Polynomial Envelope Functions for Graph Neural Networks

Mario Geiger

August 2022

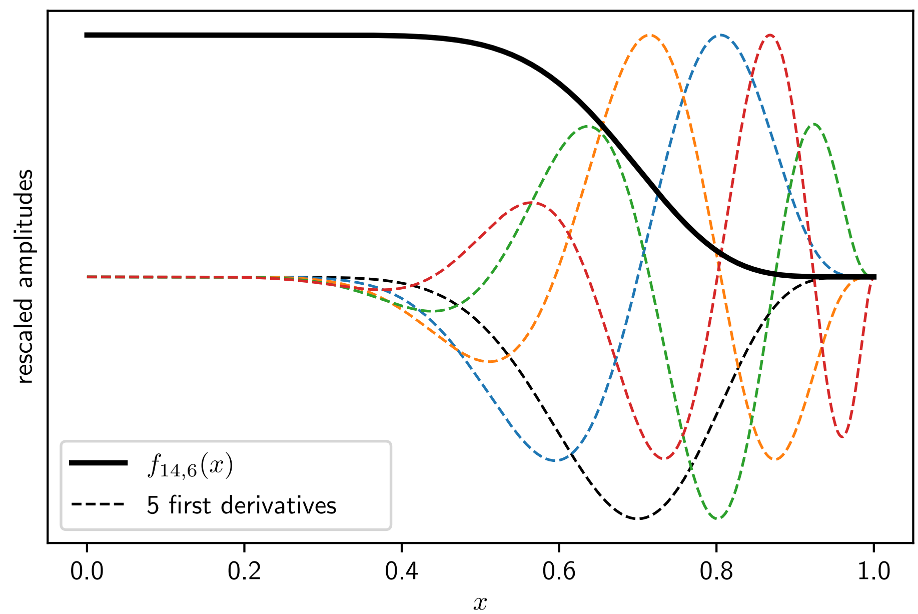

Figure 1: $f_{14,6}$ is a polynomial with its 14 first derivatives equal to zero in $x = 0$ ($f'(0) = f''(0) = \cdots = 0$) and its 6 first derivatives equal to zero in $x = 1$ ($f'(1) = f''(1) = \cdots = 0$).

1 Introduction

In the context of graph neural networks for chemistry, the nodes have a position in space and the presence of an edge is determined by the proximity between the edges.

In the case in which nodes are connected by an edge if their relative distance is smaller than a given cutoff x_c, there is a risk that your graph neural network will be discontinuous once a node enters in the proximity of another node, when the distance crosses x_c, a new edge is added, which might shift the outcome of the network.

In order to solve this shift problem, it is important to use an envelope function to ensure that the network is a smooth function of the positions of the nodes. In [1], they introduce a nice polynomial function (Eq 8) to do this job:

$$u_p(x) = 1 - \frac{(p+1)(p+2)}{2} x^p + p(p+2) x^{p+1} - \frac{p(p+1)}{2} x^{p+2} \tag{1}$$

This polynomial takes value 1 at 0 and value 0 at 1 (from now on we assume $x_c = 1$, which can always be done by evaluating in our envelope at x/x_c). u_p has $p - 1$ zero derivatives at 0 and 2 zero derivatives at 1. See graphs of this polynomial in Figure 2.

The idea behind this envelope is that you can think of your graph neural network to be defined on the fully connected graph but using an envelope that is equal to 0 for $x > x_c$. We should therefore always think of our envelope function as a piecewise function

$$f(x) = \begin{cases} u(x) & \text{for } x < x_c \\ 0 & \text{for } x > x_c \end{cases} \quad (2)$$

2 Proposition

It is therefore crucial to have a lot of zero derivatives at 1 (optimally ∞). To give flexibility to the user, we propose to generalize the polynomials u_p to the polynomials f_{n_0,n_1} (of the smallest degree) such that it has n_0 zeros derivatives at 0 and n_1 zero derivatives at 1. The relationship between f_{n_0,n_1} and u_p is:

$$u_p = f_{p-1,2} \quad (3)$$

See once more Figure 2

Seen as a piecewise function, f_{n_0,n_1} is a C^{n_1} function. Examples are shown in Figures 1 and Figure 3.

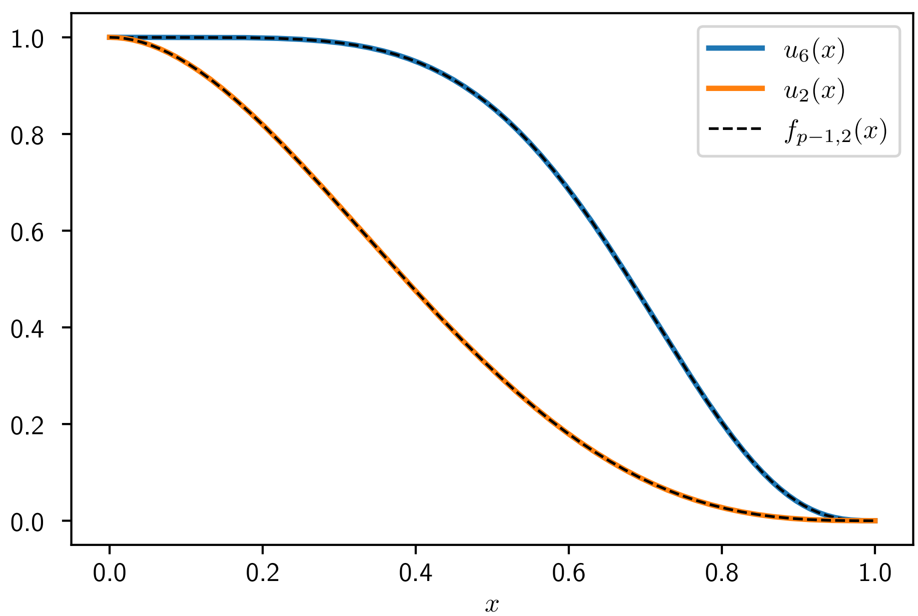

Figure 2: We can see that $u_p = f_{p-1,2}$.

3 Implementation

f_{n_0,n_1} is implemented as a polynomial of degree N,

$$f_{n_0,n_1}(x) = c_0 + c_1(x - 1/2) + c_2(x - 1/2)^2 + \dots c_N(x - 1/2)^N \quad (4)$$

where $c_0, \dots, c_N$ are determined by solving the fully determined linear system

$$\begin{bmatrix} 1 & x_0 & x_0^2 & x_0^3 & \dots & x_0^N \\ 0 & 1 & 2x_0 & 3x_0^2 & \dots & Nx_0^{N-1} \\ 0 & 0 & 2 & 6x_0 & \dots & N(N-1)x_0^{N-2} \\ 0 & 0 & 0 & 6 & \dots & \frac{N!}{(N-3)!}x_0^{N-3} \\ & & & & & \vdots \\ 0 & 0 & 0 & 0 & \dots & \frac{N!}{(N-n_0)!}x_0^{N-n_0} \\ \\ 1 & x_1 & x_1^2 & x_1^3 & \dots & x_1^N \\ 0 & 1 & 2x_1 & 3x_1^2 & \dots & Nx_1^{N-1} \\ 0 & 0 & 2 & 6x_1 & \dots & N(N-1)x_1^{N-2} \\ 0 & 0 & 0 & 6 & \dots & \frac{N!}{(N-3)!}x_1^{N-3} \\ & & & & & \vdots \\ 0 & 0 & 0 & 0 & \dots & \frac{N!}{(N-n_1)!}x_1^{N-n_1} \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_N \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \tag{5}$$

where $x_0 = -1/2$, $x_1 = 1/2$ and $N = n_0 + n_1 + 1$. See source code in this gist.

4 Numerical stability

For numerical stability we observed that it was good to express the polynomial with respect to $(x - 1/2)$.

Another idea considered was to somehow use the function $\exp(-1/x)$ that has **all** its derivatives equal to zero at $x = 0$. But this idea was abandoned due to numerical instability while trying to deform it (with compositions with smooth functions) into a good looking envelope function.

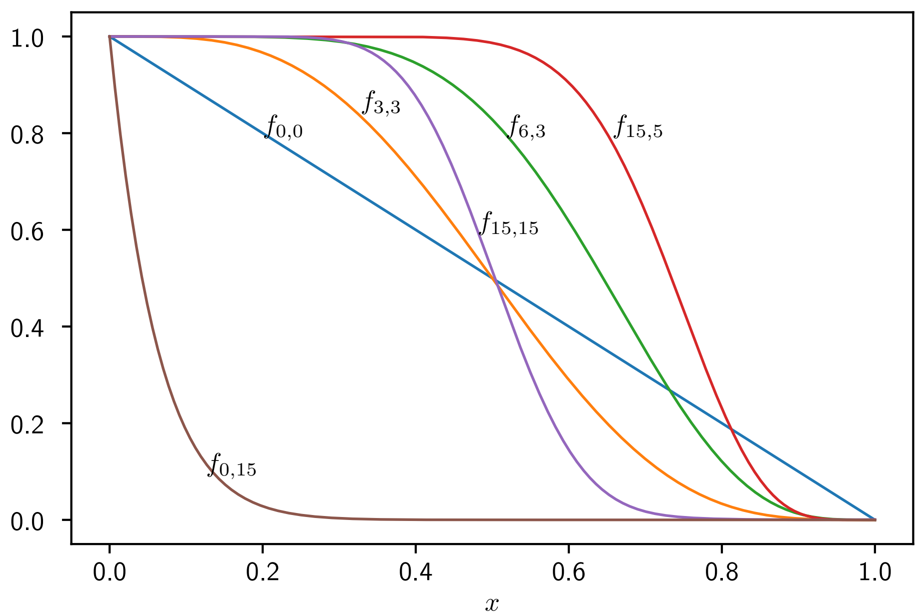

Figure 3: Examples of different f_{n_0,n_1}.

References

[1] Johannes Gasteiger, Janek Groß, and Stephan Günnemann. *Directional Message Passing for Molecular Graphs*. 2020. DOI: `10.48550/ARXIV.2003.03123`. URL: `https://arxiv.org/abs/2003.03123`.