Lab 14

Numerical Derivatives

Lab Objective: *Understand and implement finite difference approximations of the derivative. Then use finite difference quotients to find edges in images via the Sobel filter.*

Derivative approximations in one dimension

The derivative of a function f at a point x_0 is

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}. \tag{14.1}$$

In this lab we will investigate one way a computer can calculate $f'(x_0)$.

Forward difference quotients

Suppose that in Equation 14.1, instead of taking a limit, we just pick a small value for h. Then we would expect $f'(x_0)$ to be close to the quantity

$$\frac{f(x_0 + h) - f(x_0)}{h}. \tag{14.2}$$

This quotient is called the *first order forward difference approximation* of the derivative. Because $f'(x_0)$ is the limit of such quotients, we expect that when h is small, this quotient is close to $f'(x_0)$. We can use Taylor's formula to find just how close.

By Taylor's formula,

$$f(x_0 + h) = f(x_0) + f'(x_0)h + R_2(h),$$

where $R_2(h) = \left(\int_0^1 (1 - t) f''(x_0 + th) dt\right) h^2$. (This is called the *integral form* of the remainder for Taylor's Theorem; see [ref textbook] for one exposition). When we solve this equation for $f'(x_0)$ we get

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{R_2(h)}{h}. \tag{14.3}$$

Thus, the error in using the first order forward difference quotient to approximate $f'(x_0)$ is

$$\left|\frac{R_2(h)}{h}\right| \leq |h| \int_0^1 |1-t||f''(x_0+th)|dt.$$

If we assume f'' is continuous, then for any δ, set $M = \sup_{x\in(x_0-\delta,x_0+\delta)} f''(x)$. Then if $|h| < \delta$, we have

$$\left|\frac{R_2(h)}{h}\right| \leq |h| \int_0^1 M dt = M|h| = O(h).$$

Therefore, the error in using (14.2) to approximate $f'(x_0)$ grows like h.

Centered difference quotients

In fact, we can approximate $f'(x_0)$ to second order with another difference quotient, called the *centered difference quotient*. Evaluate Taylor's formula at $x_0 - h$ to derive

$$f'(x_0) = \frac{f(x_0) - f(x_0-h)}{h} + \frac{R_2(-h)}{h}. \tag{14.4}$$

The quotient that is the first term of (14.4) is called the *backward difference quotient*. This quotient also approximates $f'(x_0)$ to first order, so it is not the quotient we are looking for. When we add (14.3) and (14.4) and solve for $f'(x_0)$ (by dividing by 2), we get

$$f'(x_0) = \frac{\frac{1}{2}f(x_0+h) - \frac{1}{2}f(x_0-h)}{h} + \frac{R_2(-h) - R_2(h)}{2h} \tag{14.5}$$

The *centered difference quotient* is the first term of the right hand side of (14.5). Let us investigate the remainder term to see how accurate this approximation is. Recall from the proof of Taylor's theorem that $R_k = \frac{f^{(k)}(x_0)}{k!}h^k + R_{k+1}$. Therefore,

$$\begin{aligned}
\frac{R_2(-h) - R_2(h)}{2h} &= \frac{1}{2h}\left(\frac{f''(x_0)}{2}h^2 + R_3(-h) - \frac{f''(x_0)}{2}h^2 - R_3(h)\right) \\
&= \frac{1}{2h}(R_3(-h) - R_3(h)) \\
&= \frac{1}{2h}\left(\left(\int_0^1 \frac{(1-t)^2}{2} f'''(x_0+th)dt\right)h^3 - \left(\int_0^1 \frac{(1-t)^2}{2} f'''(x_0-th)dt\right)h^3\right) \\
&= \left(\int_0^1 \frac{(1-t)^2}{4}(f'''(x_0+th) - f'''(x_0-th))\right)h^2 \\
&= O(h^2)
\end{aligned}$$

once we restrict h to some δ-neighborhood of 0. So the error in using the centered difference quotient to approximate $f'(x_0)$ grows like h^2, which is smaller than h when $|h| < 1$.

Accuracy of approximations

Let us discuss what step size h we should plug into the difference quotients to get the best approximation to $f'(x_0)$. Since f' is defined as a limit as $h \to 0$, you may

h	1e-1	1e-3	1e-5	1e-7	1e-9	1e-11
Error	5e-3	5e-7	6e-11	6e-11	7e-9	1e-5

Table 14.1: This table shows that it is best not to choose h too small when you approximate derivatives with difference quotients. Here, "Error" equals the absolute value of $f'(1) - f_{app}(1)$ where $f(x) = e^x$ and f_{app} is the centered difference approximation to f'.

think that it is best to choose h as small as possible. In fact, dividing by very small numbers causes errors in floating point arithmetic. This means that as we decrease $|h|$, the error between $f'(x_0)$ and the difference quotient will first decrease, but then increase when $|h|$ gets too small.

Let us do an example with the function $f(x) = e^x$. A quick way to write f as a function in Python is with the `lambda` keyword.

```
>>> import numpy as np
>>> from matplotlib import pyplot as plt
>>> f = lambda x: np.exp(x)
```

In general, the line `f = lambda <params> : <expression>` is equivalent to defining a function `f` that accepts the parameters `params` and returns `expression`. Next we fix a step size `h` and define an approximation to the derivative of `f` using the centered difference quotient.

```
>>> h = 1e-1
>>> Df_app = lambda x: .5*(f(x+h)-f(x-h))/h
```

Finally, we check the accuracy of this approximation at $x_0 = 1$ by computing the difference between `Df_app(1)` and the actual derivative evaluated at 1.

```
# Since f(x) = e^x, the derivative of f(x) is f(x)
>>> np.abs( f(1)-Df_app(1) )
0.0045327354883726301
```

We note that our functions `f` and `Df_app` behave as expected when they are passed a NumPy array.

```
>>> h = np.array([1e-1, 1e-3, 1e-5, 1e-7, 1e-9, 1e-11])
>>> np.abs( f(1)-Df_app(1) )
array([  4.53273549e-03,   4.53046679e-07,   5.85869131e-11,
         5.85873572e-11,   6.60275079e-09,   1.04294937e-05])
```

These results are summarized in Table 14.1.

Thus, the optimal value of h is one that is small, but not too small. A good choice is `h = 1e-5`.

Problem 1. Write a function that accepts as input a callable function object `f`, an array of points `pts`, and a keyword argument `h` that defaults to `1e-5`. Return an array of the centered coefficient difference quotients of `f` at each point in `pts` with the specified value of `h`.

You may wonder if the forward or backward difference quotients are ever used, since the centered difference quotient is a more accurate approximation to the derivative. In fact, there are some functions that in practice do not behave well under centered difference quotients. In these cases one must use the forward or backward difference quotient.

Finally, we remark that forward, backward, and centered difference quotients can be used to approximate higher-order derivatives of f. However, taking derivatives is an *unstable* operation. This means that taking a derivative can amplify the arithmetic error in your computation. For this reason, difference quotients are not generally used to approximate derivatives higher than second order.

Derivative approximations in multiple dimensions

Finite difference methods can also be used to calculate derivatives in higher dimensions. Recall that the Jacobian of a function $f : \mathbb{R}^n \to \mathbb{R}^m$ at a point $x_0 \in \mathbb{R}^n$ is the $m \times n$ matrix $J = (J_{ij})$ defined by

$$J_{ij} = \frac{\partial f_i}{\partial x_j}(x_0).$$

The Jacobian is useful in many applications. For example, we will use the Jacobian in Lab 16 to find zeros of functions in multiple variables.

The forward difference quotient for approximating a partial derivative is

$$\frac{\partial f}{\partial x_i}(x_0) \approx \frac{f(x_0 + he_i) - f(x_0)}{h},$$

where e_i the i^{th} standard basis vector. Similarly, the centered difference approximation is

$$\frac{\partial f}{\partial x_i}(x_0) \approx \frac{\frac{1}{2}f(x_0 + he_i) - \frac{1}{2}f(x_0 - he_i)}{h}.$$

Problem 2.

1. Write a function that accepts
   (a) a function handle `f`,
   (b) an integer that is the dimension of the range of `f`,
   (c) an integer `n` that is the dimension of the domain of `f`,
   (d) an `n`-dimensional NumPy array `pt` representing a point in $\mathbb{R}^n$, and
   (e) an keyword argument `h` that defaults to `1e-5`.

   Return the approximate Jacobian matrix of `f` at `pt` using the centered coefficients difference quotient.

2. Let $f : \mathbb{R}^2 \to \mathbb{R}^2$ be defined by

$$f(x, y) = \begin{pmatrix} e^x \sin(y) + y^3 \\ 3y - \cos(x) \end{pmatrix}$$

Compare your function against the analytically computed derivative on the square $[-1, 1] \times [-1, 1]$ using ten thousand grid points (100 per side). You may apply your function to the points one at a time using a double `for` loop, but you should compute the analytic derivative in one line. What is the maximum error of your function?

Hint: The following code defines the function $f(x, y) = (x^2, x + y)$.

```
# f accepts a length-2 NumPy array
>>> f = lambda x: np.array([x[0]**2, x[0]+x[1]])
```

Application to image filters

Recall that a computer stores an image as a 2-D array of pixel values (i.e., a matrix of intensities). An image filter is a function that transforms an image by operating on it locally. That is, to compute the ij^{th} pixel value in the new image, an image filter uses only the pixels in a small neighborhood of the ij^{th} pixel in the original image.

In this lab, we will use a filter derived from the gradient of an image to find edges in an image.

Convolutions

One example of an image filter is to *convolve* an image with a filter matrix. A filter matrix is a matrix whose height and width are relatively small odd numbers. If the filter matrix is

$$F = \begin{pmatrix} f_{-1,-1} & f_{-1,0} & f_{-1,1} \\ f_{0,-1} & f_{0,0} & f_{0,1} \\ f_{1,-1} & f_{1,0} & f_{1,1} \end{pmatrix},$$

then the convolution of an image A with F is $A * F = (C_{ij})$ where

$$C_{ij} = \sum_{k=-1}^{1} \sum_{\ell=-1}^{1} f_{k\ell} A_{i+k,j+\ell}. \tag{14.6}$$

Say A is an $m \times n$ matrix. Here, we take $A_{ij} = 0$ when $i \notin \{1, \ldots m\}$ or $j \notin \{1, \ldots, n\}$. The value of C_{ij} is a linear combination of the nearby pixel values, with coefficients given by F (see Figure 14.1). In fact, C_{ij} equals the Frobenius inner product of F with the 3×3 submatrix of A centered at ij.

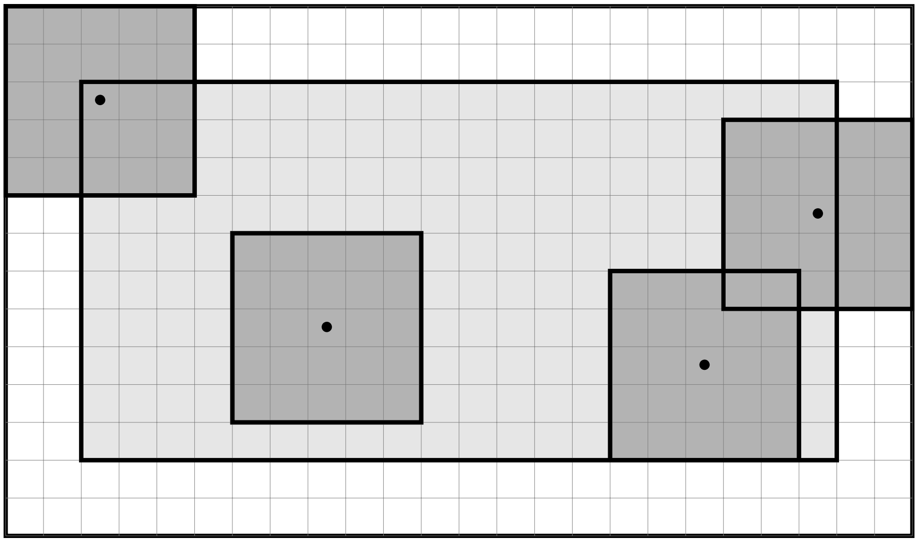


Figure 14.1: This diagram illustrates how to convolve an image with a filter. The light grey rectangle represents the original image A, and the dark grey squares are the filter F. The larger rectangle is the image padded with zeros; i.e., all pixel values in the outer white band are 0. To compute the entry of the convolution matrix C located at a black dot, take the inner product of F with the submatrix of the padded image centered at the dot.

Implementation in NumPy

Let us write a function that convolves an image with a filter. You can test this function on the image `cameraman.jpg`, which appears in Figure 14.2a. The following code loads this image and plots it with matplotlib.

```
>>> K = plt.imread('cameraman.jpg')
>>> plt.imshow(K, cmap = 'gray')
>>> plt.show()
```

Here is the function definition and some setup.

```
1. def Filter(image, filter):
2.     m, n = image.shape
3.     h, k = filter.shape
```

To convolve `image` with `filter`, we must first *pad* the array `image` with zeros around the edges. This is because in (14.6), entries A_{ij} are set to zero when i or j is out of bounds. We do this by creating a larger array of zeros, and then making the interior part of the array equal to the original image (see Figure 14.1).

For example, if the filter is a 3×3 matrix, then the following code will pad the matrix with the appropriate number of zeros.

```
 # Create a larger matrix of zeros
image_pad = np.zeros((m+2, n+2))
# Make the interior of image_pad equal to the original image
```

```
image_pad[1:1+m, 1:1+n] = image
```

We want to do this in general in our function.

```
5.    image_pad = # Create an array of zeros of the appropriate size
7.   # Make the interior of image_pad equal to image
```

Finally, we iterate through the image to compute each entry of the convolution matrix.

```
8.    C = np.empty_like(image)
9.    for i in xrange(n):
10.       for j in xrange(m):
11.           C[i, j] = # Compute C[i, j]
```

Problem 3.

1. Finish writing the function `Filter` by filling in lines 5, 7, and 10.
2. SciPy has a function that convolves two matrices just like `Filter`. Load this function with the command `from scipy.signal import convolve2d`. Then, convolve an image `img` with a filter `F` by typing `convolve2d(img, F)`. Test this function on `cameraman.jpg`.

Gaussian blur

A *Gaussian blur* is an image filter that operates on an image by convolving with the matrix

$$G = \frac{1}{159}\begin{pmatrix} 2 & 4 & 5 & 4 & 2 \\ 4 & 9 & 12 & 9 & 4 \\ 5 & 12 & 15 & 12 & 5 \\ 4 & 9 & 12 & 9 & 4 \\ 2 & 4 & 5 & 4 & 2 \end{pmatrix}.$$

We can use the function `Filter` that we wrote in Problem 3 to apply a Gaussian blur to the image `cameraman.jpg`. The result is in Figure 14.2b. Blurring an image can remove "noise", or random variation that is the visual analog of static in a radio signal (and equally undesirable).

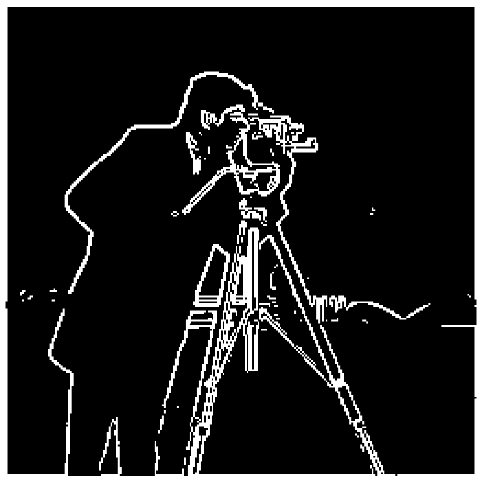
Edge detection

Automatically detecting edges in an image can be used to segment or sharpen the image. We will find edges with the Sobel filter, which computes the gradient of the image at each pixel. The magnitude of the gradient tells us the rate of change of the pixel values, and so large magnitudes should correspond to edges within the image. The Sobel filter is not a convolution, although it does use convolutions.

We can think of an image as a function from a 2×2 grid of points to $\mathbb{R}$. The image maps a pixel location to an intensity. It does not make sense to define the

(a) Unfiltered image.

(b) Image after Gaussian blur is applied.



(c) Image after the Sobel filter is applied.

Figure 14.2: Here is an example of a Gaussian blur and the Sobel filter applied to an image. This photo, known as "cameraman," is a standard test image in image processing. A database of such images can be downloaded from `http://www.imageprocessingplace.com/root_files_V3/image_databases.htm`.

derivative of this function as a limit because the domain is discrete—a step size h cannot take on arbitrarily small values. Instead, we *define* the derivative to be the centered difference quotient of the previous section. That is, we define the derivative in the x-direction at the ij^{th} pixel to be

$$\frac{1}{2}A_{i+1,j} - \frac{1}{2}A_{i-1,j}.$$

We can use a convolution to create a matrix A_x whose ij^{th} entry is the derivative of A at the ij^{th} entry, in the x-direction. In fact, $A_x = A * S$, where

$$S = \frac{1}{8}\begin{pmatrix} -1 & 0 & 1 \\ -2 & 0 & 2 \\ -1 & 0 & 1 \end{pmatrix}.$$

Note that this convolution takes a weighted average of the x-derivatives at (i, j), $(i, j+1)$, and $(i, j-1)$. The derivative at (i, j) is weighted by 2. Using a weighted average instead of just the derivative at (i, j) makes the derivative less affected by noise.

Now we can define the Sobel filter. A Sobel filter applied to an image A results in an array $B = (B_{ij})$ of 0's and 1's, where the 1's trace out the edges in the image. By definition,

$$B_{ij} = \begin{cases} 1 & \text{if } \|\nabla A(ij)\|_2 > M \\ 0 & \text{otherwise.} \end{cases}$$

Here, $\nabla A(ij) = ((A * S)_{ij}, (A * S^T)_{ij})$ is the gradient of A at the ij^{th} pixel. The constant M should be "sufficiently large" enough to pick out those pixels with the largest gradient (i.e., those pixels that are part of an edge). A good choice for M is 4 times the average value of $\|\nabla A(ij)\|_2$ over the whole image A.

When the Sobel filter is applied to `cameraman.jpg`, we get the image in Figure 14.2c. Here, the 1's in B were mapped to "white" and the 0's were mapped to "black."

Problem 4. Write a function that accepts an image as input and applies the Sobel filter to the image.