MATH 401, Graph Laplacian, FALL 2015

Let us start by observing the following relationship pertaining to the 2nd derivative on the realline.

Fact 0.1. Let f be a twice differentiable function defined on $(a, b) \subset \mathbb{R}$. Let $x \in (a, b)$. Then

$$f''(x) = \lim_{h \to 0} \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}.$$

The limit on the right hand side is sometimes called the *second symmetric derivative of f*. Please note that the above fact asserts that the second symmetric derivative exists provided the 2nd derivative in the classical sense exists. The opposite statement is false (please find a counterexample).

Proof:

First, consider the limit:

$$\lim_{h \to 0} \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}.$$

We now fix x, and treat h as variable. Apply Cauchy's mean value theorem to obtain that

$$\frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = \frac{f'(x+k) - f'(x-k)}{2k},$$

for some $0 < k < h$. Now, however, note that

$$\lim_{k \to 0} \frac{f'(x+k) - f'(x-k)}{2k} = f''(x).$$

To show this last fact, observe that for any differentiable function g, we have:

$$\begin{aligned} \lim_{k \to 0} \frac{g(x+k) - g(x-k)}{2k} &= \frac{1}{2}\left(\frac{g(x+k) - g(x)}{k} + \frac{g(x) - g(x-k)}{k}\right) \\ &= \frac{1}{2}(g'(x) + g'(x)) = g'(x). \end{aligned}$$

Now, complete this argument by taking $g = f'$.

Source of this proof: Antoni Zygmund, Trigonometric Series, Warszawa, 1935

Another Proof:

We can also use de l'Hopital's Rule to verify the existence of the limit:

$$\lim_{h\to 0} \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}.$$

We start by noting that, both, numerator and denominator converge to 0. (Since f is differentiable, it must be in particular continuous.) Moreover, the derivative of the numerator and denominator with respect to h exist. They are $f'(x+h) - f'(x-h)$ and $2h$, respectively. This shows that the derivative of the denominator is different from 0 in the neighberhood of $h = 0$. The last assumption of de l'Hopital's Rule that remains to be checkd is the existence of the limit

$$\lim_{h\to 0} \frac{f'(x+h) - f'(x-h)}{2h} = \lim_{h\to 0} \frac{f'(x+h) - f(x) + f(x) - f'(x-h)}{2h} = f''(x),$$

which follows from the existence of $f''(x)$.

Now, having defined this generalization of the 2nd derivative, we can use it to define the analog of the 2nd derivative for a function defined on $\mathbb{Z}$. In such case we let $h = 1$, note that the limit is no longer necessary for a discrete case, and we observe that

$$f''(N) = f(N+1) + f(N-1) - 2f(N), \qquad N \in \mathbb{Z}.$$

We shall now notice that both $N-1$ and $N+1$ can be viewed as neighbors of N. Denote the neighborhood of N by $nbd(N)$. This leads us to the following interpretation of 2nd derivative:

$$f''(N) = \left(\sum_{j\in nbd(N)} f(j)\right) - \left(\sum_{j\in nbd(N)} f(N)\right).$$

Observe that this definition of 2nd derivative makes sense for a function on any graph. As such we shall call it the Graph Laplacian and denote by Δ. Using textbook notation, we arrive at the following formula for the Graph Laplacian understood as a matrix acting on vectors which are functions on a (undirected) graph:

$$\Delta = A - D,$$

where A denotes the adjacency matrix and D denotes the degree matrix. (Please note that this is different form typical CS texts, where $\Delta = D - A$, for no good reason :))

We can also generalize now this notation to include weighted (undirected) graphs, i.e., graphs, where each edge (i, j) is assigned a number (weight) $w_{i,j}$:

$$\Delta(f)(N) = \left(\sum_{j \in nbd(N)} w_{j,N} f(j) \right) - \left(\sum_{j \in nbd(N)} w_{j,N} f(N) \right),$$

or, equivalently,

$$\Delta(m, n) = \begin{cases} w_{m,n} & m \neq n, m \in nbd(n) \\ -\sum_{j \in nbd(n)} w_{j,n} & m = n \\ 0 & m \notin nbd(n) \end{cases}.$$

Among some of the basic properties of the matrix Δ we find that it is symmetric, i.e.,

$$\Delta^T = \Delta,$$

and, provided the weights are chosen to be non-negative, the Laplacian is negative semidefinite, i.e.,

$$\forall v \in \mathbb{R}^d, \quad \langle \Delta v, v \rangle \leq 0.$$

These will come in handy when we shall want to compute eigendecompositions of Δ.