(n): for k in range(n): Z[i,j]
+= X[i, k] * Y[k, j] return Z
```

- Create *setup.py* with compiler commands in order to build a new python package. See example file in the same folder

setup.py file `from distutils.core import setup from Cython.Build import cythonize from distutils.extension import Extension from Cython.Distutils import build_ext`

```
setup( name = "hello", cmdclass = {"build_ext": build_ext}, ext_modules = [ Extension("hello",
["hello.pyx"], extra_compile_args = ["-O0", "-fopenmp"], extra_link_args=['-fopenmp'] ) ] )
```

Compile the *hello.pyx* file with the following command from terminal. * *python setup.py build_ext -inplace*

After your module is compiled you can import it into your notebook as usual

You can profile your cython code in order to know, either your computations are made efficiently. For the reason you may create an HTML file highlighting the line with the bad performance.

Create file profiling snapshot by calling the following command in your terminal * *cython -a hello.pyx*

Then open a new generated *hello.html* file in a browser. The lines colored yellow still need some python interactions and therefore slow, so you can still find a way to optimize them. But for now it's enough to have no yellow lines within the loops.

Generated by Cython 0.29.7

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

Raw output: [hello.c](#)

```
+01: cimport cython
+02: import numpy as np
+03: cimport openmp
+04: from cython.parallel cimport prange
+05:
+06: @cython.boundscheck(False)
+07: @cython.wraparound(False)
+08:
+09: cpdef dot(float[:, :] X, float[:, :] Y):
+10:     cdef:
+11:         int n,i,j,k
+12:         float[:, :] Z
+13:         n = X.shape[0]
+14:         Z = np.zeros((n,n), dtype = 'float')
+15:         n = len(X)
+16:         for i in prange(n, nogil = True):
+17:             for j in range(n):
+18:                 for k in range(n):
+19:                     Z[i,j] += X[i, k] * Y[k, j]
+20:         return Z
```

Import your brand new module as usual

```
In [50]: import hello
```

In []: Test the performance. It

```
In [51]: from time import time
        X = np.array(X.tolist()).astype('float32')
        Y = np.array(X.tolist()).astype('float32')
        %timeit hello.dot(X,Y)
```

783 ms ± 43.9 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)

As you already know normal python loops will take much more time to finish all the computations...

```
In [47]: st = time()
        Z = np.zeros((n,n))
        for i in range(n):
            for j in range(n):
                for k in range(n):
                    Z[i,j] += X[i, k] * Y[k, j]
        print(time() - st)
        print(np.sum(Z))
```

995.5045590400696

6907.071765647259