Approximation Theory

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1 Introduction

Currently, we observe a revolution in scientific computing associated with a qualitatively new level of artificial intelligence, machine learning, and data-driven methods. Function approximation is at the very ground level of these techniques.

This chapter will discuss classical results on function approximation with polynomials, including the Bernstein polynomials and Chebyshev interpolation, and the approximation of functions by neural networks.

1.1 The Weierstrass Approximation Theorem

The possibility of approximating a continuous function on a closed interval in a uniform norm was established by Karl Weierstrass in 1885:

Theorem 1. Suppose f is a continuous real-valued function defined on the real interval [a,b]. For every $\epsilon > 0$, there exists a polynomial p such that

$$\max_{x \in [a,b]} \|f(x) - p(x)\| < \epsilon. \tag{1}$$

1.2 The Bernstein polynomials

References for this subsection:

- [Farouki(2012)]: R. Faruoki, The Bernstein polynomial basis: A centennial retrospective, Computer Aided Geometric Design, 29/6, August 2012, pp. 379–419
- Slides by Rida T. Farouki (UC Davis)
- Slides by Richard V. Kadison (U Penn)

A simple and constructive proof of this interval was given by Sergei Bernstein in 1912. He introduced what we call now the *Bernstein polynomials*.

Consider the identity

$$1 = (x + (1 - x))^n = \sum_{k=0}^n \binom{n}{k} x^k (1 - x)^{n-k}.$$
 (2)

The polynomials in the right-hand side of (2),

$$p_{n,k}(x) \coloneqq \binom{n}{k} x^k (1-x)^{n-k},\tag{3}$$

are called the *Bernstein basis functions*. Equation (2) shows that they form a partition of unity, i.e, the sum of all Bernstein basis functions with any fixed $n \in \mathbb{N}$ is identically equal to one. It is also clear that these polynomials are nonnegative on [0,1]. The Bernstein basis functions for n = 5 are plotted in Fig. 1 Several useful identities involving Bernstein basis functions are obtained using the differentiation trick. Consider the identity

$$x\frac{d}{dy}(y+(1-x))^n\Big|_{y=x} = nx.$$
 (4)

On the other hand, using the left-hand side of (4) we get

$$nx = x\frac{d}{dy}(y + (1 - x))^n\Big|_{y = x} = x\sum_{k=1}^n \binom{n}{k} kx^{k-1}(1 - x)^{n-k}.$$
 (5)

Hence, we get the following identity:

$$\sum_{k=0}^{n} \binom{n}{k} k x^{k} (1-x)^{n-k} = nx.$$
 (6)

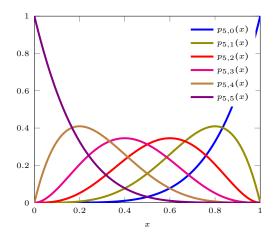


Figure 1: Bernstein basis functions $p_{n,k}$ for $n=5,\,k=0,1,2,3,4,5.$

By a similar trick, we can derive that

$$\sum_{k=0}^{n} \binom{n}{k} k^2 x^k (1-x)^{n-k} = n(n-1)x^2 + nx. \tag{7}$$

Equations (2), (4) and (6) imply the following identity that we will need to prove the Bernstein approximation theorem below:

$$\sum_{k=0}^{n} \binom{n}{k} \left(\frac{k}{n} - x \right)^2 x^k (1 - x)^{n-k} = \frac{x(1 - x)}{n}. \tag{8}$$

Definition 1. With f a real-valued function defined and bounded on the interval [0,1], let $B_n(f)$ be the polynomial on [0,1] that assigns to x the value

$$B_n(x) := \sum_{k=0}^n \binom{n}{k} x^k (1-x)^{n-k} f\left(\frac{k}{n}\right), \tag{9}$$

 $B_n(f)$ is called the nth Bernstein polynomial for f.

Using identities (2), (6), and (7) one can check that

$$B_n(1) = 1,$$
 (10)

$$B_n(x) = x, (11)$$

$$B_n(x^2) = \left(1 - \frac{1}{n}\right)x^2 + \frac{x}{n}. (12)$$

Theorem 2. (Bernstein, 1912) Let f be a real-valued function defined and bounded by M on the interval [0,1].

- 1. For each point x of continuity of f, $B_n(f)(x) \to f(x)$ as $n \to \infty$.
- 2. If f is continuous on [0,1], the Bernstein polynomial $B_n(f)$ tends uniformly to f as $n \to \infty$.
- 3. With x a point of differentiability of f, $B'_n(f)(x) \to f'(x)$ as $n \to \infty$.
- 4. If f is continuously differentiable on [0,1], then $B'_n(f)$ tends to f' uniformly as $n \to \infty$.

See R. Kadison's slides for the proof.

Thus, the Bernstein polynomial is a constructive tool for approximating any continuous function on a compact interval in \mathbb{R} in the uniform norm. However, the error of this approximation decays as $O(n^{-1})$ even for smooth functions, e.g. $B_n(x^2) = x^2(1-n^{-1}) + xn^{-1}$. In the next section, we review the Chebyshev interpolation and its application to solving boundary-value problems. You will see that the error decays faster than any power of n, the number of interpolation (or collocation) points, on smooth functions.

2 Chebyshev interpolation and Chebyshev spectral methods

2.1 Lagrangian interpolation

Suppose a continuous function f(x) defined on the interval [a,b] is given at a finite number of points x_j , j = 0, 1, 2, ..., n, a total of n + 1 points. We will denote $f(x_j)$ by f_j . The task of interpolation is to find a polynomial of degree at most n passing through all these points. Lagrange's approach to this task is to construct n + 1 polynomials $L_j(x)$ of degree n such that each $L_j(x)$ is 1 at x_j and zero at all other x_k 's. Then the linear combination

$$P(x) = f_0L_0(x) + f_1L_1(x) + \ldots + f_nL_n(x)$$

is a polynomial of degree at most n, and $P(x_j) = f_j$ for all j = 0, 1, ..., n. The polynomial P(x) written in the form above is called the Lagrange interpolation polynomial. The polynomials $L_j(x)$ are easily constructed. The error of interpolation can also be found. These results are summarized in the following theorem.

Theorem 3. Given a function f that is defined at n+1 points $x_0 < x_1 < ... < x_n \in [a,b]$ there exists a unique polynomial of degree $\leq n$ such that

$$P_n(x_j) = f(x_j), \quad j = 0, 1, 2, \dots, n.$$

This polynomial is given by

$$P_n(x) = \sum_{j=0}^n f(x_j) L_j(x),$$

where $L_j(x)$ is defined by

$$L_j(x) = \frac{\pi_{n+1}(x)}{(x-x_j)\pi'_{n+1}(x_j)} = \frac{\prod_{k=0, k\neq j}^n (x-x_k)}{\prod_{k=0, k\neq j}^n (x_j-x_k)},$$

 $\pi_{n+1}(x)$ being the nodal polynomial

$$\pi_{n+1}(x) = \prod_{k=0}^{n} (x - x_k).$$

Additionally, if f is n+1 times continuously differentiable in (a,b), then for any $x \in [a,b]$ there exists a value $\zeta_x \in (a,b)$ depending on x, such that

$$E_n(x) = f(x) - P_n(x) = \frac{f^{(n+1)}(\zeta_x)}{(n+1)!} \pi_{n+1}(x).$$
(13)

Proof. 1. Existence By construction, P_n is a polynomial of degree n passing through x_j , j = 0, 1, 2, ..., n.

- 2. Uniqueness Suppose that there are two such polynomials, $P_n(x)$ and $Q_n(x)$. Then the polynomial $d(x) := P_n(x) Q_n(x)$ is at most of degree n. On the other hand, it has at least n+1 roots x_j , $j=0,1,2,\ldots,n$. Therefore, it must be identically zero.
- 3. Error formula Consider the function

$$F(z) = f(z) - P_n(z) - [f(x) - P_n(x)] \frac{\pi_{n+1}(z)}{\pi_{n+1}(x)}.$$

This function has n+2 zeros at $z=x_j$, $j=0,1,2,\ldots,n$, and z=x. Recall Rolle's theorem that says that if a function f(z) is continuously differentiable on [a,b] and f(a)=f(b) then there is $c \in (a,b)$ such that f'(c)=0. Therefore, if we apply Rolle's theorem n+1 times we get that the function

$$F^{(n+1)}(z) = f^{(n+1)}(z) - P_n^{(n+1)}(z) - [f(x) - P_n(x)] \frac{(n+1)!}{\pi_{n+1}(x)}$$

has at least one zero in (x_0, x_n) . We denote this zero by ζ_x . Therefore, taking into account that $P_n^{(n+1)}(z) \equiv 0$, we get

$$0 = f^{(n+1)}(\zeta_x) - [f(x) - P_n(x)] \frac{(n+1)!}{\pi_{n+1}(x)},$$

and Eq. (13) follows.

Example Let us find the Lagrange interpolant p(x) passing through the points $(0, f_0)$, $(1, f_1)$, and $(2, f_2)$. The polynomial p(x) is of the form

$$p(x) = f_0 \frac{(x-1)(x-2)}{(0-1)(0-2)} + f_1 \frac{(x-0)(x-2)}{(1-0)(1-2)} + f_2 \frac{(x-0)(x-1)}{(2-0)(2-1)}$$

$$= \frac{1}{2} f_0(x^2 - 3x + 2) - f_1(x^2 - 2x) + \frac{1}{2} f_2(x^2 - x)$$

$$= f_0 + \frac{1}{2} (-3f_0 + 4f_1 - f_2)x + \frac{1}{2} (f_0 - 2f_1 + f_2)x^2.$$
(14)

2.2 The Newton interpolation polynomial

Lagrangian interpolation is convenient because it gives an explicit formula for the interpolant. However, it does not provide a convenient way to modify the polynomial to accommodate additional interpolation points. An alternative form of the interpolation polynomial, the Newton form, gives such a way. The Newton interpolation formula is used, for example, for deriving linear multistep methods with varying time step for solving ODE's. The Newton interpolation formula is defined via the divided differences. We set

$$f[x_0] = f(x_0),$$

$$f[x_0, x_1] = \frac{f[x_1] - f[x_0]}{x_1 - x_0},$$

$$f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0},$$

$$\dots$$

$$f[x_0, x_1, \dots, x_k] = \frac{f[x_1, \dots, x_k] - f[x_0, x_1, \dots, x_{k-1}]}{x_k - x_0},$$

$$\dots$$

Theorem 4. The polynomial interpolating f(x) at x_j , j = 0, 1, 2, ..., n is given by

$$P_n(x) = f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) + \dots + f[x_0, x_1, \dots, x_n](x - x_0)(x - x_1) \dots (x - x_{n-1}).$$
(15)

Example Let us find the Newton interpolant p(x) passing through the points $(0, f_0)$, $(1, f_1)$, and $(2, f_2)$. The polynomial p(x) is of the form

$$p(x) = f[0] + f[0,1](x-0) + f[0,1,2](x-0)(x-1), \tag{16}$$

where

$$f[0] = f_0, \quad f[0,1] = \frac{f_1 - f_0}{1 - 0} = f_1 - f_0, \quad f[1,2] = \frac{f_2 - f_1}{2 - 1} = f_2 - f_1,$$

$$f[0,1,2] = \frac{f[1,2] - f[0,1]}{2 - 0} = \frac{1}{2}(f_2 - f_1 - (f_1 + f_0)) = \frac{1}{2}(f_0 - 2f_1 + f_2).$$

Plugging these coefficients into Eq. (16) we get

$$p(x) = f_0 + (f_1 - f_0)x + \frac{1}{2}(f_0 - 2f_1 + f_2)x(x - 1)$$

= $f_0 + \frac{1}{2}(-3f_0 + 4f_1 - f_2)x + \frac{1}{2}(f_0 - 2f_1 + f_2)x^2$. (17)

The polynomial p(x) in Eq. (17) coincides with the one in Eq. (14) as it should.

Proof. We will proceed by induction. For n = 1 Eq. (15) holds. Suppose the polynomials $P[x_0, \ldots, x_{n-1}](x)$ and $P[x_1, \ldots, x_n](x)$ of the form of Eq. (15) interpolate f at the points x_0, \ldots, x_{n-1} and x_1, \ldots, x_n respectively. Note that both of them are of degree n-1. Hence they differ by a polynomial of degree at most n-1, and this polynomial has zeros at x_1, \ldots, x_{n-1} . Therefore,

$$P[x_1,...,x_n](x) - P[x_0,...,x_{n-1}](x) = a(x-x_1)...(x-x_{n-1})$$

where a is a number. Obviously, a is the difference of the leading coefficients of the polynomials $P[x_0, \ldots, x_{n-1}](x)$ and $P[x_1, \ldots, x_n](x)$, i.e.,

$$a = f[x_1, \dots, x_n] - f[x_0, x_1, \dots, x_{n-1}].$$

At the same time,

$$a = \frac{P[x_1, \dots, x_n](x) - P[x_0, \dots, x_{n-1}](x)}{(x - x_1) \dots (x - x_{n-1})}.$$

Now consider the polynomial

$$P[x_0, x_1, \dots, x_n](x) = P[x_0, \dots, x_{n-1}](x) + \frac{a}{x_n - x_0}(x - x_0)(x - x_1)\dots(x - x_{n-1}).$$
(18)

The last term of this polynomial is chosen so that it is zero at x_0, \ldots, x_{n-1} , and the coefficient $a/(x_n-x_0)$ is our guess that we will verify below. By construction, $P[x_0, x_1, \ldots, x_n](x)$ interpolates f at x_0, \ldots, x_{n-1} . Let us verify that it also does so at $x = x_n$. We evaluate $P[x_0, x_1, \ldots, x_n](x)$ at x_n and obtain:

$$P[x_0, x_1, ..., x_n](x_n)$$

$$=P[x_0, ..., x_{n-1}](x_n) + \frac{a}{x_n - x_0}(x_n - x_0)(x_n - x_1) ... (x_n - x_{n-1})$$

$$=P[x_0, ..., x_{n-1}](x_n) + \frac{P[x_1, ..., x_n](x_n) - P[x_0, ..., x_{n-1}](x_n)}{(x_n - x_0)(x_n - x_1) ... (x_n - x_{n-1})}(x_n - x_0)(x_n - x_1) ... (x_n - x_{n-1})$$

$$=P[x_1, ..., x_n](x_n) = f(x_n).$$

Therefore, the polynomial given by Eq. (18) interpolates f at x_j , j = 0, 1, 2, ..., n.

Remark The function $f[x_0, ..., x_n]$ is a symmetric function of its arguments i.e., it does not change if we permute $x_0, ..., x_n$. This is because the interpolation polynomial is independent of the order of nodes.

2.3 Runge phenomenon

Read Section 3.2.1 in Chapter 3 in Gil et al. [Gil et al.(2007)Gil, Segura, and Temme] and Chapter 5 in Trefethen [Trefethen(2000)].

2.4 Chebyshev polynomials

Read Section 3.3 in Chapter 3 in Gil et al. [Gil et al. (2007)Gil, Segura, and Temme].

We will study the Chebyshev polynomials in more detail as they lead to several remarkable numerical tools:

- Chebyshev interpolation, where the Runge phenomenon is eliminated [Gil et al.(2007)Gil, Segura, and Temme];
- Chebyshev least squares approximation, which is close to the minimax one;

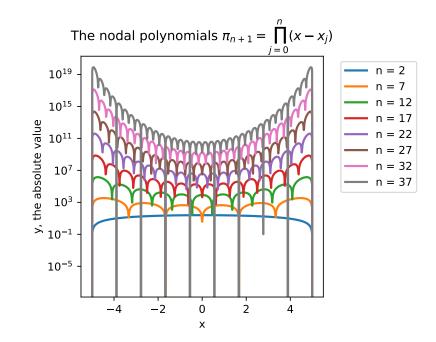


Figure 2: The nodal polynomials $\pi_{n+1}(x)$ with uniform nodes grow exponentially in the max norm.

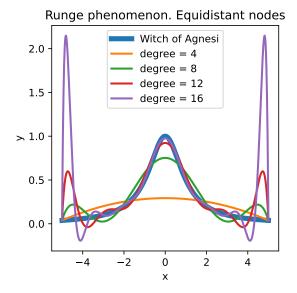


Figure 3: A demonstration of the Runge phenomenon on the example of a smooth function "Witch of Agnesi" $f(x) = (1 + x^2)^{-1}$ on the interval [-5, 5] that has poles at $\pm i$ in the complex plane.

• Chebyshev spectral methods for solving PDEs with non-periodic boundary conditions – L. N. Trefethen's book [Trefethen(2000)] Spectral Methods in Matlab.

Chebyshev polynomials are defined as follows:

$$T_n(x) = \cos[n \arccos(x)], \quad x \in [-1, 1], \quad n = 0, 1, 2, \dots$$
 (19)

It follows from the definition that

$$T_n(\cos \theta) = \cos(n\theta), \quad \theta \in [0, \pi], \quad n = 0, 1, 2, \dots$$
(20)

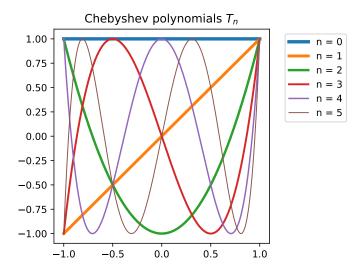


Figure 4: Graphs of the Chebyshev polynomials $T_0(x)$, $T_1(x)$, ..., $T_6(x)$.

The first few Chebyshev polynomials are

$$T_0(x) = 1,$$

$$T_1(x) = x,$$

$$T_2(x) = 2x^2 - 1,$$

$$T_3(x) = 4x^3 - 3x,$$

$$T_4(x) = 8x^4 - 8x^2 + 1,$$

$$T_5(x) = 16x^5 - 20x^3 + 5x,$$

$$T_6(x) = 32x^6 - 48x^4 + 18x^2 - 1.$$

2.5 Properties of the Chebyshev polynomials

1. The Chebyshev polynomials satisfy the following three-term recurrence relationships (TTRR):

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \quad T_0(x) = 1, \quad T_1(x) = x, \quad n = 0, 1, 2, \dots$$
 (21)

This TTRR immediately follows from Eq. (20) and the trigonometric formula

$$2\cos(a)\cos(b) = \cos(a+b) + \cos(a-b). \tag{22}$$

Indeed, let $x = \cos \theta$. Then setting $a = n\theta$ and $b = \theta$ we get (21).

2. The leading coefficient of $T_n(x)$ is 2^{n-1} . This follows from Eq. (21).

3.

$$T_n(-x) = (-1)^n T_n(x).$$

This means that if n is even, then $T_n(x) = T_n(-x)$, i.e., $T_n(x)$ is an even function, and if n is odd then $T_n(x) = -T_n(-x)$, i.e., $T_n(x)$ is an odd function. This follows from the formulas

$$\arccos(-x) = \pi - \arccos(x)$$
 and $\cos(\pi n - x) = (-1)^n \cos x$.

4. Zeros of $T_n(x)$ are

$$x_k = \cos\left(\frac{k + \frac{1}{2}}{n}\pi\right), \quad k = 0, 1, \dots, n - 1.$$
 (23)

Indeed, $T_n(\cos \theta) = \cos n\theta = 0$. Hence $n\theta = \frac{\pi}{2} + \pi k$, then $\theta = \frac{\pi}{n}(k + \frac{1}{2})$, therefore, $x = \cos \theta$ is given by (23). The values of k = 0, 1, ..., n-1 define fistinct roots.

5. Extrema of $T_n(x)$ are

$$x'_k = \cos\left(\frac{\pi k}{n}\right), \quad k = 0, 1, \dots, n. \tag{24}$$

Note that $T_n(x'_k) = (-1)^k$. Also note that x'_k follow the decreasing order and $x'_0 = 1$ and $x'_n = -1$.

6. The deviation of $2^{-n}T_{n+1}(x)$ from zero on [-1,1] is minimal possible among all polynomials with leading coefficient 1 of degree n+1. The theorem establishing this fact is below.

Theorem 5. Let

$$x_k = \cos\left(\frac{k + \frac{1}{2}}{n + 1}\pi\right), \quad k = 0, 1, \dots, n.$$

Then the monic polynomial (i.e., its leading coefficient is 1)

$$\hat{T}_{n+1} = \prod_{k=0}^{n} (x - x_k)$$

of degree n + 1 has the smallest possible uniform (maximum) norm 2^{-n} in [-1, 1] among all polynomials of degree n + 1. I.e.,

$$2^{-n} = \max_{x \in [-1,1]} |\hat{T}_{n+1}(x)| = \min_{\substack{p \in \mathcal{P}_{n+1} \\ p = x^{n+1} + \dots}} \max_{x \in [-1,1]} |p(x)|.$$

Proof. Suppose there is a monic polynomial p(x) of degree n+1 such that $|p(x)| < 2^{-n}$ for all $x \in [-1,1]$. Let x'_k , $k = 0, 1, \ldots, n+1$ be the abscissas of the extreme values of Chebyshev polynomials of degree n+1. Hence we have

$$p(x'_0) < 2^{-n} T_{n+1}(x'_0),$$

 $p(x'_1) > 2^{-n} T_{n+1}(x'_1),$
 $p(x'_2) < 2^{-n} T_{n+1}(x'_2),$

Therefore the polynomial

$$Q(x) = p(x) - 2^{-n}T_{n+1}(x)$$

changes sign between each two consecutive extrema of T_{n+1} . $T_{n+1}(x)$ has n+2 extrema on [-1,1]. Hence Q(x) has n+1 zeros. But Q(x) is of degree $\leq n$. Thus we have arrived to a contradiction. Hence there is no such monic polynomial p of degree n+1 such that $|p(x)| < 2^{-n}$ for $x \in [-1,1]$.

7. Relations with derivatives.

$$T_0(x) = T_1'(x),$$
 (25)

$$T_1(x) = \frac{1}{4}T_2'(x),\tag{26}$$

$$T_n(x) = \frac{1}{2} \left(\frac{T'_{n+1}(x)}{n+1} - \frac{T'_{n-1}(x)}{n-1} \right), \quad n \ge 2.$$
 (27)

The first two equalities are easy-to-check. The last one can be proven from the following observation:

$$T'_n(x) = \frac{n\sin(n\theta)}{\sin\theta}$$
, where $x = \cos\theta$.

Exercise Prove Eq. (27).

8. Multiplication relationship:

$$2T_r(x)T_q(x) = T_{r+q}(x) + T_{|r-q|}(x). (28)$$

Exercise Prove Eq. (28).

9. Orthogonality relationship:

$$\int_{-1}^{1} \frac{T_r(x)T_s(x)}{\sqrt{1-x^2}} dx = \begin{cases} 0, & r \neq s \\ \pi, & r = s = 0, \\ \frac{\pi}{2}, & r = s \neq 0. \end{cases}$$
 (29)

Let us prove it. We make a variable change $x = \cos \theta$. Then $dx = -\sin \theta d\theta$, $T_r(x) = \cos(r\theta)$, $T_s(x) = \cos(s\theta)$, and the integration limits are changed to: $-1 \mapsto \pi$, $1 \mapsto 0$. Therefore, using the formula

$$\cos a \cos b = 1/2 \cos(a+b) + 1/2 \cos(a-b)$$

we get:

$$\int_{-1}^{1} \frac{T_{r}(x)T_{s}(x)}{\sqrt{1-x^{2}}} dx = \int_{0}^{\pi} \cos(r\theta)\cos(s\theta)d\theta = \frac{1}{2} \int_{0}^{\pi} \left[\cos(r+s)\theta + \cos(r-s)\theta\right] d\theta$$

$$= \frac{1}{2} \begin{cases} \left[\frac{\sin(r+s)\theta}{r+s} + \frac{\sin(r-s)\theta}{r-s}\right]_{0}^{\pi}, & r \neq s \\ 2\pi, & r = s = 0, \\ \pi + \left[\frac{\sin(2r\theta)}{2r}\right]_{0}^{\pi}, & r = s \neq 0. \end{cases}$$

$$= \begin{cases} 0, & r \neq s \\ \pi, & r = s = 0, \\ \frac{\pi}{2}, & r = s \neq 0. \end{cases}$$

10. Discrete orthogonality relationship: Take the points

$$x_j = \cos\left(\frac{\pi(j+\frac{1}{2})}{n+1}\right), \quad j = 0, 1, \dots, n$$

that are the zeros of $T_{n+1}(x)$. Then for all $0 \le r, s \le n$ we have

$$\sum_{j=0}^{n} T_r(x_j) T_s(x_j) = \begin{cases} 0, & r \neq s \\ n+1, & r=s=0, \\ \frac{n+1}{2}, & r=s \neq 0, \end{cases}$$
 (30)

Exercise Prove Eq. (30). Hint: first use the trigonometric formula

$$\cos(r\theta)\cos(s\theta) = \frac{1}{2}\cos(r+s)\theta + \frac{1}{2}\cos(r-s)\theta,$$

then use the formula $\cos y = \frac{1}{2}(e^{iy} + e^{-iy})$. You will obtain four geometric series. Compute their sums.

2.6 Chebyshev interpolation

Read Section 3.4 in Gil et al. [Gil et al. (2007)Gil, Segura, and Temme]. Properties of the Chebyshev polynomials offer a nice way for computing the Chebyshev interpolant of degree

n. Fix some integer n and consider the zeros of $T_{n+1}(x)$. They are

$$x_j = \cos\left(\frac{\pi(j+\frac{1}{2})}{n+1}\right), \quad j = 0, 1, \dots, n.$$

For a given function f(x) on the interval [-1,1], the polynomial p_n of degree n interpolating f(x) at the Chebyshev points x_j , j = 0, 1, ..., n, is given by

$$p_n(x) = \sum_{k=0}^{n} c_k T_k(x) \equiv \frac{c_0}{2} + \sum_{k=1}^{n} c_k T_k(x).$$

The symbol ' indicates that the first term in the sum should be divided by two. The coefficients c_k are found from the requirement that $p_n(x_i) = f(x_i)$, j = 1, 2, ..., n, i.e.,

$$f(x_j) = \sum_{k=0}^{n} {'c_k T_k(x_j)}.$$

Then we have

$$\sum_{j=0}^{n} f(x_j) T_m(x_j) = \sum_{k=0}^{n} c_k \sum_{j=0}^{n} T_k(x_j) T_m(x_j) = \sum_{k=0}^{n} c_k \frac{n+1}{2} \delta_{mk} = \frac{1}{2} (n+1) c_k.$$

Hence the coefficients are given by

$$c_k = \frac{2}{n+1} \sum_{j=0}^{n} f(x_j) T_k(x_j), \quad x_j = \cos\left(\frac{\pi(j+\frac{1}{2})}{n+1}\right).$$
 (31)

To summarize, the Chebyshev interplant of f(x) is given by

$$p_n(x) = \frac{c_0}{2} + \sum_{k=1}^n c_k T_k(x), \tag{32}$$

where the coefficients c_k are given by Eq. (31).

2.7 Chebyshev polynomials shifted to the interval [a, b]

Suppose we need to find the Chebyshev interpolant for f(y) on the interval $y \in [a, b]$. We proceed as follows.

1. First we set up a linear map of [-1,1] onto [a,b] and map the Chebyshev points, the roots of T_{n+1} , lying in the interval [-1,1], to the interval [a,b]:

$$l(x) = \frac{b-a}{2}x + \frac{a+b}{2}; \quad x_k = \cos\left(\frac{k+1/2}{n+1}\pi\right), \quad y_k = l(x_k), \quad k = 0, 1, \dots, n. \quad (33)$$

2. Next, we compute the Chebyshev coefficients:

$$c_j = \frac{2}{n+1} \sum_{k=0}^{n} T_j(x_k) f(y_k).$$
 (34)

3. Finally, we write out the Chebyshev interpolant

$$p_n(y) = \frac{c_0}{2} + \sum_{j=1}^n c_j T_j \left(\frac{2y - a - b}{b - a} \right). \tag{35}$$

Exercise Show that the shifted Chebyshev polynomials satisfy the following orthogonality relationships

$$\int_{a}^{b} \frac{T_{r}^{[a,b]}(y)T_{s}^{[a,b]}(y)}{\sqrt{1-\left(\frac{2y-a-b}{b-a}\right)^{2}}} dy = \begin{cases} 0, & r \neq s \\ \frac{b-a}{2}\pi, & r = s = 0, \\ \frac{(b-a)\pi}{4}, & r = s \neq 0. \end{cases}$$
(36)

2.8 Clenshaw's method for evaluating Chebyshev sums

Chebyshev interpolant can be evaluated at the point $y \in [a, b]$ directly from Eq. (32)

$$p_n(y) = \frac{c_0}{2} + \sum_{k=1}^n c_k \cos(k \arccos(y)), \text{ where } x = \frac{2y - a - b}{b - a}.$$
 (37)

This formula has a shortcoming in that it requires evaluation of cos and arccos which are typically built-in functions, but their evaluation is time-consuming in comparison with basic floating-point operations.

An elegant way to evaluate Chebyshev interpolant that avoids calculations of cos and arccos was proposed by Clenshaw (1955). A detailed description of Clenshaw's algorithm is given in Chapter 3 "Chebyshev Expansions" from "Numerical Methods for Special Functions" by Amparo Gil, Javier Segura, and Nico Temme (see pages 75-76). Here, we show how one can implement it in MATLAB.

Suppose we need to evaluate the sum

$$p_n(y) = \frac{c_0}{2} + \sum_{k=1}^n c_k T_k(x)$$
, where $x = \frac{2y - a - b}{b - a}$.

We rewrite this sum in the vector form:

$$p_n(y) = \mathbf{c}^{\mathsf{T}} \mathbf{t} - \frac{c_0}{2},$$

where $\mathbf{c} := [c_0, c_1, \dots, c_n]^{\mathsf{T}}$, $\mathbf{t} := [T_0(x), T_1(x), \dots, T_n(x)]^{\mathsf{T}}$. Recall that the Chebyshev polynomials satisfy TTRR (21) that can be written in the matrix form as

$$\begin{bmatrix} 1 & & & & & & \\ -2x & 1 & & & & & \\ 1 & -2x & 1 & & & & \\ & 1 & -2x & 1 & & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2x & 1 \end{bmatrix} \begin{bmatrix} T_0(x) \\ T_1(x) \\ T_2(x) \\ \vdots \\ T_n(x) \end{bmatrix} = \begin{bmatrix} 1 \\ -x \\ 0 \\ \vdots \\ 0 \end{bmatrix} \equiv A\mathbf{t} = \mathbf{d}.$$

Let **b** be a vector such that

$$\mathbf{b}^{\mathsf{T}} A = \mathbf{c}^{\mathsf{T}}, \quad \text{or} \quad A^{\mathsf{T}} \mathbf{b} = \mathbf{c}. \tag{38}$$

Note that **b** is readily found starting from b_n as A^{T} is upper-triangular. Then

$$p_n(y) = \mathbf{c}^{\mathsf{T}} \mathbf{t} - \frac{c_0}{2} = \mathbf{b}^{\mathsf{T}} A \mathbf{t} - \frac{c_0}{2}$$

= $\mathbf{b}^{\mathsf{T}} \mathbf{d} - \frac{c_0}{2} = b_0 - b_1 x - \frac{c_0}{2}$.

From (38) we find

$$c_0 = b_0 - 2xb_1 + b_2$$

Therefore,

$$p_n(y) = b_0 - b_1 x - \frac{c_0}{2} = b_0 - b_1 x - \frac{1}{2} (b_0 - 2xb_1 + b_2) = \frac{1}{2} (b_0 - b_2).$$
 (39)

3 Approximation of functions with neural networks

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3.1 What is a neural network?

A feed-forward fully connected neural network with l hidden layers is a composition of functions of the form

$$\mathcal{N}(x;\theta) = \mathcal{L}_{l+1} \circ \sigma_l \circ \mathcal{L}_l \circ \sigma_{l-1} \circ \dots \circ \sigma_1 \circ \mathcal{L}_1. \tag{40}$$

The symbol \mathcal{L}_k denotes the k's affine operator of the form $\mathcal{L}_k(x) = A_k x + b_k$, while σ_k denotes a nonlinear function called an *activation function*. The activation functions act entry-wise on vector arguments.

The user chooses the activation functions, the dimensions of matrices A_k , and the number of hidden layers l and called the *hyperparameters* of the neural network.

The matrices A_k and shift vectors (or bias vectors) b_k are encoded into the argument θ : $\theta = \{A_k, b_k\}_{k=1}^{l+1}$. They are called the *parameters* of the neural network. The term *training*

neural network means optimizing $\{A_k, b_k\}_{k=1}^{l+1}$ with respect to a certain objective function called the loss function. The loss function is set up by the user so that it is minimized if the neural network $\mathcal{N}(x;\theta)$ satisfies certain conditions. For example, one might want the neural network to assume certain values f_j at certain points x_j , $j = 1, \ldots, N$. These points x are called the training data. In this case, a common choice of the loss function is the least squares error:

$$Loss(x;\theta) = \frac{1}{n} \sum_{j=1}^{n} ||N(x_j;\theta) - f_j||^2.$$
(41)

The activation functions σ_k can be arbitrary **non-polynomial** functions. Popular choices are (Fig. 3.1)

• sigmoid:

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

• hyperbolic tangent:

$$\tanh(x) = \frac{e^x + e^{-x}}{e^x - e^{-x}};\tag{42}$$

• rectified linear unit:

$$ReLU(x) = \begin{cases} x, & x \ge 0 \\ 0, & x < 0. \end{cases}$$

There are many other possible choices for the activation functions.

3.2 Approximation of continuous functions in \mathbb{R}^n by neural networks with one hidden layer

Ref.: [Pinkus(1999)]

Definition 2. We will say that a set of functions \mathcal{M} is **dense** in the set of continuous functions $C(\mathbb{R}^n)$ in the **topology of uniform convergence on compacta** if for any $\epsilon > 0$, any compact set $K \subset \mathbb{R}^n$, and any continuous function $f(x) : \mathbb{R}^n \to \mathbb{R}$, there exists a function $g(x) \in \mathcal{M}$ such that

$$\max_{x \in K} |f(x) - g(x)| < \epsilon. \tag{43}$$

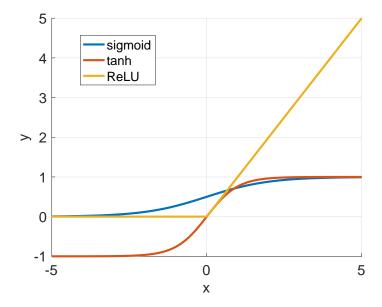


Figure 5: Common activation functions for neural networks.

We will consider the sets \mathcal{M} of the form

$$\mathcal{M}(\sigma) := \operatorname{span} \left\{ \sigma(w \cdot x - \theta) \mid w \in \mathbb{R}^n, \ \theta \in \mathbb{R} \right\}. \tag{44}$$

The question whether $\mathcal{M}(\sigma)$ is dense in $C(\mathbb{R})$ in the topology of uniform convergence on compacta addresses the necessary part of the function approximation. If the answer is yes, then, in principle, one can approximate a function $f \in C(\mathbb{R}^n)$ with a function $g \in \mathcal{M}(\sigma)$ with any given accuracy. However, it does not mean that this approximation will be efficient regarding the number of parameters involved, and it does not give us a good recipe to construct such an approximation. We will address these questions in later sections.

The earliest works addressing the density of $\mathcal{M}(\sigma)$ are Hecht-Nielsen (1987), Gallant and White (1988), and Irie-Miyake (1988).

The first proofs of density of $\mathcal{M}(\sigma)$ in $C(\mathbb{R}^n)$ in the uniform topology on compacta belong to Cybenko (1989) [Cybenko(1989)] and Funahashi (1989). Cybenko and Funahashi independently proved very similar results using different methods. Cybenko proved it for any continuous sigmoidal function, which is not necessarily monotone, while Funahashi proved it for any continuous monotone sigmoidal function. Hornik, Stinchcombe,

and White (1989) proved almost the same results for σ bounded and monotone, but not necessarily continuous. Their method of proof is also different.

The main theorem in [Pinkus(1999)] is

Theorem 6. Let $\sigma \in C(\mathbb{R})$. Then $\mathcal{M}(\sigma)$ is dense in $C(\mathbb{R}^n)$, in the topology of uniform convergence on compacta, if and only if σ is not a polynomial.

If σ is a polynomial of degree r, then \mathcal{M} is a set of polynomials of degree r and hence not dense in $C(\mathbb{R}^n)$.

If σ is not a polynomial, the proof of the density property of \mathcal{M} is quite long and consists of several stages. The following proposition reveals the two components that we need to prove to establish the density of (σ) in $C(\mathbb{R}^n)$, in the topology of uniform convergence on compacta.

Proposition 1. Assumptions:

1. $\Lambda, \Theta \subset \mathbb{R}$ are such that the set

$$\mathcal{N}(\sigma; \Lambda, \Theta) := \operatorname{span}\{\sigma(\lambda t - \theta) \mid \lambda \in \Lambda, \theta \in \Theta\},\tag{45}$$

is dense in $C(\mathbb{R})$ in the topology of uniform convergence on compacta.

2. Let $A \subset \mathbb{S}^{n-1}$ be a set of unit vectors in \mathbb{R}^n , where \mathbb{S}^{n-1} is the unit sphere in \mathbb{R}^n , such that the set of ridge functions

$$\mathcal{R}(A) = \operatorname{span} \left\{ g(a \cdot x) : g \in C(\mathbb{R}), \ a \in A \right\} \tag{46}$$

is dense in $C(\mathbb{R})$ in topology of uniform convergence on compacta.

Then

$$\mathcal{M}(\sigma; \Lambda \times A, \Theta) := \operatorname{span}\{\sigma(w \cdot x - \theta) \mid w \in \Lambda \times A, \theta \in \Theta\}$$

$$\tag{47}$$

is dense in $C(\mathbb{R})$ in topology of uniform convergence on compacta.

Proof. Let $f \in C(K)$ for some compact set in \mathbb{R}^n . Since $\mathcal{R}(A)$ is dense in C(K), given $\epsilon > 0$ there exist $g_i \in C(\mathbb{R} \text{ and } a^i \in A, i = 1, ..., r \text{ such that}$

$$\left| f(x) - \sum_{i=1}^{r} g_i(a^i \cdot x) \right| < \frac{\epsilon}{2} \quad \forall x \in K.$$
(48)

Since K is compact,

$$\{a^i \cdot x \mid x \in K\} \subseteq [\alpha_i, \beta_i],$$

for some finite interval $[\alpha_i, \beta_i]$, i = 1, ..., r. Because $\mathcal{N}(\sigma; \Lambda, \Theta)$ is dense in $C([\alpha_i, \beta_i])$, i = 1, ..., r, there exist constants $c_{ij} \in \mathbb{R}$, $\lambda_{ij} \in \Lambda$, and $\theta_{ij} \in \Theta$, $j = 1, ..., m_i$, i = 1, ..., r, for which

$$\left| g_i(t) - \sum_{j=1}^{m_i} c_{ij} \sigma(\lambda_{ij} t - \theta_{ij}) \right| < \frac{\epsilon}{2r} \quad \forall t \in [\alpha_i, \beta_i], \quad i = 1, \dots, r.$$

$$(49)$$

Therefore,

$$\left| f(x) - \sum_{i=1}^{r} \sum_{j=1}^{m_i} c_{ij} \sigma(\lambda_{ij} a^i \cdot x - \theta_{ij}) \right| < \epsilon \quad \forall x \in K.$$
 (50)

The question of whether the set $\mathcal{R}(A)$ of ridge functions is dense in $C(\mathbb{R}^n)$ was answered in 1961 by Vostrecov and Kreines:

Theorem 7. $\mathcal{R}(A)$ is dense in $C(\mathbb{R}^n)$ in topology of uniform convergence on compacta, if and only if there is no nontrivial (not identically zero) homogeneous (all terms have the same total degree) polynomial that vanishes on A.

Note that a ridge function $g(a \cdot x)$ is constant on all hyperplanes normal to the direction of a.

The proof of the density of $\mathcal{N}(\cdot)$ in $C(\mathbb{R})$ is conducted in a series of propositions that gradually extend the set of permissible σ and shrink the sets Λ and Θ .

Proposition 2. Let $\sigma \in C^{\infty}(R)$ and is not a polynomial. Then $\mathcal{N}(\sigma; \mathbb{R}, \mathbb{R})$ is dense in \mathbb{R} .

We will need the following lemma by Corominas and Sunyer Balaguer (1954):

Lemma 1. Let $\sigma \in C^{\infty}(R)$ and is not a polynomial. Let I be any open interval in \mathbb{R} . Then there exists a point $t \in I$ such that $\sigma^{(k)}(t) \neq 0$ for all $k \in \{0\} \cup \mathbb{N}$.

Proof. (Proposition 2.) Set $-\theta_0 = t$ where t is the point from Lemma 1. We have that

$$\frac{1}{h} \left[\sigma((\lambda + h)t - \theta_0) - \sigma(\lambda t - \theta_0) \right] \in \mathcal{N}(\sigma; \mathbb{R}, \mathbb{R}).$$

Therefore, letting $h \to 0$ and choosing $\lambda = 0$, we obtain

$$\frac{d}{d\lambda}\sigma(\lambda t - \theta_0)\Big|_{\lambda=0} = t\sigma'(-\theta_0) \in \overline{\mathcal{N}(\sigma; \mathbb{R}, \mathbb{R})}.$$

Inductively applying the same argument, we establish that

$$\frac{d^k}{d\lambda^k}\sigma(\lambda t - \theta_0)\Big|_{\lambda=0} = t^k \sigma^{(k)}(-\theta_0) \in \overline{\mathcal{N}(\sigma; \mathbb{R}, \mathbb{R})} \quad \forall k \in \{0\} \cup \mathbb{N}.$$

Since $\sigma^{(k)}(-\theta_0) \neq 0$ for any k, the set $\overline{\mathcal{N}(\sigma;\mathbb{R},\mathbb{R})}$ contains all monomials t^k , $k = 0, 1, \ldots$, hence all polynomials. Hence, it is dense in C(K) for any compact set K by the Weierstrass theorem.

Note that the proof of Proposition 2 only requires that Λ contains a sequence tending to zero. In the further series of propositions, Pinkus [Pinkus(1999)] relaxes the requirements on σ . I am referring interested students to his paper.

3.3 Approximation of differentiable functions in \mathbb{R}^n by neural networks with one hidden layer

Notation:

 $D^{\mathbf{m}} := \frac{\partial^{|\mathbf{m}|}}{\partial^{m_1} \dots \partial^{m_n}}, \quad |m| = m_1 + \dots + m_n, \quad m_1, \dots, m_n \in \mathbb{Z}_+^n \equiv \{0\} \cup \mathbb{R}^n;$

$$C^{\mathbf{m}^1,\dots,\mathbf{m}^s}(\mathbb{R}^n) = \bigcap_{j=1}^s C^{\mathbf{m}^j}(\mathbb{R}^n).$$

Definition 3. We say that $\mathcal{M}(\sigma)$ is dense in $C^{\mathbf{m}^1,\dots,\mathbf{m}^s}$ if, for any $f \in C^{\mathbf{m}^1,\dots,\mathbf{m}^s}(\mathbb{R}^n)$, any compact set $K \subset \mathbb{R}^n$, any $\epsilon > 0$, there exists $g \in \mathcal{M}(\sigma)$ such that

$$\max_{x \in K} \left| D^{\mathbf{k}} f(x) - D^{\mathbf{k}} g(x) \right| < \epsilon \quad \forall \mathbf{k} \in \mathbb{Z}_{+}^{n} \quad \text{s.t.} \quad \mathbf{k} \le \mathbf{m}^{i} \quad for \ some \quad i.$$
 (51)

Theorem 8. Let $\mathbf{m}^i \in \mathbb{Z}_+^n$, $1 \le i \le s$, and set $m = \max_{1 \le i \le s} |\mathbf{m}^i|$. Assume $\sigma \in C^m(\mathbb{R})$ and sigma is not a polynomial. Then $\mathcal{M}(\sigma)$ is dense in $C^{\mathbf{m}^1,\dots,\mathbf{m}^s}(\mathbb{R}^n)$.

This result was established as a results of a series of works by various authors in the 1990s: Hornik, Stinchcombe and White (1990), Hornik (1991), Ito (1993), Li (1996). Pinkus's review paper contains an outline of its proof.

3.4 How many neurons do we need?

Pinkus [Pinkus(1999)] reviews the results on the number of neurons in one-hidden-layer neural networks required to approximate a given function $f \in \mathcal{B}_p^s(\mathbb{R}^n)$, where

$$\mathcal{B}_p^s(\mathbb{R}^n) \coloneqq \left\{ f \in \mathcal{W}_p^s \mid \|f\|_{s,p} \le 1 \right\}. \tag{52}$$

Here \mathcal{W}_p^m is the Sobolev space consisting of all functions with weak derivatives up to order m such that their L_p -norm over the unit ball in \mathbb{R}^n is finite. Note that \mathcal{W}_p^m includes all functions with continuous derivatives up to order m that have finite L_p -norm over the unit ball in \mathbb{R}^n . It also includes all functions with continuous derivatives up to order m-1 that have finite L_p -norm over the unit ball in \mathbb{R}^n , and the (m-1)st derivative is Lipschitz-continuous.

Hence, we define the set

$$\mathcal{M}_r(\sigma) := \left\{ \sum_{i=1}^r c_i \sigma(w_i \cdot x - \theta_i) \mid c_i, \theta_i \in \mathbb{R}, \ w_i \in \mathbb{R}^n \right\}.$$
 (53)

The infimum of the approximation error of f in $\mathcal{M}_r(\sigma)$ in a normed space X is denoted by

$$E(f, \mathcal{M}_r(\sigma), X) := \inf_{g \in \mathcal{M}_r(\sigma)} \|f - g\|_X.$$
(54)

The following two theorems reveal how the lower and upper bounds on $E(\cdot)$ scale with s and n.

Theorem 9. Maiorov and Meir, 1999. Lower bound. Let $p \in [1, \infty]$, $s \ge 1$, $n \ge 2$, and

$$\sigma(t) = \frac{1}{1 + e^{-t}},$$

or σ be a polynomial spline of a fixed degree with a finite number of knots. Then

$$E(\mathcal{B}_p^s(\mathbb{R}^n), \mathcal{M}_r(\sigma), L_p) \ge C(r \log r)^{-s/n}$$
(55)

for some constant C independent of r.

Theorem 10. Mhaskar, 1996. Upper bound. Assume that $\sigma : \mathbb{R} \to \mathbb{R}$ is $C^{\infty}(\mathbb{R})$ and not a polynomial. For any $p \in [1, \infty]$, $s \ge 1$, $n \ge 2$,

$$E(\mathcal{B}_p^s(\mathbb{R}^n), \mathcal{M}_r(\sigma), L_p) \le Cr^{-s/n}$$
(56)

for some constant C independent of r.

This theorem can be derived using the fact that the error of approximating a function by a polynomial scales with its degree as k as k^{-s} , as follows from the Chebyshev interpolation and its connection with the Fourier theory. The number of neurons r such that the closure of \mathcal{M}_r contains a polynomial of degree k in 1D scales as k, as can be seen from the proof of Proposition 2. The number of monomials of degree k in \mathbb{R}^n is

$$\begin{pmatrix} k+n-1 \\ k \end{pmatrix} \equiv \begin{pmatrix} k+n-1 \\ n-1 \end{pmatrix} = \frac{(k+n-1)(k+n-2)\dots(k+1)}{(n-1)!}.$$

If $k \gg n$, the number of monomials scales at k^n .

The upper bound in Theorem 10 was generalized on other classes of activation functions.

3.5 Benefits of depth of neural networks

The first work that addresses the benefits of depth is the PhD dissertation by Johan Hastad (MIT,1986) [Hastad(1987)] who has shown that Boolean circuits with only or and and operations require exponential size in order to represent a parity function well. The parity function takes a boolean vector as input and outputs one if the input vector has odd number of ones and zero otherwise.

Matus Telgarsky [Telgarsky(2015)] considered the sawtooth function

$$g(x) \equiv g_1(x) := \begin{cases} 2x, & x \in [0, 1/2), \\ 2(1-x), & x \in [1/2, 1], \\ 0, & \text{otherwise.} \end{cases}$$
 (57)

This function can be iterated as

$$g_m(x) = \underbrace{g \circ \dots \circ g}_{\text{m times}}(x).$$
 (58)

For example, the functions $g_2(x)$ and $g_3(x)$ are

$$g_2(x) = g(g(x)), \quad g_3(x) = g(g(g(x))).$$
 (59)

The graphs of g, g_2 , and g_3 are shown in Fig. 6. The function $g_m(x)$ has 2^{m-1} teeth.

It is easy to check that g(x) can be expressed as a linear combination of three ReLU functions:

$$g(x) = 2\text{ReLU}(x) - 4\text{ReLU}(x - 1/2) + 2\text{ReLU}(x - 1). \tag{60}$$

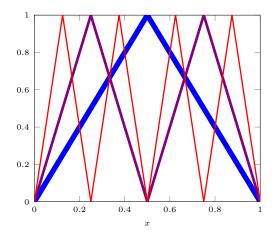


Figure 6: Sawtooth functions g_m for m = 1, 2, 3.

Indeed,

$$2\mathsf{ReLU}(x) - 4\mathsf{ReLU}(x - 1/2) + 2\mathsf{ReLU}(x - 1) = \begin{cases} 0, & x \le 0, \\ 2x, & x \in [0, 1/2), \\ 2x - 4x + 2 = 2(1 - x), & x \in [1/2, 1], \\ 2x - 4x + 2 + 2x - 2 = 0, & x > 1 \end{cases}$$

Therefore, the function g_2 can be represented as a two-layer ReLU neural network with three neurons in each layer. In fact, g_2 can be represented as a linear combination of five ReLU functions, i.e., as a one-layer ReLU neural network with 5 neurons:

$$g_2(x) = 4 \text{ReLU}(x) - 8 \text{ReLU}(x-1/4) + 8 \text{ReLU}(x-1/2) - 8 \text{ReLU}(x-3/4) + 4 \text{ReLU}(x-1).$$
 (61)

The number of ReLU functions required to represent g_m , if composition is not allowed, is $1+2^m$. Indeed, we need 2 ReLUs to represent each tooth and one more ReLU to flatten the function for x > 1. However, using function composition, $g_m(x)$ is represented by m layers with three ReLUs in each layer.

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