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APPLIED APPROXIMATION THEORY

PUBLISHED BY

TUFTE-LATEX.GOOGLECODE.COM

First printing, March 2024

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Introduction

At its heart, approximation theory is concerned with understanding and quantifying the extent to which one function can be approximated by elements of another *given* collection of functions. As one would expect, it plays a central role in many fields, *inter alia* numerical analysis, differential equations, statistics, and data science. It is intimately related to the geometry of function spaces and compressibility. Indeed, a motif throughout these notes is the role that smoothness plays in the effective dimension of a function space, understood in a suitable sense.

It has a long history, dating at least back to Euler's 1777 work on minimizing errors in distances on maps of Russia; continuing through Laplace's work in 1843 on determining the best ellipsoidal approximation to the Earth; and Bernstein's work on constructive function theory in the 20th century, to today, where it underpins modern approaches to everything from PDE solvers, fast linear algebra, signal processing, and neural networks. In all of this, a key figure is Pafnuty Chebyshev, who in 1853 considered the following problem which arose in the study of locomotives:

Given an interval $[a, b]$ *a function* $f : [a, b] \to \mathbb{R}$, *and a natural number* n, *solve*

$$\min_{p \in \mathcal{P}_n} \max_{a \leq x \leq b} |f(x) - p(x)|,$$

where $\mathcal{P}_n$ *denotes the set of polynomials of degree* at most n.

Understanding this innocuous-looking optimization problem will be a central focus of these notes and, as we shall see, has far ranging implications, extensions, and applications. When considering an approximation problem, there are three fundamental mathematical questions to consider: what functions are we approximating? With

what? In what sense? Additionally, from a computational perspective, when assessing a method for approximation, there are three fundamental computational traits that are desirable for a method to possess: is it accurate? Is it numerically stable? Can it be carried out in a reasonable amount of time?

A motivating example

As a first example that will highlight many of the themes of these notes, let us first consider the example of numerical integration. That is to say, we want to obtain information ($\int_0^1 f(x)\,\mathrm{d}x$) from samples. This leads to a problem of *quadrature*.

One of the simplest approaches to approximate such an integral would be through either the left-hand or right-hand Riemann rules:

$$L_n(f) := \frac{1}{n}\sum_{k=0}^{n-1} f(k/n), \quad R_n(f) := \frac{1}{n}\sum_{k=1}^{n} f(k/n),$$

respectively. Note that both of these approximations take the general form

$$\sum_{k=0}^{n} f(x_k)w_k,$$

where $x_k = k/n$ and $w_k = 1/n$ except at the right endpoint (for L_n) or the left endpoint (for R_n). The x_k are called *quadrature points* and the w_k are referred to as the corresponding *quadrature weights.* The error is clearly dependent on the smoothness of f. Indeed, it is easy to construct a function for which the integral, in a Lebesgue sense, exists and is equal to zero, but the left-hand and right-hand Riemann rules with equispaced points take on any desired value for all n.

Thus, we must buy convergence at the price of imposing more assumptions on our function f. One way to think about this is that the space of all functions, even all bounded functions, is too large to allow for numerical integration. Instead, we might consider restricting our attention to a subset of functions which are almost low dimensional. Indeed, approximation theory is fundamentally about function "compression" - the extent to which a given set of functions can be well-approximated by a finite dimensional subspace. One mechanism for a function space to be compressible is smoothness. An old game in numerical analysis (or analysis in general) is to buy decay at the cost of derivatives.

Returning to our example, we see that from Taylor's theorem, if f is smooth enough, then

$$|R_n(f) - I(f)| \leq C\|f'\|_\infty n^{-1}.$$

Here $\|\cdot\|_\infty$ denotes the L^∞ norm, C is a constant independent of f, and $I(f)$ is the true integral of f

$$I(f) := \int_0^1 f(x)\,\mathrm{d}x.$$

A similar result holds for the left-hand sum. These rules have a classical interpretation: if the integral denotes the (signed) area under the curve $y = f(x)$, then $R_n(f)$ is the area under the piecewise constant approximation to f which is equal to $f(k/n)$ for all $x \in ((k-1)/n, k/n]$, $k = 1, \ldots, n$.

Using this intuition, generalizing is rather straightforward. Rather than piecewise constant, we could instead use a piecewise linear approximant, giving us the trapezoid rule:

$$T_n(f) := \frac{f(0)+f(1)}{2n} + \frac{1}{n}\sum_{k=1}^{n-1} f(k/n).$$

For smooth enough functions this looks much better. And it is! Indeed, one can easily show that

$$|T_n(f) - I(f)| \leq C\|f''\|_\infty n^{-2}.$$

Exercise 1. *Prove this. Note that the increase in accuracy relies on smoothness.*

Exercise 2. *Can you find a counterexample when the function is differentiable, but not twice differentiable?*

Clearly, one could continue on in this way. But, there is a more subtle point that the geometric picture misses. Looking at the formulae for the three rules, we get

$$T_n(f) = \frac{L_n(f) + R_n(f)}{2},$$

and so the trapezoid rule is the average of the left and right. So far, so reasonable. Generically speaking, one "overshoots" the other "undershoots" and the two errors almost cancel. But, returning to the formula for T_n,

$$T_n(f) = \frac{f(0/n)}{2n} + \frac{1}{n}\sum_{k=1}^{n-1} f(k/n) + \frac{f(n/n)}{2n}.$$

In particular, only the endpoints are affected. From this, we conclude that almost all of the error comes only from the endpoints. How should we interpret this?

A first approach: Fourier series

In the following, we will assume that f is smooth, and it, along with all of its derivatives, is periodic (i.e. $f(0) = f(1)$, $f'(0) = f'(1)$, $\cdots$). Then it can be shown that f can be expressed as a Fourier series

$$f(x) = \sum_{m\in\mathbb{Z}} e^{2\pi imx} f_m,$$

where

$$f_m = \int_0^1 e^{-2\pi imx} f(x)\,\mathrm{d}x.$$

In general, one needs much less regularity for the Fourier representation to exist. Later in these notes we will revisit decompositions of this type, exploring under what conditions they are defined and in what sense they converge to f. For now, we will not worry too much about these issues.

After substituting our expression for f into the formula for $T_n(f)$, we find that

$$T_n(f) = \sum_{j=0}^{n-1} \left(\sum_{m\in\mathbb{Z}} e^{2\pi imx_j} f_m \right) \frac{1}{n} = \sum_{m\in\mathbb{Z}} \frac{f_m}{n} \sum_{j=0}^{n-1} \left(e^{2\pi im/n}\right)^j.$$

Here $x_j = j/n$, and we have used the periodicity of f to equate the contributions from $j = 0$ and $j = n$. In particular, as a first sign that there is something interesting happening, for equispaced points the left-hand Riemann rule, the right-hand Riemann rule, and the trapezoid rule all give the same result.

The inner sum on the right-hand side of the previous expression is a truncated geometric series, and can be explicitly summed, which gives

$$\sum_{j=0}^{n-1} \left(e^{2\pi im/n}\right)^j = \begin{cases} n, & e^{2\pi im/n} = 1, \\ \frac{e^{2\pi im}-1}{e^{2\pi im/n}-1}, & e^{2\pi im/n} \neq 1. \end{cases}$$

So,

$$T_n(f) = \sum_{m\in n\mathbb{Z}} f_m.$$

Now, $I(f) = f_0$ and hence

$$E_n(f) := |T_n(f) - I(f)| = \left| \sum_{m\in n\mathbb{Z},\, m\neq 0} f_m \right|.$$

Thus, the speed of the convergence is directly related to the rate of decay of the Fourier coefficients. How does this relate to smoothness?

We begin by observing that if we take the expression for f_m and integrate by parts, for $m \neq 0$,

$$f_m = -\frac{1}{2\pi im} \int_0^1 \frac{\mathrm{d}}{\mathrm{d}x} \left(e^{-2\pi imx}\right) f(x)\,\mathrm{d}x = \frac{1}{2\pi im} \int_0^1 e^{-2\pi imx} f'(x)\,\mathrm{d}x.$$

The boundary conditions arising in the integration by parts disappear because of the periodicity of f and its derivatives. Indeed, now we see an explanation for the heuristic observation that the error is dominated by the endpoints. If f is not periodic then we must keep the boundary terms, which would in turn contribute to slower decay in the Fourier coefficients.

Naturally, if f is smooth enough, then we can iterate, to obtain

$$f_m = \frac{1}{(2\pi i m)^k} \int_0^1 e^{-2\pi i m x} f^{(k)}(x)\, \mathrm{d}x.$$

This formula yields the following bound for f_m

$$|f_m| \leq \frac{1}{2\pi |m|^k} \|f^{(k)}\|_1,$$

and hence

$$E_n \leq \frac{\|f^{(k)}\|_1}{(2\pi)^k} \sum_{j \in \mathbb{Z}, j \neq 0} \frac{1}{|jn|^k} \leq \frac{2\|f^{(k)}\|_1}{(2\pi n)^k} \sum_{j=1}^{\infty} \frac{1}{j^k}.$$

The last sum is independent of f and n, and converges for all $j > 1$. A crude bound can be obtained by comparing it to the integral of $1/x^k$ on $[1, \infty)$, which gives the upper bound $k/(k-1)$. So, for all $n \geq 2$,

$$E_n \leq C \frac{\|f^{(k)}\|_1}{(2\pi n)^k}.$$

Here we see the trade-off between smoothness and integration error very clearly.

A second approach: the Euler-Maclaurin formula

For our next approach, we will use the Euler-Maclaurin formula to bound the error in our quadrature rules. To do so, we need a little bit of notation. Given integers m, n and an integrable function $g : [m, n] \to \mathbb{R}$, we set

$$I_{m,n}(g) = \int_m^n g(x)\, \mathrm{d}x$$

and

$$S_{m,n}(g) = g(m+1) + \cdots + g(n).$$

Theorem 1. *If $k \in \mathbb{N}$ and $g \in C^k([m, n])$ then*

$$S_{m,n} - I_{m,n} = \sum_{j=1}^{k} \frac{B_j}{j!} \left[f^{(j-1)}(n) - f^{(j-1)}(m) \right] + R_k.$$

Here, B_k are the Bernoulli numbers (see Table 1). The remainder term, R_k, is bounded by

$$|R_k| \leq \frac{2\zeta(k)}{(2\pi)^k} \int_m^n |f^{(k)}(x)|\, \mathrm{d}x$$

if k is even. For odd k the Riemann zeta function, $\zeta(k)$, can be omitted.

n	B_n
0	1
1	1/2
2	1/6
4	-1/30
6	1/42
8	-1/30
10	5/66
12	-691/2730
14	7/6
16	-3617/510
18	43867/798
20	-174611/330
⋮	⋮

Table 1. *Bernoulli numbers. All odd Bernoulli numbers greater than one are zero.*

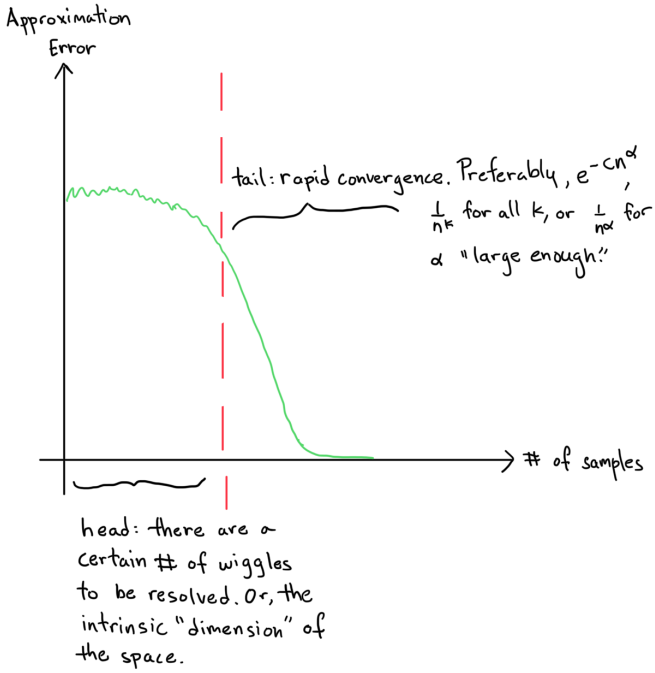
Rescaling to $[0,1]$ and setting $k=2$, $m=0$, we see that

$$T_n(f) - I(f) = \frac{n^{-2}}{12}|f'(1) - f'(0)| + R_2 \in O(n^{-2}).$$

Again, higher-order error terms come from the failure of derivatives of f to be periodic.

Summary

For periodic, smooth functions, the trapezoid, left-hand, and right-hand rules are the gold standard. They converge faster than any power of n (though one has to be a little bit careful with interpreting this). Schematically, the approximation error of an ideal scheme looks like the plot below.



For the trapezoid rule, we use differentiability to get compressibility. Finally, the error is not spread uniformly throughout the interval.

Additional Exercises

Exercise 3. *Assuming that $f \in C^4(0,1)$, construct an improved quadrature rule which computes the integral of f on $(0,1)$ with an error which is $O(h^4)$. Your rule should only involve a constant number of modifications to the standard left-hand or right-hand Riemann sums as $n \to \infty$. Implement your quadrature rule and plot the convergence for: i) $f(x) = e^x$*

and ii) $f(x) = \sqrt{x}$ (of course this isn't differentiable up to the boundary!). Compare your numerical results with those obtained from Simpson's rule – using a cubic approximation on each subinterval, where the cubic is chosen to agree with f at the two endpoints and the midpoint of each subinterval.

The Basics of Bases

In this chapter, our goal will be to formulate means of describing, classifying, and quantifying spaces of functions and notions of distance therein. The properties of the functions we wish to approximate and those with which we approximate them, determine the rate of convergence, the algorithm, and the manner of the proofs. Generic theorems (or algorithms) work for broad classes of functions but then do not typically exploit the unique structure of a specific problem. The same considerations apply to measures of distance, our definition of "success".

More importantly, in applications there is typically a natural "budget" for accuracy of certain quantities, which induce natural objective functions for approximation problems. Do we care about outliers (i.e. catastrophic failure due to rare events, machining parts, etc.)? Or, do we care about the average, or a weighted average, being small (like antenna design)?

One of the most natural and convenient ways of specifying collections of functions is through *bases*. Every finite dimensional linear vector space, E, has a basis - a maximal linearly independent collection of vectors in E. This generalizes (rather unsatisfyingly) to infinite dimensions in the following way.

Definition 1. *A subset $\mathcal{X}$ of a vector space E is a Hamel basis if every vector $v \in E$ can be expressed uniquely as a finite linear combination of elements in $\mathcal{X}$. That is to say, for every $v \in E$, there exist $\alpha_1, \ldots, \alpha_n \in \mathbb{R}$, $v_1, \ldots, v_n \in \mathcal{X}$ such that*

$$v = \sum_{i=1}^{n} \alpha_i v_i.$$

Without more, we are limited to finite sums. In particular, we need a notion of convergence to use infinite sums. Even for relatively pedestrian spaces, $\mathcal{X}$ is typically uncountable.

Proposition 1. *Every linear vector space has a Hamel basis.*

Proof. A somewhat sterile application of Zorn's lemma which we leave to the reader. Note that linear independence involves only finite linear combinations. □

Still, this gives us our first approximation result. We now impose additional structure on our vector spaces, with the hope of obtaining more useful results. In particular, we now focus on the case in which E is a Banach space.

Moving to Banach spaces

Definition 2. *A sequence $\{v_j\}_1^\infty$ in a Banach space X is called a Schauder basis if for all $v \in X$ there exist unique coefficients $\alpha_1, \alpha_2, \dots$ such that*

$$v = \sum_{j=1}^{\infty} \alpha_j v_j,$$

where implicitly we require the sum on the right-hand side in the last expression to converge.

It is easy to show that X must be separable to have a Schauder basis. Unfortunately, this is not sufficient (though finding counterexamples is non-trivial - see Enflo 1973).

The next result allows us to control the size of the partial sums in terms of the norm of v.

Theorem 2. *Suppose $\{v_j\}_1^\infty$ is a Schauder basis of the Banach space X. Then there exists a constant M such that for all $v \in X$,*

$$\left\| \sum_{j=1}^{N} \alpha_j v_j \right\| \leq M \|v\|$$

for all $N = 1, 2, \cdots$. Here, the α_j's are the coefficients such that

$$v = \sum_{j=1}^{\infty} \alpha_j v_j.$$

The minimal M for which the above inequality holds for all M and N is called the basis constant.

Proof. We define a new space E and show that it is isomorphic to X. In particular, set

$$E := \left\{ \{\alpha_j\}_1^\infty \mid \sum_{j=1}^{\infty} \alpha_j v_j \text{ converges in } X \right\}.$$

Moreover, for $\alpha \in E$, set

$$\|\alpha\|_E := \sup_{N \in \mathbb{N}} \left\| \sum_{j=1}^{N} \alpha_j v_j \right\|.$$

It is easily verified that, equipped with this norm, E is a Banach space. Moreover, clearly there is a bounded bijection from E to X. Thus, by the inverse mapping theorem, this is an isomorphism. □

Now, for each positive integer N we can define the operator $S_N : X \to \mathbb{R}$ by

$$S_N(v) := \sum_{j=1}^{N} \alpha_j v_j,$$

where again $\{v_j\}_1^\infty$ is a Schauder basis and the $\{\alpha_j\}_1^\infty$ are the corresponding coefficients of v. Note that the α_j are independent of N. Clearly S_N is a projection onto the span of $\{v_1, \ldots, v_N\}$ and, by the previous theorem, all the S_N's are uniformly bounded. It follows that that the coefficients are linear functionals on X, called *biorthogonal functionals*, and are denoted by v_j^*. Hence,

$$v = \sum_{j=1}^{\infty} v_j v_j^*(v).$$

Clearly,

$$\|v_j\||v_j^*(v)| = \|v_j v_j^*(v)\| = \|\|S_j(v) - S_{j-1}(v)\| \leq 2M\|v\|$$

and so $\|v_j\|\,\|v_j^*\| \leq 2M$ for all j.

This gives a slick characterization of compactness.

Theorem 3. *A subset $A \subset X$ is compact if and only if A is bounded and the basis expansions converge uniformly, i.e.*

$$\|v - S_N(v)\| \leq \epsilon_N \to 0,$$

for all $v \in A$.

Note here that the ϵ_N do not depend on v.

Proof. Necessity: from above, we know that S_N converges to the identity operator pointwise. Using a standard ϵ-net argument, since convergence is uniform on compact sets, it follows that S_N converges uniformly to the identity on A.
Sufficiency: For any ϵ, there exists an N such that $\|v - S_N(v)\| \leq \epsilon$ for all $v \in A$. The image of S_N is a finite dimensional subspace and $A \subset \mathcal{N}_\epsilon(S_N)$ (A is contained within an ϵ-neighborhood of the image of S_N). □

We now impose even more mathematical structure to obtain stronger results. For Banach spaces we added a notion of length. Going to Hilbert spaces, we now also add a notion of angle.

Hilbert spaces

Definition 3. *A set $\{v_j\}_1^\infty$ in H (a Hilbert space) is an orthogonal system if $\langle v_j\,,\, v_k\rangle = 0$ for all $j \neq k$. It is orthonormal if additionally $\|v_j\| = 1$ for all j.*

Theorem 4. *Let $\{v_j\}_1^\infty$ be an orthogonal system. The following are equivalent:*

i $\sum_j \alpha_j v_j$ *converges in* H

ii $\sum_j |\alpha_j|^2 \|v_j\|^2 < \infty$

iii $\sum_j \alpha_j v_j$ *converges unconditionally*

If there is convergence then

$$\|\sum_j \alpha_j v_j\|^2 = \sum_j |\alpha_j|^2 \|v_j\|^2.$$

Proof. We leave the proof as an exercise. □

Definition 4. *Let $\{v_j\}_1^\infty$ be an orthonormal system in H. The* Fourier series *of v with respect to $\{v_j\}_1^\infty$ is*

$$\sum_{j=1}^{\infty} \langle v_j, v\rangle v_j.$$

The scalar quantities $\langle v_j, v\rangle$ are called the Fourier coefficients.

We end this section with several useful results about orthonormal systems on Hilbert spaces.

Lemma 1. *If $\{v_j\}_1^\infty$ is an orthonormal system then for each N, S_N is an orthogonal projection.*

Lemma 2 (Bessel's inequality)**.** *If $\{v_j\}_1^\infty$ is again an orthonormal system in a Hilbert space H,*

$$\sum_{j=1}^{\infty} |\langle v_j, v\rangle|^2 \leq \|v\|^2.$$

We also have the following optimality result.

Lemma 3. *Among all convergent sequences $s = \sum_j \alpha_j v_j$, $\|v - s\|$ is minimized by the Fourier series of v. The same is true of partial sums.*

Thus, finding a best approximation from a subspace is easy in a Hilbert space provided we have an orthonormal system. Here we should add that "best" is being measured with respect to the norm of the Hilbert space. A natural follow-up question is how to find orthonormal systems. If H is separable, it's easy, at least in practice. Just apply Gram-Schmidt to the countably dense set.

Projections

Projection operators arise naturally in approximation theory. Here we briefly review some general theory of projections which will be useful throughout these notes.

Definition 5. *Given a Banach space E, the linear operator $P : E \to E$ is called a* projection *if it is bounded and* idempotent, *i.e. $P^2 = P$.*

The following theorem gives a handy characterization of projections.

Theorem 5. *Suppose $P : E \to E$ is a projection and $\mathcal{R}(P) = V$. Then V is a closed subspace of E, and $V = \ker(I - P)$. Here I is the identity operator on E.*

Proof. To prove the first assertion, note that $I - P$ is continuous, so its kernel is closed. Thus, it suffices to show that $V = \ker(I - P)$. To see this, observe that if $v \in V$, then there exists a $u \in E$ such that $Pu = v$. Then $Pv = P^2u = Pu = v$. Thus $v \in \ker(I - P)$ and hence $V \subseteq \ker(I - P)$. Similarly, if $w \in \ker(I - P)$ then $Pw = w$ and so $w \in V$, implying the reverse inclusion. □

Given a projection P, there are a few other natural projections we can construct.

Proposition 2. *Let $P : E \to E$ be a projection. Then $(I - P) : E \to E$ is also a projection. So is the adjoint of P, $P^* : E^* \to E^*$.*

Proof. Both are clearly linear and bounded. For idempotency, for $I - P$, we observe that $(I - P)^2 = I - 2P + P^2 = I - P$. For the adjoint, recall that it is defined by: $(P^*\ell)(v) = \ell(Pv)$, for all $v \in E$. Hence, $((P^*)^2\ell)(v) = (P^*\ell)(Pv) = \ell(P^2v) = \ell(Pv) = (P^*\ell)(v)$. □

Given two projections, $P, Q : E \to E$ it is natural to ask whether it is possible to combine them. Unfortunately, in general, neither PQ nor QP are projections. The following result gives some conditions on which certain new projections can be created from two existing ones.

Proposition 3. *Let $P, Q : E \to E$ be two projections. Define the operator $P \oplus Q = P + Q - PQ$. Suppose $PQP = QP$. Then*

1. *$P \oplus Q$ is a projection onto $\mathcal{R}(P) + \mathcal{R}(Q)$.*
2. *QP is a projection onto $\mathcal{R}(P) \cap \mathcal{R}(Q)$.*

Proof. The proof follows by a direct calculation.

$$\begin{aligned}(P \oplus Q)^2 &= (P + Q - PQ)^2 = (P^2 + PQ - P^2Q) + (QP + Q^2 - QPQ) - (PQP + PQQ - PQPQ) \\ &= P + QP + Q - QPQ - PQP - PQ + (PQP)Q = P + Q - QPQ - PQ + QPQ \\ &= P + Q - PQ.\end{aligned}$$

Moreover, $(P \oplus Q)P = P$, and so $(P \oplus Q)u = u$ for all $u \in \mathcal{R}(P)$. Similarly, $(P \oplus Q)Q = Q$ and hence $(P \oplus Q)v = v$ for all $v \in \mathcal{R}(Q)$. If $w \in \mathcal{R}(P) + \mathcal{R}(Q)$ then $w = u + v$ where $u \in \mathcal{R}(P)$ and $v \in \mathcal{R}(Q)$. From above, both u and v are fixed by $P \oplus Q$. □

Remark 1. *The operator $P \oplus Q$ is called the* Boolean sum *of the linear operators.*

We finish our discussion with the following result which shows that if we are willing to consider only a finite-dimensional subspace U, a projection onto U always exists, and the norm is not too big.

Theorem 6. *Let U be an n-dimensional subspace of a Banach space E. There exists a projection $P : E \to U$ with norm at most n.*

Proof. Before proving the main result we need the following tool from functional analysis (it is a simplified version of Auerbach's theorem):

If U is an n-dimensional normed space, then there exist vectors $u_1, \cdots, u_n$ and functionals $\ell_1, \cdots, \ell_n$ such that $\|u_i\| = 1$, $\|\ell_i\|_1, 1, \cdots, n$, and $\ell_j(u_i) = \delta_{i,j}$.

We sketch the proof briefly. Let $v_1, \cdots, v_n$ be a basis of U. Define $M : (U^*)^{\otimes n} \to \mathbb{R}$, by $M(\nu_1, \cdots, \nu_n) = |\det(\nu_j(v_i))|$. Since U^* is finite-dimensional, M attains its maximum m_* in the unit ball $B_{U^*} \times \cdots B_{U^*}$ at some point $(\ell_1, \cdots, \ell_n)$. Note that $m_* > 0$ since otherwise $A_{i,j} = \nu_j(v_i)$ would have a left nullvector for any choice of ν's. This in turn would imply that there is a v such that $\ell(v)$ for all $\ell \in U^*$ (just choose $\nu_1, \cdots, \nu_n$ to be a basis of U^* for example).

Now set $A_{j,i} = \ell_i(v_j)$ and let $C = A^{-1}$. We set $u_j = \sum_{k=1}^n C_{j,k} v_k$. It is easy to see that $\ell_i(u_j) = \delta_{i,j}$, $1 \le i, j \le n$. To show the bound on $\|u_j\|$, note that for any $\psi \in E^*$,

$$\psi(u_i) = \sum_{j=1}^n C_{i,j} \psi(v_j).$$

Next, we observe that $C_{i,j}\psi(v_j)$ (as a vector) is a solution to the equation $Ax = \psi(\vec{v})$. By Cramer's rule,

$$\sum_{j=1}^n C_{i,j} \psi(u_j) = \frac{\det A_i}{\det(A)},$$

where A_i is the matrix formed by replacing the ith column with $\psi(u_j)$. In particular,

$$|\psi(u_i)| = \left| \frac{M(\ell_1, \cdots, \ell_{i-1}, \psi, \ell_{i+1}, \cdots, \ell_n)}{M(\ell_1, \cdots, \ell_n)} \right| \le \|\psi\|.$$

Thus, since ψ was arbitrary, $\|u_i\| \le 1$.
We now turn to the proof of the theorem. From Auerbach's theorem, we can find $u_1, \cdots, u_n \in U$ and $\ell_1, \cdots, \ell_n \in U^*$. By Hahn-Banach, the latter can be extended to act on all of E, while not increasing the

norm. Then, set $P(v) = \sum_i u_i \ell_i(v)$. Clearly, $\mathcal{R}(P) = U$ and $P^2 = P$. Finally,

$$\|Pv\| = \|\sum_i u_i \ell_i(v)\| \leq \sum_i \|u_i\|\|\ell_i\|\|v\| \leq n\|v\|.$$

□

Further reading

There are many good functional analysis textbooks which cover this. See the notes from R. Vershynin, for example. For projections, see *A Comprehensive Course in Analysis, Volume 5* by B. Simon. For a more applied approach, see *A Course in Approximation Theory* by W. Cheney and W. Light.

Additional Exercises

Exercise 4. *Let $\{v_j\}_{j=1}^{\infty}$ be an orthonormal basis of a Hilbert space H. Let A be a bounded operator from H to itself with bounded inverse. Consider the sequence of vectors $w_j := Av_j$. Is $\{w_j\}_1^{\infty}$ an orthonormal basis? A Schauder basis? If so, can you bound its basis constant?*

Exercise 5. *Let $\psi : \mathbb{R} \to \mathbb{R}$ be the function defined by*

$$\psi(x) = \begin{cases} 0, & x \notin (0,1), \\ 2x, & x \in [0, 1/2], \\ 2(1-x), & x \in [1/2, 1]. \end{cases}$$

For $i = 0, \cdots, \infty$ and $k = 0, \cdots, 2^i - 1$ define $\psi_{i,k}$ by

$$\psi_{i,k}(x) = \psi(2^i x + k).$$

Consider the collection of functions $\mathcal{X} = \{1, x, \psi_{0,0}, \psi_{1,0}, \psi_{1,1}, \psi_{2,0}, \cdots\}$. Sketch the first five functions of $\mathcal{X}$ on $[0,1]$. Show that $\mathcal{X}$ is a Schauder basis of $C([0,1])$.

Exercise 6. *Let H be a Hilbert space and let $P, Q : H \to H$ be two projections. In the following, set $C = i[P,Q] = i(PQ - QP)$. We also assume that P and Q are* orthogonal, *i.e. $P^* = P$ and $Q^* = Q$.*

a) Find explicit examples of P and Q which do not commute. Make sure to give clear definitions of both them and H. Sketch a geometric characterization of when this happens.

b) Show that $0 \leq \langle v, Pv \rangle \leq 1$ for all $v \in H$.

c) For any $v \in H$, set $\bar{P}(v) = \langle v, Pv \rangle$, $\bar{Q}(v) = \langle v, Qv \rangle$, $\sigma_P^2(v) = \langle v, (P - \bar{P}\, I)^2 v \rangle$ and $\sigma_Q^2(v) = \langle v, (Q - \bar{Q}\, I)^2 v \rangle$. Show that $\sigma_P, \sigma_Q \leq \|v\|/2$. Here I is the identity operator on H.

d) If C is the commutator of P and Q, show that $\frac{1}{4}|\langle v, Cv\rangle|^2 \leq \sigma_P^2(v)\sigma_Q^2(v)$. Argue that $\|C\| \leq 1/2$. Hint: use Cauchy-Schwarz. For the last part, you can use without proof that $\|C\| = \sup_{\|v\|\leq 1} |\langle v, Cv\rangle|$ (this follows from the fact that C is Hermitian).

Some General Principles of Approximation Theory

In the following, we take X to be a Banach space. If A is a nonempty subset of X, we set

$$d(v, A) := \inf_{u \in A} \|v - u\|.$$

Notation 1. *Given $v \in X$, let $P_A(v)$ denote the set of nearest points to v in A, i.e. the set of best approximations to v in A.*

$$P_A(v) := \{u_0 \in A \mid \|v - u_0\| = d(v, A)\}.$$

Definition 6. *A set A is called an* existence set *if $P_A(v)$ is nonempty for all $v \in A$, and a* uniqueness set *if the cardinality of $P_A(f)$ is always at most one. A is called a* Chebyshev set *if it is an existence and uniqueness set.*

Clearly, existence sets are closed, but closed does not imply existence.

Example 1. *Set $X = \ell_2$, $A = \{(1 + 1/j)e_j\}_1^\infty$ where e_j denotes the jth canonical basis vector. This is closed, but not an existence set.*

Example 2. *Set $X = \ell_\infty$, $A = \{v \in \ell_\infty \mid \|v\|_\infty \leq 1\}$. This is an existence set, but not a uniqueness set.*

Example 3. *Set X to be a normed vector space and A any finite dimensional linear subspace. Then A is an existence set. This follows from a theorem by F. Riesz that says that if $v \in X$, then $B_{2\|v\|} \cap A$ is compact. B_r here denotes the ball of radius at r centered at the origin.*

Lemma 4. *If A is convex, then $P_A(v)$ is always convex.*

Proof. Given $v \in X$ suppose u_0 and u_1 in $P_A(v)$. For any $\lambda \in [0, 1]$ set $u_\lambda = \lambda u_0 + (1 - \lambda)u_1$. Then

$$\begin{aligned} \|v - u_\lambda\| &= \|\lambda(v - u_0) + (1 - \lambda)(v - u_1)\| \\ &\leq \lambda\|v - u_0\| + (1 - \lambda)\|v - u_1\| \\ &= d(v, A). \end{aligned}$$

□

In order to get more control on existence and uniqueness, we can introduce some additional geometric assumptions on the space X. Let $S = \partial B$ where B is the unit ball in X.

- X is *strictly convex* if for all $u, v \in S$ with $u \neq v$, $\|u + v\| < 2$.
- X is *uniformly convex* if, given $\epsilon > 0$, there is a $\delta = \delta(\epsilon)$ such that for any $u, v \in S$ with $\|u + v\| > 2 - \delta$ then $\|u - v\| < \epsilon$.
- X is *smooth* if for each $v \in S$, there is a unique supporting functional (i.e. $\ell \in X^*$ with $\|\ell\| = 1$ and $\ell(v) = \|v\|$).

As a counterexample, consider the space of $\{\alpha_j\}$ equipped with the norm

$$\|\{\alpha_j\}\| := \left(\sum_{j=1}^{\infty} \frac{1}{j^2} |\alpha_j|^2\right)^{1/2} + \sum_{j=1}^{\infty} \left(1 - \frac{1}{j}\right) |\alpha_j|$$

Lemma 5. *If M is convex and the space is strictly convex, then M is a uniqueness set.*

Remark 2. *Note that $C(X)$ is not strictly convex (exercise: prove this). To characterize uniqueness in this space, other tools are required.*

A geometric criterion for best approximations

Using geometric tools from functional analysis, we now formulate a general criterion for best approximations.

Theorem 7. *Suppose M is a convex set in a Banach space X, and $v \in X$, $v \notin \overline{M}$. Then u_0 is a best approximation to v in M if and only if there is a linear functional $\ell \in X^*$ satisfying the following conditions:*

i) $\|\ell\|_{X^*} = 1$,

ii) $\ell(v - u_0) = \|v - u_0\|$

iii) $\Re\, \ell(u - u_0) \leq 0$ *for all* $u \in M$.

Proof. The main ingredient of the proof in the forward direction will be the geometric Hahn-Banach theorem, a simplified version of which states:

Suppose A and B are disjoint non-empty convex subsets of a Banach space X. Moreover, suppose A is open. There exists a bounded linear functional $\ell \in X^*$, and a real number α such that

$$\Re\, \ell(u) < \alpha \leq \Re \ell(v)$$

for all $u \in A$ and $v \in B$.

Now, we suppose u_0 is a best approximation to v from M. We set $r = \|u_0 - v\|$ and let $\mathring{B}_r(v)$ denote the interior of the ball of radius r in X which is centered at v. Then $\mathring{B}_r(v)$ and $\overline{M}$ are disjoint and so, by the geometric Hahn-Banach theorem, there exists an $\tilde{\ell} \in X^*$

and $\alpha \in \mathbb{R}$ with $\Re\,\tilde{\ell}(\mathring{B}_r(v)) > \alpha$ and $\Re\tilde{\ell}(\overline{M}) \leq \alpha$. In particular, $\Re\tilde{\ell}(B_r(v)) \geq \alpha$.

Now we set $\beta = \Re\tilde{\ell}(v - u_0)$ and $\ell = \frac{r}{\beta}\tilde{\ell}$. Clearly, by linearity

$$\Re\,\ell(v - u_0) = \|v - u_0\|.$$

This is a start, but we still need to: a) prove boundedness, b) remove the '$\Re$' from the previous equality. We argue by contradiction: suppose $\|\ell\| > 1$. Then, there exists $w \in B_r(0)$ with $\ell(w) > r$. Setting $z = v - w$, we observe that $z \in B_r(v)$, but

$$\Re\,\tilde{\ell}(z) = \Re\,\tilde{\ell}(v - u_0) + \Re\,\tilde{\ell}(u_0) - \Re\,\tilde{\ell}(w) \leq \beta + \alpha - \frac{\beta}{r}\ell(w) < \alpha.$$

This yields a contradiction, since $z \in B_r(v)$ implies that $\Re\,\tilde{\ell}(z) \geq \alpha$. Thus, $\|\ell\| = 1$ and hence $\ell(v - u_0) = \|v - u_0\|$.

In the other direction, assume such an ℓ exists. Then for any $u \in M$,

$$\|u - v\| \geq \Re\,\ell(v - u) = \Re\,\ell(v - u_0) - \Re\,\ell(u_0 - u) \geq \|v - u_0\|.$$

□

Remark 3. *This can be modified to allow for the choice of a different functional for each element of M. In this form it is called the* generalized Kolmogorov criterion.

Example 4. *$X = H$ a Hilbert space. A point u_0 in a convex set M is a best approximation to $v \in H$ if and only if*

$$\Re\langle v - u_0, u - u_0\rangle \leq 0,$$

for any $u \in M$.

Example 5. *$X = L_p(X, \mu)$, $1 < p < \infty$. If M is a* subspace *of X, then $u_0 \in M$ is a best approximation to $v \in L_p(X, \mu)$ if and only if*

$$\int_X |v(x) - u_0(x)|^{p-2}(\overline{v}(x) - \overline{u_0}(x)) = 0$$

for all $u \in M$.

In the next section we dive into the theory for approximation of continuous functions in a little more detail.

Haar subspaces and continuous functions

For spaces of continuous functions equipped with the supremum norm, *Haar subspaces* give a convenient characterization of when a unique best approximation to a given function exists in a subspace.

Definition 7. *A Haar subspace M is an n-dimensional subspace of $C(\Omega)$ such that any $u \in M$ has at most $n-1$ zeros in Ω.*

Lemma 6. *M is an n-dimensional Haar subspace if and only if for any n points $x_1, \ldots, x_n \in \Omega$ and $\beta_1, \ldots, \beta_n \in \mathbb{C}$ the interpolation problem:*

$$\text{Find } u \in M \text{ such that } u(x_i) = \beta_i,\ i = 1, \ldots, n$$

always has a solution.

Remark 4. *This is equivalent to saying that given any bais $u_1, \ldots, u_n$, the $n \times n$ matrix Φ defined by $(\Phi)_{i,j} = u_j(x_i)$ is invertible for any distinct points $x_1, \ldots, x_n$.*

A natural question is: who cares? The answer is given in the following theorem (which we won't prove here).

Theorem 8 (Haar's uniqueness theorem)**.** *If X is locally compact, then a finite dimensional subspace M of $C(\Omega)$ is a Haar subspace if and only if every $f \in C(\Omega)$ has a unique best approximation in M, i.e. M is a Chebyshev set.*

Unfortunately, as it turns out, having high-dimensional Haar subspaces is somewhat difficult.

Theorem 9 (Mairhuber-Curtis theorem)**.** *Suppose $\Omega \subseteq \mathbb{R}^d$, $d \geq 2$ contains an interior point. Then there is no Haar subspace of $C(\Omega)$ of dimension $n \geq 2$.*

Proof. Given a basis $u_1, \ldots, u_n$ consider the function $d(x_1, \ldots, x_n) = \det(u_j(x_i))$. Since the u_j are continuous, so is d. Consider two points x_1 and x_2 lying in a ball $B_r(x_*) \subset \Omega$ for some $r > 0$ and $x_* \in \Omega$. Note that the existence of such a ball is guaranteed by the condition that Ω have non-empty interior. Let $x_3, \ldots, x_n$ be arbitrary in Ω. Consider two non-intersecting continuous paths $\gamma_{1,2} : [0,1] \to \Omega$ with $\gamma_1(0) = x_1, \gamma_1(1) = x_2, \gamma_2(0) = x_2, \gamma_2(1) = x_1$ chosen so that both γ_1 and γ_2 do not pass through $x_3, \ldots, x_n$. Then, since $d(x_1, x_2, \ldots, x_n) = -d(x_2, x_1, \ldots, x_n)$ and $d(\gamma_1(t), \gamma_2(t), x_3, \ldots, x_n)$ is continuous as a function of t, there exists a $t_* \in [0,1]$ for which d vanishes. □

In fact this has deeper implications. It shows that for interpolation in dimensions $d \geq 2$, one cannot in general used a fixed data for arbitrary scattered data. We will see more about Haar spaces later in these notes when we discuss polynomial approximations of continuous functions.

Interpolation in finite dimensional subspaces

In the last section, we reached a somewhat depressing conclusion: colloquially, except in one dimension given a fixed basis there always exists a set of points for which the interpolation problem is

not solvable. But, we could take the opposite perspective: given a finite dimensional subspace, find points $x_1, \ldots, x_n$ which are good for interpolation.

Let us be a bit more precise. Let S be an arbitrary set with $|S| \geq n$ and $u_1, \ldots, u_n : S \to \mathbb{C}$ be bounded and linearly independent. Moreover, suppose $u : S \to \mathbb{C}$ is defined by

$$u(x) = \sum_{j=1}^{n} \alpha_j u_j(x)$$

for some (unknown) coefficients α_j. For interpolation our goal is the following:

Given points $x_1, \ldots, x_n \subseteq S$ and samples $u^{(1)} = u(x_1), \ldots, u^{(n)} = u(x_n)$, find functions $v_j : S \to \mathbb{C}$ such that

$$u(x) = \sum_{j=1}^{n} v_j(x) u^{(j)}.$$

Clearly, a necessary and sufficient condition is

$$d(x_1, \ldots, x_n) := \det(u_j(x_i)) \neq 0.$$

Also, clearly for generic problems many choices of $x_1, \ldots, x_n$ are possible. Are some better than others computationally?

Idea 1: We could try to choose sample points $x_1^*, \ldots, x_n^*$ such that

$$(x_1^*, \ldots, x_n^*) = \operatorname{argmin}_{(x_1, \ldots, x_n) \in S^n} \kappa(u_j(x_i))$$

if possible. Here κ denotes the condition number of the matrix with (i, j)th entry $u_j(x_i)$. Of course many related conditions are possible. This approach tries to make the *coefficient recovery problem* as stable as possible. Note that even with optimal points, this might still be very poorly conditioned! For example, choosing $u_j(x) = 1 + \epsilon \sin(j\pi x)$. Though this seems rather pathological, situations like this arise frequently in applications. This is also somewhat roundabout since we only need v_j, though of course we could find it by setting

$$v_j(x) := \sum_{j=1}^{n} A_{i,j}^{-1} u_i(x),$$

where $A_{i,j} = u_j(x_i)$.

Idea 2: Using the previous definition of A it is easy to show that for any $x \in S$,

$$\sum_{j=1}^{n} A_{i,j} v_j(x) = f_i(x), \quad i = 1, \ldots, n.$$

Cramer's rule then gives

$$v_j(x) = \frac{d(x_1, \ldots, x_{i-1}, x, x_{i+1}, \ldots, x_n)}{d(x_1, \ldots, x_n)}.$$

The interpolation will be numerically unstable if $\|v_j\|_\infty \gg 1$. In particular, oscillations in signs of the v_j will lead to numerical catastrophic cancellation. A natural goal then is to try to make the norms of the v_j small.

We first claim that

$$B := \sup_{(x_1,\ldots,x_n)\in S^n} < \infty$$

and $B > 0$.

Next, we claim that for any $0 < \epsilon < 1$ there exist points $x_1^*, \ldots, x_n^*$ with

$$d(x_1^*, \ldots, x_n^*) \geq B \max(1/2, 1 - \epsilon/2).$$

Choosing these points, and using our formula for v_j, together with the identity

$$\frac{B}{d} - 1 \leq \epsilon,$$

we find that

$$|v_j(x)| \leq \frac{B}{d} \leq 1 + \epsilon.$$

Remark 5. *For continuous functions we can choose $\epsilon = 0$.*

Two fundamental approximation problems

In the last two sections we have seen two fundamental problems in approximation theory:

- The "measurement" or "sampling" problem: given the value of a function at a collection of points, approximate its value at another location. Colloquially,

  given points, choose functions

- The "experimental" or "design" problem: given a collection of functions, choose points which allow stable interpolation. Colloquially

  given functions, choose points

Exercises

Exercise 7. *Assume that u_1 and u_2 are two best L_1 approximations to f from a convex set M. Moreover, assume that all three functions are continuous. Show that*

$$\operatorname{sgn}(f - u_1)(x) = \operatorname{sgn}(f - u_2)(x),$$

for all $x \in X$. Here we assume that f and all the functions in M are real-valued.

Exercise 8. *Prove or give a counter-example: every subspace of a Haar subspace is a Haar subspace.*

Exercise 9. *Show that if Ω contains a subset homeomorphic to the letter 'Y' then $C(\Omega)$ cannot contain a Haar subspace of dimension greater than one.*

Exercise 10. *Given $x_1, \ldots, x_n \in \mathbb{R}$, find an expression for the determinant of the $n \times n$ matrix V with (i, j)th entry x_i^{j-1}. Use this to show that the monomials form a Haar subspace. Hint: argue that the determinant is a polynomial in each x_i and the total degree is at most $n(n+1)/2$. Show that $(x_1 - x_2)$ must be a factor of the determinant and use this to guess a general form for the determinant.*

Exercise 11. *Let $\lambda_1, \ldots, \lambda_n \in \mathbb{R}_+$ and consider the set of functions $u_j : \mathbb{R}_+ \to \mathbb{R}$ with $u_j(x) = e^{-\lambda_j x}$. Show that the u_j are linearly independent and form a Haar subspace of $C(\mathbb{R}_+)$. Hint: use induction and Rolle's theorem.*

Continuous Functions

So far we have discussed a variety of results related to the existence and uniqueness of best approximations. We have even discussed a little bit about how to represent them and how to use them. One glaring hole in all this is that we so far haven't actually said much about how good these "best approximations" are! Of course, this is intimately related to the existence of "good" bases and the decay of coefficients in those bases.

In this part, we focus on continuous functions and give several results on when a given collection of functions can approximate an arbitrary one.

Our first goal is as follows: prove (and define the terms in) the following result.

Theorem 10 (Stone-Weierstrass[1])**.** *Let X be a compact metric space and $\mathcal{A}$ be a subalgebra of $C(X)$. If $\mathcal{A}$ separates points in X and vanishes at no point in X then $\mathcal{A}$ is dens in $C(X)$. Here $\mathcal{A}$ and $C(X)$ consist of real-valued functions.*

[1] Marshall H. Stone was chair of the mathematics department of the University of Chicago from 1946-1952. He was partly responsible for bringing André Weil, Antoni Zygmund, Saunders MacLane, Shiing-Shen Chern, Paul Halmos, Irving Segal and Edwin Spanier to Chicago. This period is sometimes called the "Stone age".

Before proving the theorem we recall some definitions. Firstly, a vector space $\mathcal{A}$ is an algebra if there is a multiplication operation such that

i) $(fg)h = f(gh)$

ii) $f(g+h) = fg + fh$ where "$+$" denotes the vector space addition operation

iii) $\alpha(fg) = (\alpha f)g = f(\alpha g)$ for any scalar α.

We say: $\mathcal{A}$ is commutative if $fg = gf$; has an identity if there exists $e \in \mathcal{A}$ with $ef = fe = f$ for all $f \in \mathcal{A}$; and is normed if $\|\cdot\|$ satisfies the usual norm properties *and* $\|fg\| \leq \|f\|\,\|g\|$. If $\mathcal{A}$ is normed and complete then it is a Banach algebra.

We say that $\mathcal{A}$ *separates points* if for any $x, y \in X$, with $x \neq y$ there is an $f \in \mathcal{A}$ with $f(x) \neq f(y)$.

We now turn to the proof.

Proof. The proof consists of three parts:

1. First, we show that for all $f \in \mathcal{A}$, $|f| \in \overline{\mathcal{A}}$. From this we deduce that for any $f_1, \ldots, f_n \in \mathcal{A}$, the function $\max\{f_1, \ldots, f_n\} \in \overline{A}$.
2. Next, we show that for any $\epsilon > 0$, for any $f \in C(X)$, and for any $x \in X$, there exists a function $f_x \in \overline{\mathcal{A}}$ such that $g_x(x) = f(x)$, and
$$g_x(y) > f(x) - \epsilon, \quad \forall y \in X.$$
3. Finally, we show that using a finite number of the g_x functions constructed in the previous step, we can construct a function $g \in \overline{\mathcal{A}}$ with $|f(y) - g(y)| < \epsilon$ for all $y \in X$.

We sketch some details of these steps below.

1: Given $f \in \mathcal{A}$ we wish to show that $|f|$ can be approximated from within $\mathcal{A}$. Here we use a neat idea. Given any polynomial p, since $\mathcal{A}$ is an algebra, $fp(f) \in \mathcal{A}$. Thus, it suffices to find a polynomial $x\,p(x)$ which approximates $|\cdot|$ on $[-\|f\|_\infty, \|f\|_\infty]$. Without loss of generality we set $\|f\| = 1$. In particular, the problem has been reduced from finding an approximation from a continuous function defined on an *arbitrary* compact metric space from a general algebra, to approximating a *specific* function (absolute value) from a *specific* algebra (namely polynomials restricted to the interval $[-1, 1]$).

We begin by observing that for any $s \in [-1, 1]$,
$$|s| = \sqrt{1 - (1 - s^2)} = \sum_{n=0}^{\infty} (1 - s^2)^n (-1)^n \binom{\frac{1}{2}}{n},$$
which converges uniformly on $[-1, 1]$.

Letting q_N denote the N^{th} partial sum, then we have that for any $\epsilon > 0$ there exists an N such that $|q_N(s) - |s|| < \epsilon$ for any $s \in [-1, 1]$. Now, it follows that $q_N(0)| < \epsilon$ and so $|q_N(s) - q_N(0) - |s|| < 2\epsilon$. Finally, since $q_N(s) - q_N(0) = s p_N(s)$ for some polynomial p_N, we have that $q_N(f) - q_N(0) \in \mathcal{A}$.

2: For any x, y with $x \neq y$ there exists an $h_{y,x} \in \mathcal{A}$ with $h_{y,x}(x) = f(x)$, $h_{y,x}(y) = f(y)$. To see this, we note that $\tilde{\mathcal{A}} := \{(g(x), g(y)),\, g \in \mathcal{A}\}$ is a subalgebra of $\mathbb{R}^2$. It is easy to argue that it must in fact be all of $\mathbb{R}^2$, since $\mathcal{A}$ separates points and vanishes at no point in X.

Now, we argue by compactness that there are a finite number of y's such that
$$g_x(t) := \max\{h_{y_1,x}(t), \ldots, h_{y_n,x}(t)\} \geq f(t) - \epsilon, \quad \forall t \in X.$$

3: Finally, we argue by compactness of X that there are a finite number of x's such that
$$\min\{g_{x_1}(t), \ldots, g_{x_n}(t)\} \leq f(t) + \epsilon, \quad \forall t \in X.$$

□

Remark 6. *For the complex case, $\mathcal{A}$ should be self-conjugate (i.e. if $f \in \mathcal{A}$ then $\overline{f} \in \mathcal{A}$).*

Corollary 1. *The set of all functions $f(x,y) = f(x)g(y)$ with $f \in C(X), g \in C(Y)$ is dense in $C(X \times Y)$.*

Corollary 2. *If K is a compact subset of $\mathbb{R}^n$, then the set of all n-variate polynomials is dense in $C(K)$.*

This is great in that it gives us a (sort of) constructive way of obtaining an approximation of arbitrary fidelity. For polynomials (particularly in one dimension) it is overkill and the construction is a bit clunky. For polynomials on $[0,1]$ we will now give a few alternate proofs. Apart from being more constructive, they highlight interesting techniques that are frequently used in other contexts.

Theorem 11 (Weierstrass approximation theorem)**.** *For any $f \in C[0,1]$ and $\epsilon > 0$ there exists a polynomial p such that $\|f - p\| < \epsilon$.*

proof (Bernstein): For any bounded f on $[0,1]$ define the *Bernstein polynomial of f* by

$$B_n(f)(x) = \sum_{k=0}^{n} f\left(\frac{k}{n}\right) \binom{n}{k} x^k (1-x)^{n-k}, \quad 0 \le x \le 1.$$

In particular,

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

Also,

$$\begin{aligned} B_n(x)(x) &= \sum_{k=0}^{n} \binom{n}{k} \frac{k}{n} x^k (1-x)^{n-k} = \sum_{k=0}^{n} \binom{n-1}{k-1} x^k (1-x)^{n-k} \\ &= \sum_{k=0}^{n-1} \binom{n-1}{k-1} x^{k+1} (1-x)^{n-1-k} \\ &= x. \end{aligned}$$

Finally,

$$\begin{aligned} B_n(x^2)(x) &= \sum_{k=0}^{n} \binom{n}{k} \frac{k^2}{n^2} x^k (1-x)^{n-k} \\ &= \frac{s}{n} \frac{\partial}{\partial s} s \frac{\partial}{\partial s} (s+t)^n \Big|_{s=x,t=1-x} = s(s+t)^{n-1} \Big|_{s=x,t=1-x} - \frac{n-1}{n} st(s+t)^{n-2} \Big|_{s=x,t=1-x} \\ &= x - x(1-x)\frac{n-1}{n} \\ &= x^2 \left(1 - \frac{1}{n}\right) + \frac{x}{n}. \end{aligned}$$

So, B_n is exact on 1 and x and converges like $1/n$ for x^2.

Continuing, given a $\delta > 0$ we let F denote the set of $k \in \{0, \ldots, n\}$ for which

$$\left| \frac{k}{n} - x \right| \geq \delta.$$

Then

$$\begin{aligned}
\sum_{k \in F} \binom{n}{k} x^k (1-x)^{n-k} &\leq \frac{1}{\delta^2} \sum_{k \in F} \binom{n}{k} \left(\frac{k}{n} - x \right)^2 x^k (1-x)^{n-k} \\
&\leq \frac{1}{\delta^2} \sum_{k=0}^{n} \binom{n}{k} \left(\frac{k}{n} - x \right)^2 x^k (1-x)^{n-k} \\
&\leq \frac{1}{\delta^2} \left[x^2 B_n(1)(x) - 2x B_n(x) + B_n(x^2)(x) \right] \\
&= \frac{1}{\delta^2} \left[x^2 - 2x^2 + x^2 \left(1 - \frac{1}{n} \right) + \frac{x}{n} \right] \\
&= \frac{x - x^2}{n\delta^2} \\
&\leq \frac{1}{4n\delta^2}.
\end{aligned}$$

Then,

$$\begin{aligned}
|f(x) - B_n(f)(x)| &\leq \left| f(x) - \sum_{k=0}^{n} \binom{n}{k} f\left(\frac{k}{n} \right) x^k (1-k)^{n-k} \right| \\
&= \left| \sum_{k=0}^{n} \binom{n}{k} \left(f(x) - f\left(\frac{k}{n} \right) \right) x^k (1-k)^{n-k} \right|.
\end{aligned}$$

Now, for any $\epsilon > 0$ there exists a δ such that $|f(x) - f(y)| < \epsilon$ whenever $|x - y| < \delta$. Thus, with that choice of δ,

$$\begin{aligned}
|f(x) - B_n(f)(x)| &\leq \sum_{k \in K} 2\|f\| \binom{n}{k} x^k (1-x)^{n-k} + \epsilon \sum_{k \neq F} \binom{n}{k} x^k (1-k)^k \\
&\leq \frac{2\|f\|}{4n\delta^2} + \epsilon.
\end{aligned}$$

Choosing $n > \|f\|/(2\delta^2)$, we see that

$$\|f - B_n(f)\|_\infty \leq 2\epsilon.$$

□

This has the following interpretation. Suppose that one has a biased coin with probability of heads equal to x. At each turn, you take a step to the right if heads and stay put if tails. Then the probability you are at "k" after n turns is given by

$$\binom{n}{k} x^k (1-x)^{n-k}.$$

Thus,

$$B_n(f)(x) = \mathbb{E}\left[f\left(\frac{k(n,x)}{n}\right)\right] = \mathbb{E}\left[f\left(\frac{\sum_{i=1}^n X_i}{n}\right)\right]$$

where the X_i are independent Bernoulli random variables with $P(X_i = 1) = x$ and $P(X_i = 0) = 1 - x$. Convergence implies that

$$f(x) = \lim_{n\to\infty} \mathbb{E}[f(\bar{X})].$$

We now turn to another proof, due to Weierstrass.

proof (Weierstrass). Extend f to $\tilde{f}$, continuous on all of $\mathbb{R}$ with compact support. Solve the heat equation

$$\frac{\partial}{\partial t}u(x,t) = \Delta u(x,t)$$

with initial data $\tilde{f}$. It can be shown that $\lim_{t\to 0} u(x,t) = f(x)$ for all $x \in [0,1]$. Now,

$$u(x,t) = \int_{\mathbb{R}} \frac{e^{-(x-y)^2/4t}}{\sqrt{4\pi t}}\tilde{f}(y)\,\mathrm{d}y.$$

For $t > 0$, this is entire in x and hence has a uniformly convergent Taylor series on $[0,1]$. □

We conclude our proofs with one attributed to Landau.

proof (Landau). Let $f \in C[0,1]$ and consider $\tilde{f} = f - [f(0) + x(f(1) - f(0)]$. We note that $\tilde{f}(0) = \tilde{f}(1) = 0$ and $\tilde{f}$ differs from f by a polynomial. We now extend $\tilde{f}$ to all of $\mathbb{R}$, setting $\tilde{f} \equiv 0$ outside of $[0,1]$. Set

$$L_n(x) = c_n \int_{-1}^{1} \tilde{f}(x-t)(1-t^2)^n\,\mathrm{d}t$$

where c_n is a normalization constant chosen so that

$$c_n \int_{-1}^{1} (1-t^2)^n\,\mathrm{d}t = 1.$$

Making the change of variables $s = x - t$ in the definition of L_n, we see that

$$L_n(x) = c_n \int_{x-1}^{x+1} \tilde{f}(s)(1-(x-s)^2)^n\,\mathrm{d}s.$$

Now, since $\tilde{f}$ vanishes outside of $[0,1]$, for $x \in [0,1]$,

$$L_n(x) = c_n \int_{0}^{1} \tilde{f}(s)(1-(x-s)^2)^n\,\mathrm{d}s$$

which is a polynomial in x. Moreover,

$$\psi_n(t) := c_n(1-t^2)^n\chi_{[-1,1]}$$

is an approximate identity, and hence $\tilde{f} \star \psi_n \to \tilde{f}$ as $n \to \infty$. More concretely, for $|t| < 1/\sqrt{n}$,

$$(1-t^2)^n \geq 1 - nt^2$$

and hence $c_n < \sqrt{n}$. For $0 < \delta < 1$,

$$c_n \int_{[-1,1]\setminus(-\delta,\delta)} (1-t^2)^n \, \mathrm{d}t \leq 2c_n(1-\delta^2)^n \to 0$$

as $n \to \infty$. So,

$$\begin{aligned} \left|L_n(x) - \tilde{f}(x)\right| &= c_n \left| \int_{-1}^{1} [\tilde{f}(x-t) - \tilde{f}(x)] \, (1-t^2)^n \, \mathrm{d}t \right| \\ &\leq c_n \int_{-\delta}^{\delta} (1-t^2)^n |\tilde{f}(x-t) - \tilde{f}(x)| \, \mathrm{d}t \\ &\quad + c_n \int_{[-1,1]\setminus(-\delta,\delta)} (1-t^2)^n 2 \, \|\tilde{f}\|_\infty \, \mathrm{d}t. \end{aligned}$$

If we choose δ small enough so that $|\tilde{f}(x-y) - \tilde{f}(x)| < \epsilon$ for all $|y| < \delta$ and $x \in [0,1]$ and choose n large enough so that $2\|f\|_\infty \sqrt{n}(1-\delta^2)^n < \epsilon/2$, then we obtain

$$|L_n(x) - \tilde{f}(x)| \leq 2\epsilon, \quad \forall x \in [0,1].$$

□

There is a common theme in these last two proofs. Convolve f with a "nice" function. Prove that the new function satisfies the required property. Pass to the limit to obtain the required result for the original function.

The Weierstrass (or Stone-Weierstrass) approximation theorem guarantees that given a continuous function, we can find an arbitrarily close polynomial approximation. In principle one could back out precise bounds on convergence depending on the regularity of f (say for Hölder spaces) and even back out an algorithm of sorts for constructing these approximations. In practice, they can be far from optimal. In the next chapter we begin our quest to rectify this deficiency by first trying to establish useful properties of best polynomial approximations.

Additional exercises

Exercise 12. *In this problem we will explore weighted spaces. In the following, assume f is a continuous function on an interval $[a,b]$ and w is a positive continuous weight function on $[a,b]$. For $p \in [1,\infty]$, let $\|\cdot\|_p$ be defined by*

$$\|f\|_p = \left(\int_a^b |f(x)|^p \, w(x) \, \mathrm{d}x \right)^{1/p}.$$

For $p = 2$ we also define $\langle , \rangle_w$ by

$$\langle f, g \rangle_w = \int_a^b f(x)\, g(x)\, w(x)\, \mathrm{d}x.$$

1. *Show that for any $f \in C[a,b]$, $\|f\|_1 \leq c\|f\|_2$ and $\|f\|_2 \leq c\|f\|$ where*

$$c = \left(\int_a^b w(t)\, \mathrm{d}t \right)^{1/2}.$$

   Here $\|\cdot\|$ denotes the usual sup *norm for $C[a,b]$.*

2. *Show that polynomials are dense in $C[a,b]$ under all three norms $\|\cdot\|$, $\|\cdot\|_1$, $\|\cdot\|_2$. Show that $C[a,b]$ is not complete under $\|\cdot\|_1$ or $\|\cdot\|_2$.*

Where have all the errors gone?

In this chapter we pick up our story of polynomial approximations, and try to answer the simple question: what are the properties of the best polynomial approximation, and how do we find them? The following remarkable result is attributed to Chebyshev, though special cases were known to Laplace and, before him, to Euler.

Equioscillations

Theorem 12 (Equioscillation)**.** *The space of polynomials of degree at most n on $[-1,1]$, which we denote by P_n, is a Chebyshev set in $C[-1,1]$, i.e. a best approximation always exists and is always unique. Moreover, if f is real, the best approximation p_* is real, and $f - p_*$ equioscillates in at least $n+2$ extreme points. That is to say, there exist points $-1 \leq x_0 < x_1 < \cdots < x_n < x_{n+1} \leq 1$ such that*

$$p_*(x_i) - f(x_i) = -[p_*(x_{i+1}) - f(x_{i+1})], \quad i = 0, \ldots, n,$$

and $|p_*(x_i) - f(x_i)| = \|p_* - f\|_\infty$ for $i = 0, \ldots, n+1$.

Aside 1. *A set of such points is also sometimes referred to as an* alternant.

Proof. Existence: $0 \in P_n$ so $d(f, P_n) \leq \|f\|$. So, it suffices to consider $S = \{p \in P_N \,|\, \|p - f\| \leq \|f\|\}$. This is a compact set and $\|p - \|f$ is continuous. So it attains its minimum.

Equioscillation implies optimality: We argue by contradiction. Suppose $f - p$ equioscillates at $x_0 < x_1 < x_{n+1}$ and suppose there exists a $q \in P_n$ with $\|f - q\| < \|f - p\|$. In particular, we mean that $|f(x_i) - p(x_i)| = \|f - p\|_\infty$ for all $i = 0, \ldots, n+1$. It follows that $q - p = f - p - (f - q)$ alternates in sign at $x_0, \ldots, x_{n+1}$ and hence changes sign between each pair of consecutive equioscillation points. Thus $q - p$ has $n+1$ roots and (since they are polynomials of degree at most n) we have $q = p$ which is a contradiction.

Optimality implies equioscillation: We once again argue by contradiction. Suppose p_* is a best approximation but $f - p_*$ equioscillates

at $-1 \leq x_0 < \cdots < x_{k+1} \leq 1, k < n$, and no longer alternating sequence exists. We are done if we can find a polynomial which is positive near the points x_i at which $f - p_* > 0$ and negative near the remaining x_i for which $f - p_* < 0$. Conceptually, this is easy - simply take a point between each x_i, x_{i+1}, call it s_i and form the polynomial $p(x) = (-1)^k(x - s_0)\dots(x - s_k)$. Here we have assume that $f(x_0) - p_*(x_0) > 0$. For the opposite sign, we multiply p by -1. Then for δ small enough,

$$\|f - (p_* + \delta p)\|_\infty \leq \|f - p_*\|_\infty$$

but $p_* + \delta p \in P_n$, since $p \in P_{k+1}$ and $k < n$. This gives our contradiction.

The only care comes in choosing the s_i and δ. Assuming without loss of generality that $f(x_0) - p_*(x_0) > 0$, the s_i should be chosen so that

$$(-1)^i(f(x) - p_*(x)) > -(1 - \epsilon)\|f - p_*\|_\infty$$

for all $x \in [s_{i-1}, s_i]$, $i = 0, \dots, k+1$ with $s_{-1} = -1$ and $s_{k+1} = 1$. Let $w_i = \max_{x \in [s_{i-1}, s_i}(-1)^{i-1}(f(x) - p_*(x))$, $i = 0, \dots, k$ and $w = \max\{w_i\}$. Then, setting $\delta = 1/2w$, $p(x) = (-1)^k(x - s_0)\dots(x - s_k)$, and $\tilde{p} = p_* + \delta p$ gives the required contradiction.

Uniqueness: Suppose p and q are both optimal. Set $r = (p + q)/2$. By the equioscillation characterization, there exist $-1 \leq x_0 < \cdots < x_{n+1} \leq 1$ with $(f - r)(x_i) = (-1)^i\|f - r\|$ for all $i = 0, \dots, n+1$ or $(f - r)(x_i) = (-1)^{i-1}\|f - r\|$ for all $i = 0, \dots, n+1$.

But

$$\begin{aligned} |f(x_i) - r(x_i)| &= \left|\frac{1}{2}(f(x_i) - p(x_i)) + \frac{1}{2}(f(x_i) - q_(x_)\right| \\ &\leq \frac{1}{2}|f(x_i) - p(x_i)| + \frac{1}{2}|f(x_i) - q(x_i)| \\ &\leq \frac{1}{2}\|f - p\| + \frac{1}{2}\|f - q\|. \end{aligned}$$

Where equality holds if and only if the signs are the same, or either are zero.

Also, $|f(x_i) - r(x_i)| = \|f - p\| = \|f - q\|$ so it follows that

$$|f(x_i) - p(x_i)| = \|f - p\| = \|f - q\| = |f(x_i) - q(x_i)|$$

and $\operatorname{sgn}(f(x_i) - p(x_i)) = \operatorname{sgn}(f(x_i) - q(x_i))$. Thus, $p(x_i) = q(x_i)$ for $i = 0, \dots, n+1$, and hence $p \equiv q$. □

The next theorem gives a lower bound on the error of the best approximation.

Theorem 13 (de la Vallée Poussin)**.** *Given $f \in C[a, b]$, suppose $q \in P_n$ and $f(x_i) - q(x_i)$ alternates in sign at $a \leq x_0 < x_1 < x_{n+1} \leq b$. If $E_n(f)$ denotes the error of the best approximation in P_n then*

$$E_n(f) \geq \min_{i=0,\dots,n+1} |f(x_i) - q(x_i)|.$$

Proof. We argue by contradiction. Setting p_* to be the best polynomial approximation to f in P_n, and suppose that

$$E_n(f) < \min_{i=0,\ldots,n+1} |f(x_i) - q(x_i)|.$$

Then, $q - p_*$ has $n+1$ roots which is a contradiction. □

Remez exchange algorithm

The results of the previous section suggest a simple algorithm for finding the best polynomial approximation. We only sketch the details here. As input it takes a function f and an interval $[a, b]$ together with an initial guess for the equioscillation points, call them $x_0^{(0)}, \ldots, x_{n+1}^{(0)}$. The idea is to find the equioscillation points of p_* iteratively using the de la Vallée Poisson theorem as a criterion or "monitor function". The output will be the candidate equioscillation points and coefficients in a monomial expansion.

The algorithm proceeds as follows. For each iteration $i = 1, 2, \ldots$ we solve the linear system

$$\begin{pmatrix} 1 & x_0 & x_0^2 & \ldots & x_0^n & 1 \\ 1 & x_1 & x_1^2 & \ldots & x_1^n & -1 \\ 1 & x_2 & x_2^2 & \ldots & x_2^n & 1 \\ 1 & x_3 & x_3^2 & \ldots & x_3^n & -1 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 1 & x_{n+1} & x_{n+1}^2 & \ldots & x_{n+1}^n & (-1)^{n+1} \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \\ \vdots \\ \\ \alpha_n \\ E \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \\ \\ \vdots \\ \\ f_n \\ f_{n+1} \end{pmatrix}.$$

Here $x_0 = x_0^{(i-1)}, \ldots, x_{n+1} = x_{n+1}^{(i-1)}$ are the current guesses for the equioscillation points, $\alpha_0 = \alpha_0^{(i-1)}, \ldots, \alpha_n = \alpha_n^{(i-1)}$ are the current guesses for the coefficients, $E = E^{(i)}$ is the current guess for $\|f - p_*\|$ and $f_0 = f(x_0), \ldots, f(x_{n+1})$.
Next, we compute

$$e^{(i)}(x) = f(x) - \sum_{j=0}^{n} \alpha_j^{(i)} x^j$$

and find its maximum (in absolute value). We move the adjacent $x_j^{(i-1)}$ for which $e^{(i)}(x_j^{(i-1)})$ has the same sign, to that point. Set $x_k^{(i)} = x_k^{(i-1)}$ for all other points.

We exit when $\max_j |e^{(i)}(x_j^{(i)})| - \min_j |e^{(i)}(x_j^{(i-1)})| < \epsilon$, a prespecified tolerance.

Remark 7. *It is easy to update this algorithm to move multiple points at the same time. Also, rather than solve the coefficients in a monomial bases, one can use other representations / bases.*

This is nice, and very useful, if there is one (or a small number) of functions you wish to approximate, at a fixed polynomial order. With many functions and multiple orders it can quickly become computationally infeasible. In the next chapter we relax the optimality criteria and see if we can get something almost optimal but more flexible.

General equioscillation theorems

Looking at the proof of the equioscillation theorem and the de la Vallée Poussin theorem, we can see that both proofs hinged on the repeated use of the property that a polynomial $p \in P_n$ can have at most n roots. This, however, is a property shared by any n-dimensional Haar subspace. So, a natural question is whether or not we can extend our equioscillation and de la Vallée Poussin theorems to this more general setting. The answer is an emphatic yes.

Theorem 14. *Suppose V is an $(n+1)$-dimensional Haar subspace of $C[-1,1]$. Given $f \in C[-1,1]$, let u_* denote the best approximation to f from V. Then u_* is unique and $f - u_*$ equioscillates in at least $n+2$ extreme points.*

Proof. Equioscillation implies optimality: This is exactly identical to the case of polynomials.

Optimality implies equioscillation: The intuition is the same as for polynomials, though we have to work a bit harder. Again we argue by contradiction. Suppose u_* is a best approximation, but $f - u_*$ has an alternant of length $k+1$, $-1 \leq x_0 < \cdots < x_{k+1} \leq 1, \quad k < n$, and no longer alternant exists. Set $E = \|f - u_*\|_\infty$.

Without loss of generality, suppose that $f(x_0) - u_*(x_0) > 0$. Fix $\epsilon > 0$. Since f and u_* are continuous, and no longer alternant exists, there exists an $s_0 \in [x_0, x_1]$ such that $f(x) - u_*(x) > -(1-\epsilon)E$ for all $x \in [-1, s_0]$ and $f(x) - u_*(x) < (1-\epsilon)E$ for all $x \in [s_0, x_1]$. Colloquially, s_0 is chosen between the last time $f - u_* = E$ and the first time $f - u_* = -E$ on the interval $[x_0, x_1]$. Proceeding to the next interval, we select $s_1 \in (x_1, x_2)$ so that $f - u_* < (1-\epsilon)E$ for all $x \in [s_0, s_1]$ and $f - u^* > -(1-\epsilon)E$ on $[s_1, x_2]$. We can continue in this way to obtain $s_0, s_1, \ldots, s_k$. Note that by construction $s_0 \neq -1$ and $s_k \neq 1$.

Now, for polynomials the proof involved constructing a polynomial which changed sign only at $s_0, \ldots, s_k$ and nowhere else. For polynomials this is trivial. For Haar subspaces this is a bit more subtle.

Suppose $k = n-1$. Since V is a Haar subspace, we know that there is a unique function $v \in V$ with $v(s_i) = 0, i = 0, \ldots, n-1$, $v(-1) =$

$\operatorname{sgn}(f(-1) - u_*(-1))$. One remaining concern is as to whether or not the function v changes sign at each of the s_i. By adjusting $v(s_i)$ one can argue that if there is no sign change then it would be possible to create a function in V with more than n roots - a contradiction. The function v so constructed has n roots and hence changes sign only at the s_i.

Suppose $k = n - 2$. We choose v to be the unique function in V such that $v(s_i) = 0, i = 1, \ldots, n-2$, $v(-1) = 1$, and $v(1) = -1$. Once again, the function only changes signs at the s_i.

Suppose $k < n - 2$. For any of the i we can redo the construction of s_i to obtain two new distinct points $s_{i,a}$ and $s_{i,b}$ which satisfy the same conditions required by s_i, and add them to our set. Proceeding in this way, we arrive either at the $k = n - 2$ or $k = n - 1$ case. Letting $\{\tilde{s}_i\}$ denote this new set. As before we construct a $v \in V$ which changes sign at each $\tilde{s}_i$, and nowhere else.

Thus, for any $k < n$ we can construct a $v \in V$ which alternates in sign at each x_i. We can assume that $\operatorname{sgn}(v(x_i)) = \operatorname{sgn}(f(x_i) - u_*(x_i))$ for all $i = 0, \ldots, k$, otherwise we replace v by $-v$. Setting $\hat{u} = u_* - \delta v$ with $\delta < \epsilon/(2\|v\|_\infty)$, we see that $\|f - \hat{u}\|_\infty < \|f - u\|_\infty$, which gives us our contradiction.

Uniqueness: The proof is identical to the polynomial case. □

We also have an analog of the de la Vallé Poussin theorem. The proof is once again identical to the polynomial case.

Theorem 15 (Generalized de la Vallée Poussin)**.** *Given $f \in C[a, b]$, suppose $q \in P_n$ and $f(x_i) - q(x_i)$ alternates in sign at $a \leq x_0 < x_1 < x_{n+1} \leq b$. If $E_n(f)$ denotes the error of the best approximation in P_n then*

$$E_n(f) \geq \min_{i=0,\ldots,n+1} |f(x_i) - q(x_i)|.$$

Best polynomial approximations of 'x^n'

We conclude our discussion of best approximations by returning to polynomials and considering a simple example, due to Chebyshev. The question is:

What is the best approximation to x^n in P_{n-1} on the interval $[-1, 1]$?

Colloquially, the question then is asking to what extent x^n may be considered a polynomial of degree at most $n - 1$ if we measure distance in the supremum norm.

We first note that this is equivalent to finding the monic polynomial in P_n which is closest to 0. Indeed, this is one of the simplest cases of a general class of problems related to finding functions 'least deviating from zero'. It was a particularly popular line of research in

the Russian school of approximation theory associated with Chebyshev.

Let $p_* \in P_{n-1}$ denote the best polynomial approximation to x^n and $\hat{p} = x^n - p_*$. Then, by the equioscillation thoerem, there exist $n+1$ points $-1 \le x_0 < x_1 < \cdots < x_n \le 1$ with

$$|x_i^n - p_*(x_i)| = \|x^n - p_*(x)\|_\infty = \|\hat{p}\|_\infty$$

and the sequence alternates. It follows that $\hat{p}'(x_i) = 0$ for all $x_i \in (-1,1)$. Since $\hat{p}' \in P_{n-1}$ only has $n-1$ zeros, and there are $n+1$ points x_i that $x_0 = -1$ and $x_n = 1$ (if either were inside the interval, then $\hat{p}'$ would have at least n roots). Thus, for some constant c,

$$\hat{p}'(x) = c(x - x_1)\dots(x - x_{n-1}).$$

On the other hand, if we set $E = \|\hat{p}\|$, then $q := E^2 - \hat{p}^2$ has double roots at $x_1, \dots, x_n$ and simple roots at $x = \pm 1$. This last follows from the fact that q has $2n$ roots counting multiplicity and the fact that $E^2 - p^2$ is non-negative on $[-1,1]$. Thus, for some constant $\tilde{c}$,

$$E^2 - \hat{p}^2 = \tilde{c}(1 - x^2)\prod_{i=1}^{n-1}(x - x_i)^2$$

and hence

$$\beta(1 - x^2)(\hat{p}')^2 = E^2 - \hat{p}^2$$

for some constant β. Comparing leading coefficients it is clear that $\beta = 1/n^2$. So,

$$\frac{\hat{p}'}{\sqrt{E^2 - \hat{p}^2}} = \pm\frac{n}{\sqrt{1 - x^2}}.$$

This is a separable ordinary differential equation and can be integrated to obtain

$$\arccos\frac{\hat{p}}{E} = \pm n \arccos x + C,$$

and hence $p = E\cos(n\arccos x + C)$. At $x = -1$, $p = \pm E$ and so $\pm 1 = \cos(n\pi + C)$ from which it follows that $C = k\pi$ for some $k \in \mathbb{Z}$. Thus,

$$p = \pm E\cos(n\arccos x).$$

Now,

$$z^n + \frac{1}{z^n} = \left(z^{n-1} + \frac{1}{z^{n-1}}\right)(z + 1/z) - \left(z^{n-2} + \frac{1}{z^{n-2}}\right)$$

and hence

$$\cos(nt) = 2\cos(t)\cos((n-1)t) - \cos((n-2)t)$$

from which it follows that

$$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$$

where $T_n(x) = \cos(n \arccos x)$. These are called *Chebyshev polynomials*. From the above identity, it is easy to see that the leading order coefficient of T_n is 2^{n-1}. Thus

$$p = \frac{1}{2^{n-1}} T_n$$

and so the error of approximating x^n by a polynomial of degree at most $(n-1)$ is $1/2^{n-1}$.

We can see immediately from the formula that if x_i are the zeros of T_n then

$$x_i = \cos\left(\frac{m\pi}{n} + \frac{\pi}{2n}\right).$$

The previous result has the following nice interpretation. The roots of T_n minimize

$$\max_{x\in[-1,1]} |(x - x_1)\dots(x - x_n)|$$

which is equivalent to minimizing

$$\max_{x\in[-1,1]} \sum_{j=1}^{n} \log|x - x_j|.$$

Now, up to a scaling, log is the Green's function for the Laplace equation in two dimensions. Roughly speaking $-\log|\mathbf{x} - \mathbf{x}'|/(2\pi)$ is the (2D) electrostatic potential due to a unit charged placed at $\mathbf{x}'$. So the Chebyshev roots are the places you should put n unit charges to minimize the maximum electrostatic potential on $[-1, 1]$. Obviously one can generalize this problem to more general subsets of $\mathbb{C}$, or even more generally to arbitrary manifolds, as well as adding weight functions.

Finally, we are left with the following additional amusing interpretation: on $[-1, 1]$, for large enough n, x^n "is" a polynomial of degree at most $n - 1$. Here we mean that for any ϵ there exists an n (logarithmic in ϵ!) for which

$$\inf_{p\in P_{n-1}} \|x^n - p\| < \epsilon.$$

One can extend this to more general orders. The following is due to Rivlin and Newman (1976):

Theorem 16. *Let $k < n$ and set*

$$E_k(x^n) := \max_{p\in P_k} \|x^n - p\|_{L^\infty([-1,1])}.$$

Then

$$E_k(x^n) \le 2e^{-\frac{k^2}{2n}}.$$

We thus obtain a rather shocking result: measured in the supremum norm, x^n is approximately a polynomial of order $\sim c\sqrt{n}$.

Additional Exercises

Exercise 13. *For any $n \geq 0$ show that the mapping which takes the function $f \in C[-1,1]$ to its best polynomial approximation $p_* \in P_n$ is continuous with respect to the ∞-norm on $C[-1,1]$. Hint: uniqueness follows from above. Combine with compactness.*

Exercise 14. *In this problem we will explore best approximations on L^2.*

1. *For $n \geq 1$ let p_* denote the best approximation to f from P_{n-1} in the least-squares sense, i.e.*

$$p_* = \operatorname{argmin}_{p \in P_{n-1}} \|f - p\|_2.$$

   Show that $\langle f - p_*, p \rangle_w = 0$ for all $p \in P_{n-1}$. Moreover, show that if $q \in P_{n-1}$ and $\langle f - q, p \rangle_w = 0$ for all $p \in P_{n-1}$ then q is the unique best approximation to f from P_{n-1} in the least-squares sense. Hint: for uniqueness, use the parallelogram law applied to $f - q$ and $f - p$.

2. *Show that if p_* is the best least-squares approximation to f then $f - p_*$ has at least n zeros on $[a,b]$. Hint: use the previous part.*

3. *Let $p_{*,2}^{(n)}$ denote the best least-squares approximation to f from P_{n-1} and $p_{*,\infty}^{(n)}$ denote the best uniform approximation. Show that*

$$\|f - p_{*,2}^{(n)}\|_2 \leq \|f - p_{*,\infty}^{(n)}\|_2$$

   and hence $\|f - p_{*,2}^{(n)}\|_2 \to 0$ as $n \to \infty$.

4. *If p_n denotes the nth Legendre polynomial, and α_n is its leading coefficient (i.e. the coefficient of x^n) then show that p_n/α_n is the smallest monic polynomial in P_n (measured in the $\|\cdot\|_2$ norm).*

Exercise 15. *A (simplified) Remez algorithm works by doing the following: Choose "control" points $x_0, \ldots, x_{n+1}$ in the interval $[0,1]$ to initialize. For each iteration, form the system*

$$\begin{bmatrix} 1 & x_0 & x_0^2 & \ldots & x_0^n & -1 \\ 1 & x_1 & x_1^2 & \ldots & x_1^n & 1 \\ \vdots & \vdots & \ddots & \vdots & & \\ 1 & x_{n+1} & x_{n+1}^2 & \ldots & x_{n+1}^n & (-1)^{n+2} \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \vdots \\ \alpha_n \\ E \end{bmatrix} = \begin{bmatrix} f(x_0) \\ \vdots f(x_{n+1}) \end{bmatrix}$$

and solve it. Find the location of the maximum of $e(x) = f(x) - \sum_{j=0}^n \alpha_j x^j$ on the interval $[0,1]$. Call it x_*. Move the closest control point x_i (for which the signs of $e(x_*)$ and $e(x_i)$ agree) to x_* and move to the next iteration.

1. *Perform one iteration of the Remez algorithm to compute the best polynomial approximation to x^5 by polynomials of degree at most 3 on the interval $[0,1]$. Start with equispaced nodes $x_0 = 0, \ldots, x_5 = 1$.*

2. *Write a code to use the Remez algorithm to compute the best polynomial approximation to x^5 by polynomials of degree at most 3 on the interval $[0,1]$. Plot the equioscillation points and the error as a function of iteration number. Show plots for initialization both with equispaced points and random initial points. Hint: in Matlab, the commands vander, polyval, and roots might be helpful.*

3. *Extend your code in some way (multiple points at once, more general function, more stable formulae for solving the linear system, some different experiments, etc.).*

Exercise 16. *Recall the formula for Chebyshev polynomials:*

$$T_n(x) = \cos(n \operatorname{acos} x).$$

1. *Let $p \in P_n$ be a polynomial given by a finite Chebyshev series*

$$p(x) = \sum_{k=0}^{n} \alpha_k T_k(x)$$

and let $s \in [-1,1]$. Show that $p(s)$ can be evaluated using the following algorithm. Set $u_{n+1} = 0$, $u_n = \alpha_n$ and

$$u_k = 2su_{k+1} - u_{k+2} + \alpha_k, \quad k = n-1, m-2, \ldots, 0.$$

Then $p(s) = \frac{1}{2}(\alpha_0 + u_0 - u_2)$.

2. *Show that T_n satisfies the ODE $(1-x^2)y'' - xy' + n^2 y = 0$.*

Exercise 17. *In this problem, we will give a brief proof of Theorem 16 (see Sachdeva and Vishnoi 2013).*

a) *For $i = 1, 2, \cdots$, let X_i be the Bernoulli random variable which takes values ± 1 with equal probability. For $n < 0$, define $T_n = T_{-n}$. Prove that*

$$x^n = \mathbb{E}\left[T_{X_1 + \cdots + X_n}(x)\right].$$

Hint: use induction and the three-term recurrence for Chebyshev polynomials.

b) *One simple version of Hoeffding's inequality states that for $Z_1, \cdots, Z_n$ i.i.d. bounded random variables, $a \le Z_i \le a + L$ almost surely, if S_n denotes their sum, then for all $t > 0$,*

$$\mathbb{P}\left[S_n - \mathbb{E}(S_n) \ge t\right] \le e^{-t^2/(nL^2)}.$$

Using this, bound the probability that $|X_1 + \cdots + X_n| > c\sqrt{n}$ for any $c > 0$.

c) *Using (a), (b), and the bound $\|T_m\|_{L^\infty([-1,1])} \le 1$ for all m, argue that x^n can be written as a linear combination of Chebyshev polynomials up to order $c\sqrt{n}$ plus an error term. Give an explicit bound for the error.*

d) *Check this numerically. Take x^{100} and compute the Chebyshev coefficients for $m = 10, 20, 30, 40, 50$. What is the error for each m?*

Convergence of Chebyshev Polynomial Approximations

Previously, we saw how Chebyshev polynomials arose naturally in the contexts of best approximations to monomials and electrostatics. Here we explore in more detail their utility for approximating more general functions, and take our first steps toward practical and provable algorithms for polynomial approximation and interpolation.

Convergence of Chebyshev series

Our first result establishes the representability of Lipschitz functions on $[-1, 1]$ by Chebyshev series.

Theorem 17. *Suppose we are given a function f which is Lipschitz continuous on $[-1, 1]$. Then f has a unique representation as a Chebyshev series,*

$$f(x) = \sum_{k=0}^{\infty} \alpha_k T_k(x),$$

which is absolutely continuous and uniformly convergent. Moreover, the coefficients are given by the following formula,

$$\alpha_k = \frac{2}{\pi} \int_{-1}^{1} \frac{f(x) T_k(x)}{\sqrt{1-x^2}} \, \mathrm{d}x, \quad k > 0,$$
$$\alpha_0 = \frac{1}{\pi} \int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} \, \mathrm{d}x.$$

Proof. The intuition of the proof echoes the construction of the Chebyshev polynomials themselves, and their roots.
Let's map f to the unit circle. Given $z \in \mathbb{Z}$, $|z| = 1$, set $x = \frac{1}{2}(z + \frac{1}{z})$. Then $z = e^{i\theta}$ implies $x = \cos\theta$. Define F by $F(z) = f(x(z))$. Then

$$\mathrm{d}x = \frac{1}{2}\left(1 - \frac{1}{z^2}\right) \mathrm{d}z = \frac{i/z}{2i}\left(z - \frac{1}{z}\right) \mathrm{d}z = \pm \frac{i}{z}\sqrt{1-x^2},$$

where we take the $+$ if $\mathrm{Im}(z) \geq 0$ and the $-$ if $\mathrm{Im}(z) \leq 0$.

If f is Lipschitz, so is F. In fact, the regularity is better near ± 1. In this case, F can be uniquely written as a Laurent series which is absolutely and uniformly convergent on the unit circle.

$$F(x) = \frac{1}{2} \sum_{k=0}^{\infty} a_k \left(z^k + \frac{1}{z^k}\right) = \frac{1}{2} \sum_{k=0}^{\infty} a_k T_k(x),$$

where the first equality follows from the symmetry of F ($z \mapsto 1/z$) and the second follows from making the substitution $= e^{i\theta}$ and the definition of T_k.

The coefficient of z^k ($a_k/2$) can be easily computed using the Cauchy integral formula, to obtain

$$a_k = \frac{1}{i\pi} \int_{|z|=1} z^{-1-k} F(z)\, \mathrm{d}z, \quad k > 0.$$

Similarly, for z^{-k}, for which the coefficient is also $a_k/2$, one finds that

$$a_k = \frac{1}{i\pi} \int_{|z|=1} z^{-1+k} F(z)\, \mathrm{d}z.$$

So, averaging the two expressions,

$$a_k = \frac{1}{2\pi i} \int_{|z|=1} \frac{1}{z} \left(z^k + z^{-k}\right) F(z)\, \mathrm{d}z = \frac{1}{\pi i} \int_{|z|=1} \frac{1}{z} T_k(x(z))\, F(z)\, \mathrm{d}z.$$

Changing variables to x, and noting that the part involving $\mathrm{Im}(z) > 0$ comes in with an extra minus sign, we obtain

$$\begin{aligned} a_k &= \frac{1}{i\pi} \int_{|z|=1} \frac{1}{z} T_n(x(z))\, f(x(z))\, \mathrm{d}z \\ &= \frac{-1}{i\pi} \int_{-1}^{1} T_k(x) f(x) \frac{1}{\sqrt{1-x^2}} \frac{\mathrm{d}x}{i} + \frac{1}{i\pi} \int_{-1}^{1} T_k(x) f(x) \frac{1}{-\sqrt{1-x^2}} \frac{\mathrm{d}x}{i}. \end{aligned}$$

So,

$$a_k = \frac{2}{\pi} \int_{-1}^{1} \frac{T_k(x) f(x)}{\sqrt{1-x^2}}\, \mathrm{d}x, \quad k > 0.$$

The case where $k = 0$ is left as an exercise. □

Chebyshev and Best Approximations

The next theorem gives some further justification for all of this bother about Chebyshev polynomials. It follows by a 1967 result of MJD Powell (thought related results appear elsewhere).

Theorem 18. *Suppose f is bounded and continuous on $[-1, 1]$ and let p_* denote its best polynomial approximation from P_n. Let p denote its truncated Chebyshev expansion (truncated after $n + 1$ terms). Then*

$$\frac{\|f - p\|_\infty}{\|f - p_*\|_\infty} \sim \frac{4}{\pi^2} \log n, \quad \text{as } n \to \infty.$$

Proof. We actually start with proving a much more general result. Suppose we are given a finite dimensional subspace M of E, and moreover that this space is equipped with an inner product $\langle\, , \rangle_E$. Let $\phi_1, \ldots, \phi_m$ be an orthonormal basis of M (with respect to that inner product).

Given $f \notin M$, let p denote the orthonormal projection of f onto M and p_* denote the best approximation to f in M. We emphasize here that $\langle u, u\rangle_E^{1/2} \neq \|u\|_E$ in general, i.e. that the norm on E is not necessarily the norm induced by the inner product. R need not be complete with respect to $\langle\ ,\ \rangle_E$.

The trick boils down to this: $(f-p)-(f-p_*) \in M$. Thus for some coefficients α_i,

$$(f-p)-(f-p_*) = \sum_{i=1}^{m} \alpha_i \phi_i.$$

Taking inner products against ϕ_i,

$$\alpha_i = -\langle \phi_i, f-p_*\rangle_E,$$

where we have used the fact that $f-p$ is orthogonal to M. Then

$$f-p = f-p_* + P_m(f-p_m), \quad \text{with} \quad P_m(u) = \sum_{i=1}^{m} \phi_i \langle \phi_i, u\rangle_E,$$

and hence

$$\|f-p\|_E \leq \|f-p_*\|_E + \|P_M\|_{E\to E}\|f-p_*\|_E,$$

and hence

$$\frac{\|f-p\|_E}{\|f-p_*\|_E} \leq 1 + \|P_M\|_{E\to E}.$$

For Chebyshev polynomials, the natural inner product is

$$\langle u, v\rangle := \int_{-1}^{1} \frac{uv}{\sqrt{1-x^2}}\,\mathrm{d}x,$$

and the basis is $\phi_0 = 1/\sqrt{\pi}$, $\phi_k = \sqrt{2/\pi}T_k$, $k>0$. Thus, in order to use the above result with $E = L^\infty([-1,1])$, $M = P_n$, and the inner product defined above, we need to estimate the operator norm (as a map from $L^\infty \to L^\infty$) of the projection P defined by

$$P(u)(x) = \int_{-1}^{1} \sum_{i=0}^{n} \frac{\phi_i(x)\phi_i(y)}{\sqrt{1-y^2}} u(y)\,\mathrm{d}y.$$

Our bound on $\|P\|$ will mostly consist of truncated geometric series combined with trigonometric identities. And so we begin,

$$\|P\| \leq \sup_x \int_{-1}^{1} \left| \sum_{i=0}^{n} \frac{\phi_i(x)\phi_i(y)}{\sqrt{1-y^2}} \right| \mathrm{d}y.$$

The sum is given explicitly by

$$sum_{i=0}^{n} \phi_i(x)\phi_i(y) = \frac{2}{\pi} \sum_{k=0}^{n} \cos(k \arccos x)\cos(k \arccos y) - \frac{1}{\pi}.$$

We observe that $\cos(ks)\cos(kt) = \frac{1}{2}[\cos(k(s-t)) + \cos(k(s+t))]$ and

$$\sum_{k=0}^{n} \cos(k\alpha) - \frac{1}{2} = \frac{\sin((n+\frac{1}{2})\alpha)}{2\sin(\alpha/2)}.$$

So,

$$I(s) := \int_{-1}^{1} \left| \sum_{i=0}^{n} \frac{\phi_i(x)\phi_i(y)}{\sqrt{1-y^2}} \right| \mathrm{d}y = \frac{1}{2\pi} \int_{-1}^{1} \left| \frac{\sin((n+\frac{1}{2})(s-t))}{\sin(\frac{s-t}{2})} + \frac{\sin((n+\frac{1}{2})(s+t))}{\sin(\frac{s+t}{2})} \right| \frac{1}{1-y^2}\,\mathrm{d}y$$

where we have set $s = \arccos x$, and $t = t(y) = \arccos y$. Changing variables to from y to t, we find

$$\begin{aligned}
I(s) &= \frac{1}{2\pi} \int_{0}^{\pi} \left| \frac{\sin((n+\frac{1}{2})(s-t))}{\sin(\frac{s-t}{2})} + \frac{\sin((n+\frac{1}{2})(s+t))}{\sin(\frac{s+t}{2})} \right| \mathrm{d}t \\
&= \frac{1}{4\pi} \int_{-\pi}^{\pi} \left| \frac{\sin((n+\frac{1}{2})(s-t))}{\sin(\frac{s-t}{2})} + \frac{\sin((n+\frac{1}{2})(s+t))}{\sin(\frac{s+t}{2})} \right| \mathrm{d}t \\
&\le \frac{1}{2\pi} \int_{-\pi}^{\pi} \left| \frac{\sin((n+\frac{1}{2})(s-t))}{\sin(\frac{s-t}{2})} \right| \mathrm{d}t \\
&\le \frac{1}{2\pi} \int_{-\pi}^{\pi} \left| \frac{\sin((n+\frac{1}{2})t}{\sin(\frac{t}{2})} \right| \mathrm{d}t
\end{aligned}$$

We break the region of integration up into two pieces, $R_1 = [-\alpha, \alpha]$ and $R_2 = [-\pi, \pi] \setminus R_1$. Here $\alpha \in (0, \pi)$ is left free and will be chosen later.

On R_1, we observe that $|\sin((n+1/2)t)| < (n+1/2)|t|$ and

$$\frac{1}{|\sin(t/2)|} \le \frac{1}{|t|/2 - |t|^3/(3!8)} = \frac{2}{|t|} + O(\alpha^2).$$

Then,

$$\frac{1}{2\pi} \int_{R_1} \left| \frac{\sin((n+\frac{1}{2})t}{\sin(\frac{t}{2})} \right| \mathrm{d}t \le \frac{2n+1}{2\pi} \int_{-\alpha}^{\alpha} 1\,\mathrm{d}t + O(n\alpha^3) = \frac{2n+1}{\pi}\alpha + O(n\alpha^3).$$

Away from R_1, we use the bound $|\sin((n+1/2)t)| < 1$ and hence

$$\frac{1}{2\pi} \int_{R_2} \left| \frac{\sin((n+\frac{1}{2})t}{\sin(\frac{t}{2})} \right| \mathrm{d}t \le \frac{1}{\pi} \int_{\alpha}^{\pi} \frac{1}{\sin(t/2)}\,\mathrm{d}t = \frac{2}{\pi} \log \frac{\tan(\pi/4)}{\tan(\alpha/4)} = -\frac{2}{\pi}\log(\alpha/4) + O(\alpha^2 \log(\alpha)).$$

Setting $\alpha = 1/(n+1/2)$ and putting together our bounds on R_1 and R_2, we find

$$\|P\|_{\infty\to\infty} \le \frac{2}{\pi}\left(1 + \log\left(\frac{n+1/2}{4}\right)\right) + O(n^{-2}\log(n)).$$

□

To recap, we know that for Lipschitz functions, truncated Chebyshev series provide uniformly convergent polynomial approximations. Moreover, they are within a log factor of optimal! It is remarkable, given the nonlinear nature of best approximations, that a nonadaptive linear method should get so close. Now that we know how good they are, let's try to get a more quantitative estimate on the rate of convergence. To do this we will impose more regularity and see how that regularity yields compressibility.

Regularity and decay

We begin our discussion about the interplay between regularity of a function and the decay of its Chebyshev coefficients with the following theorem.

Theorem 19. *For an integer $p \geq 0$, let $f, f', '$ dots, $f^{(p-1)}$ be absolutely continuous and suppose $f^{(p)}$ is of bounded variation with total variation V. Then, for $k \geq p+1$, the Chebyshev coefficients α_k of f satisfy*

$$|\alpha_k| \leq \frac{2V}{\pi k(k-1)\dots(k-p)} \leq \frac{2V}{\pi(k-p)^{p+1}}.$$

Proof. We begin by recalling that

$$\alpha_k = \frac{2}{\pi}\int_0^\pi f(\cos(\theta))\,\cos(k\theta)\,\mathrm{d}\theta.$$

Set

$$F_{j,n} = \int_0^\pi f^{(j)}(\cos(\theta))\,\cos(n\theta)\,\mathrm{d}\theta.$$

Integration by parts, together with the identity $\sin(x)\,\sin(ax) = \frac{1}{2}\left[\cos((a-1)x) - \cos((a+1)x)\right]$, yields

$$F_{j,n} = \frac{1}{2n}\left[F_{j+1,n-1} - F_{j+1,n+1}\right].$$

In particular,

$$F_{0,k} = \frac{1}{2^{p+1}}\sum_{i_1,\dots,i_{p+1}=1}^{2}(-1)^{p+1+i_1+\cdots i_{p+1}}\frac{F_{p+1,k+(-1)^{i_1}+\cdots+(-1)^{i_{p+1}}}}{k(k+(-1)^{i_1})\times\cdots\times(k+(-1)^{i_1}+\cdots+(-1)^{i_p})}.$$

Let Z_j be the Bernoulli random variable which is ± 1 with probability $1/2$ in each case. Let $U_j = \sum_{i=1}^{j} Z_j$. Then,

$$F_{0,k} = \frac{1}{k}\mathbb{E}\left[\frac{(-1)^{p+1+U_{p+1}}F_{p+1,k+U_{p+1}}}{e^{\sum_1^p \log(k+U_i)}}\right].$$

We observe that the denominator inside the expectation is always bounded below by

$$(k-1)\cdots(k-p).$$

Moreover, an elementary estimate of the numerator gives an upper bound of

$$\|f^{(p)}\|_{TV} =: V.$$

Hence,

$$|\alpha_k| = \frac{2}{\pi}|F_{0,k}| \leq \frac{2V}{\pi k(k-1)\cdots(k-p)}.$$

□

Corollary 3. *If f satisfies the conditions of the previous theorem, then*

$$\|f - f_n\| \leq \frac{2V}{\pi(n-p)^p},$$

where f_n is the Chebyshev projection of f obtained by keeping the first $n+1$ terms in the Chebyshev series.

When f is analytic in a neighborhood of $[-1,1]$ this result can be dramatically improved with an elegant proof.

Definition 8. *Consider the "Joukowsky" map $x = \frac{1}{2}(z + 1/z)$. For $\rho > 1$, the image of the circle of radius ρ, under this map, is an ellipse with foci at ± 1. These ellipses are called* Bernstein ellipses *and we will denote their interiors by E_ρ.*

Theorem 20. *Suppose f defined on $[-1,1]$ is analytically continuable to the open Bernstein ellipse E_ρ and $|f(x)| \leq M$ on that ellipse. If α_k denotes its Chebyshev coefficients then*

$$|\alpha_0| \leq M$$
$$|\alpha_k| \leq 2M\rho^{-k}.$$

Proof. The case $k = 0$ is easy. For $k > 0$,

$$\begin{aligned}\alpha_k &= \frac{1}{\pi i}\int_{|z|=1} z^{-1-k}F(z)\,\mathrm{d}z \\ &= \frac{1}{\pi i}\int_{|z|=\rho} z^{-1-k}F(z)\,\mathrm{d}z,\end{aligned}$$

where the last equality follows from Cauchy's integral formula. Hence

$$|\alpha_k| \leq 2\pi\rho M\rho^{-k-1}.$$

□

Corollary 4. *If f satisfies the conditions of the previous theorem,*

$$\|f - f_m\| \leq \frac{2M\rho^{-n}}{\rho - 1}.$$

Additional Exercises

Exercise 18.

In this problem we will explore Chebyshev interpolation. Consider the function $f(x) = e^x$ *on the interval* $[-1, 1]$.

1. *Interpolate* f *using* $2, 5, 10, 15$ *and* 20 *Chebyshev polynomials. Do this in two ways: firstly, by computing projections using the equation derived in class for coefficients in a Chebyshev expansion; and secondly, by forming the matrix* $V_{i,j} = T_j(x_i)$, $i, j = 0, \ldots, n$ *and using it to find the coefficients in the Chebyshev expansion. Include plots of the functions (all in the same plot), and errors.*

2. *Write down an explicit formula for the Bernstein ellipse with parameter* ρ *in terms of the real and imaginary parts of* x.

3. *Find a bound on the rate of convergence as a function of* n. *Use the bound based on Bernstein ellipses and choose the* ρ *depending on* n.

Exercise 19. *The Chebyshev polynomials can be expressed in the monomial basis as*

$$T_n(x) = \frac{n}{2} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k \frac{(n-k-1)!}{k!(n-2k)!} (2x)^{n-2k}, n > 0.$$

Verify that this gives the correct polynomials for $n = 1$ *and* $n = 2$.

1. *Prove that this expression satisfies the Chebyshev recurrence relation*

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x).$$

2. *Implement this formula numerically for* $n = 2, 5, 10, 15, 20, 40$ *and* 80 *and plot the solutions and the errors compared with computing them via the formula* $T_n(x) = cos(n \operatorname{acos}(x))$. *Is the result surprising?*

Exercise 20. *In this problem, we will examine some of the ramifications of approximation theory for linear algebra.*

1. *Write a code to find the best polynomial approximation to* $f(x) = 1/x$ *on the interval* $[1, 5]$ *for* $n = 4$.

2. *Construct a* 1000×1000 *symmetric random matrix* A *with eigenvalues all lying between* $[1, 5]$ *and a random vector* $b \in \mathbb{R}^{1000}$. *Use your answer from part (a) to approximate the solution of the linear system* $Ax = b$. *Give guarantees on the norm of the error (be careful with which norm you are using, though you can use any norm you want, to measure the error). Compute the actual error and compare. Note: the distribution of the random variables you use is up to you, as long as* A *has the right properties.*

3. *Find the coefficients in the (shifted and scaled) Chebyshev expansion for* $1/x$ *on the interval* $[1, 5]$ *for* $n = 5, 10, 20$. *Be careful about the mapping from* $[-1, 1]$ *to* $[1, 5]$ *and back.*

4. *Use the same* A *and* b *from part (b). Use your answer from part (c) to approximate the solution of the linear system* $Ax = b$. *Note: given a matrix* M *and a vector* v *you can compute* $T_n(M)v$ *from* $T_{n-1}(M)v$ *and* $T_{n-2}(M)v$ *using the recurrence relation! You do not need to calculate it each time, nor should you compute it using the cosine representation of* T_n. *What guarantees can you give on the accuracy of your solution?*

Interpolation and its Interpretations

So far we have considered the question of finding a "good" polynomial approximation to a given function f. We have not been overly concerned with computational considerations (finding maxima, integration, and the number of evaluations of f, for example). In this section we (partially) fill this gap. Our setup is the following:

Suppose we are given points $x_0, \ldots, x_n \in [-1, 1]$ and samples $f_1, \ldots, f_n$ taken from an unknown function f with certain known properties (Lipschitz,p-times differentiable, continuous, etc.).

Then, we ask the following questions:

- Given $x \in [-1, 1]$ can we find $\tilde{f} \approx f(x)$?
- How do we construct $\tilde{f}$ from the given data?
- What is the accuracy of $\tilde{f}$ and how does that depend on the locations of the points and the properties of f?
- When can we do this in practice (on a computer with finite precision arithmetic)?
- Can we characterize good points?

Let's start with polynomials. Why? Well, previously we have found error bounds for polynomial approximation. If we can understand how to (stably!) interpolate polynomials, then we can try to use the face that for smooth enough functions f there is a nearby polynomial.

Idea 1: Compute the Vandermonde matrix

$$\underbrace{\begin{pmatrix} 1 & x_0 & \ldots & x_0^n \\ 1 & x_1 & & x_1^n \\ \vdots & \vdots & & \vdots \\ 1 & x_n & \ldots & x_n^n \end{pmatrix}}_{V} \underbrace{\begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix}}_{\vec{\alpha}} = \underbrace{\begin{pmatrix} f_0 \\ f_1 \\ \vdots \\ f_n \end{pmatrix}}_{\vec{f}}$$

For each x, set $\delta_x = (1, x, x^2, \dots, x^n)^T$. Then, if $f \in P_n$,

$$f(x) = \delta_x^T \vec{\alpha}.$$

We have seen this idea (in a much more general context) before. There are some immediately visible drawbacks and natural questions. In general, V will be poorly-conditioned, so V^{-1} will magnify errors (rounding, experimental, etc.) by a large factor, leading to large errors in $\vec{\alpha}$. Does this affect the final result? The answer is somewhat surprising and depends on the points x_i. See Shen & Serkh 2023 for a good analysis of this approach.
Cosmetically, it requires computing the coefficients $\vec{\alpha}$ (which are auxiliary) and takes $O(n^2) - O(n^3)$ operations.

Remark 8. *Nothing stops us from using a different basis, besides monomials that is, and re-running the above arguments. In practice this works great, provided we can find points for which the associated "Vandermonde matrix" $V_{i,j} = \phi_j(x_i)$ is well-conditioned.*

Idea 2: Lagrange interpolation.
We will first go through the naïve approach and then fix it. Construct

$$\ell_i(x) = \frac{\prod_{j \neq i}(x - x_j)}{\prod_{j \neq i}(x_i - x_j)}, \quad i = 0, \dots, n.$$

Clearly, ℓ_i is a polynomial of degree n, vanishing at all x_j except for x_i at which it is one. Using this basis, if $f \in P_n$,

$$f(x) = f_0 \ell_0(x) + \cdots + f_n \ell_n(x).$$

To see this, note that both sides are in P_n and agree at $n+1$ points.
A natural question is how stable this is.

Definition 9. *Given $x_1, \dots, x_n$ the* Lebesgue constant Λ *is defined via*

$$\Lambda = \sup_{f \in C([a,b])} \frac{\|p_f\|}{\|\vec{f}\|_\infty} = \sup_{f \in C([a,b])} \frac{\|p_f\|}{\|f\|}$$

where $\vec{f} = (f_0, \dots, f_n)^T$ and

$$p_f = \sum_{j=0}^{n} f_j \ell_j(x).$$

The function

$$\lambda(x) = \sum_{j=0}^{n} |\ell_j(x)|,$$

is called the Lebesgue function. *Noe that here we assume the x_i's are in an interval $[a, b]$ and the ∞-norms are taken over that interval.*

Proposition 4. *If the x_i are all distinct then $1 \leq \Lambda < \infty$.*

Proof. It is easy to argue that $\|p_f\|$ is a continuous function of $f_0, \ldots, f_n$. By scaling, it suffices to consider $\|\vec{f}\|_\infty \leq 1$. By compactness then, Λ is finite. □

Our next result relates the Lebesgue constant to the best polynomial approximation.

Theorem 21. *Let $x_0, \ldots, x_n \in [a, b]$ and Λ be the Lbesgue constant. Given $f \in C([a, b])$, let p be its Lagrange approximation and p_* be the best polynomial approximation in P_n. Then*

$$\|f - p\| \leq (1 + \Lambda)\|f - p_*\|.$$

Remark 9. *We have seen a very similar result before.*

Proof. We could argue by noting that $P : f \mapsto p_f$ is a projection of $C([a, b])$ to P_n and $\|P\|_\infty = \Lambda$. The result then follows the first part of the proof for Chebyshev errors versus best approximation errors.

More concretely, we note that $p - p_*$ is a polynomial. So

$$\begin{aligned} f - p - (f - p_*) &= \sum_{j=0}^{n} ((f - p) - (f - p_*))|_{x_j} \ell_j(x) \\ &= -\sum_{j=0}^{n} (f - p_*)|_{x_j} \ell_j(x), \end{aligned}$$

and hence

$$\|f - p\| \leq \|f - p_*\| \left(1 + \max_x \sum_{j=0}^{n} |\ell_j(x)|\right) = (1 + \Lambda)\|f - p_*\|.$$

□

Thus the Lebesgue constant is closely tied to how well Lagrange interpolation works at approximating continuous functions, at least relative to their best polynomial approximation.

Theorem 22. *On the interval $[-1, 1]$, if Λ_n is the Lebesgue constant for any set of $n + 1$ distinct points in $[-1, 1]$, then*

a) $\Lambda_n \geq \frac{2}{\pi} \log(n + 1) + \frac{2}{\pi} \left(\gamma + \log\left(\frac{4}{\pi}\right)\right)$.

b) For Chebyshev roots,

$$\Lambda_n \leq \frac{2}{\pi} \log(n + 1) + 1.$$

Proof. We do not prove (a) here. See the paper of Erdös (1961) and Brutman (1978).

For (b) we proceed as in Powell. The proof, though it is certainly not optimal, involves combining trigonometric identities with truncated geometric expansions. We begin by recalling that the roots of the Chebyshev polynomial T_{n+1} are

$$x_m = \cos\left(\frac{(m+1/2)}{n+1}\pi\right).$$

Then

$$\sum_{k=0}^{n}{}' T_k(x_j)T_k(x_i) = \sum_{k=0}^{n}{}' \cos\left(k\frac{(j+1/2)}{n+1}\pi\right)\cos\left(k\frac{(i+1/2)}{n+1}\pi\right) = \frac{(n+1)}{2}\delta_{i,j}.$$

We leave the last equality as an exercise. Here the prime is used to denote that the first term in the sum should be halved.

Thus,

$$\sum_{k=0}^{n}{}' T_k(x_j)T_k(x) = \frac{2}{(n+1)}\ell_j(x).$$

Now, setting $\theta_j = \arccos(x_j)$ and $\theta = \arccos(x)$,

$$\begin{aligned}\sum_{k=0}^{n}{}' T_k(x_j)T_k(x) &= \sum_{k=0}^{n}{}' \cos(k\theta_j)\cos(k\theta) \\ &= \frac{1}{4}\frac{\sin((n+1/2)(\theta+\theta_j))}{\sin((\theta+\theta_j)/2)} + \underbrace{\frac{1}{4}\frac{\sin((n+1/2)(\theta-\theta_j))}{\sin((\theta-\theta_j)/2)}}_{S_n(\theta-\theta_j)}.\end{aligned}$$

Summing over j we obtain

$$\sum_{j=0}^{n}|\ell_j(x)| = \frac{1}{2(n+1)}\sum_{j=0}^{n}|S_n(\theta-\theta_j)+S_n(\theta+\theta_j)|.$$

Next we use the identity

$$\sin((n+1/2)(\theta\pm\theta_j)) = \pm(-1)^j\left[\cos((n+1)\theta)\cos\left(\frac{\theta\pm\theta_j}{2}\right)+\sin((n+1)\theta)\sin\left(\frac{\theta+\theta_j}{2}\right)\right].$$

Substituting this into our expression for $\lambda(x)$, we obtain the bound

$$\sum_{j=0}^{n}|\ell_j(x)| \le \frac{|\cos((n+1)\theta)|}{2(n+1)}\sum_{j=0}^{n}\left|\cot\left(\frac{\theta+\theta_j}{2}\right)-\cot\left(\frac{\theta-\theta_j}{2}\right)\right|.$$

We claim that is suffices to optimize over $[0, \frac{\pi}{2(n+1)}]$. On this interval all $|\ell_j(x(\theta))|$ are decreasing, so the right hand side is bounded above by

$$\begin{aligned}\frac{2}{n+1}\sum_j\left|\cot\left(\frac{\theta_j}{2}\right)-\cot\left(\frac{-\theta_j}{2}\right)\right| &= \frac{1}{n+1}\sum_j\left|\cot\left(\frac{\theta_j}{2}\right)\right| \\ &\le \frac{1}{n+1}\cot\left(\frac{\theta_0}{2}\right)+\frac{1}{\pi}\int_{\theta_0}^{\pi}\cot(x/2)\,\mathrm{d}x \\ &= \frac{1}{n+1}\cot\left(\frac{\theta_0}{2}\right)+\frac{2}{\pi}\log\frac{\sin(\pi/2)}{\sin(\theta_1/2)}.\end{aligned}$$

Setting $\theta_1 = \pi/(4(n+1))$, we arrive at the bound

$$\Lambda \leq \frac{4}{\pi} + \frac{2}{\pi} \log\left(\frac{4(n+1)}{\pi}\right) + O(n^{-2}).$$

□

This is somewhat encouraging. What about equispaced?

Theorem 23. *For equispaced points, Λ_n satisfies*

$$\Lambda_n > \frac{2^{n-2}}{n^2}, \quad \Lambda_n \sim \frac{2^{n+1}}{en \log n}.$$

Proof. Try to get a bound as close as you can. □

Runge Phenomena

The blow up of the Lebesgue constant for equispaced interpolation is associated with a behavior known as *Runge phenomena*. Polynomial interpolation from equispaced points is exponentially ill-conditioned. Typically, the interpolant is relatively fine in the middle of the interval but oscillates wildly near the endpoints.

Example 6. *The witch of Agnesi. Consider the function*

$$f(x) = \frac{1}{1 + a^2 x^2}.$$

To make this more precise, set $\ell(x) = \prod_{j=0}^{n}(x - x_j)$ and let $p_f(x)$ be the Lagrange interpolant of f, which is assumed to be sufficiently smooth. For $x \neq x_j$, $j = 0, 1, 2, \ldots, n$, we define

$$\phi_x(t) = f(t) - p_f(t) - \frac{f(x) - p_f(x)}{\ell(x)} \ell(t).$$

Note that $\phi_x(x_i) = 0$ and $\phi_x(x) = 0$. Since ϕ_x is a polynomial in t, the interlacing of roots then says that $\phi_x^{(n_1)}$ has a root on $[-1, 1]$ at ξ_x, say. Then

$$\phi_x^{(n+1)}(\xi_x) = f^{(n+1)}(\xi_x) - 0 - \frac{f(x) - p_f(x)}{\ell(x)}(n+1)! = 0.$$

The zero arises since $p_f \in P_n$. After rearranging, we find

$$|f(x) - p_f(x)| = \frac{1}{(n+1)!} |\ell(x)| \, |f^{(n+1)}(\xi_x)|.$$

Example 7. *The witch continued. It is clear that*

$$\|\ell\|_\infty \leq h^{n+1} n!.$$

Also,

$$\|f^{(n+1)}\|_\infty \leq a^n n!$$

and so the bound becomes

$$|f(x) - p_f(x)| \leq \frac{h^{n+1}(n!)^2 a^n}{(n+1)!} \sim \frac{1}{n^{3/2}} \sqrt{8\pi} \left(\frac{2a}{e}\right)^n.$$

So $\|f - p_f\|$ converges if $2a/e < 1$. Of course this is an upper bound only, but it gives some reasonable intuition.

How do we avoid Runge phenomena?

i) Change the points.

i) Change the problem. Sacrifice passing through every point using, for example, least squares.

i) Change the approximation space, i.e. use piecewise polynomials or other, more general, approaches (see "radial basis functions" for example).

Potential theory, the Hermite integral formula, and interpolation

In this section we recast Lagrange interpolation as a contour integral. Apart from its aesthetic appeal, the resulting formula gives a relatively slick way of bounding interpolation errors, and introduces deep connections to *potential theory*. Given $x_0, \ldots, x_n$ let ℓ_j denote the j^{th} Lagrange interpolant. Set

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

Then, it is easy to check that

$$\ell_j(x) = \frac{\ell(x)}{\ell'(x_j)\,(x - x_j)}.$$

If f is analytic in a suitable region, we can get a nice formula for the Lagrange interpolant. We begin by recalling that the interpolating polynomial to f passing through $x_0, \ldots, x_n$ is given by

$$p(x) = \sum_{j=0}^{n} f(x_j)\, \ell_j(x).$$

Now, by Cauchy's formula,

$$\ell_j(x) = \frac{1}{2\pi i} \int_{\Gamma_j} \frac{\ell(x)}{\ell(t)\,(x - t)}\, \mathrm{d}t$$

where Γ_j encloses x_j but no other x_i nor x. It is an exercise to show that the residue of the pole at $t = x_j$ is given by $1/(\ell'(x_j)\,(x - x_j))$. Then, if f is analytic in a neighborhood containing Γ_j,

$$\ell_j(x) f(x_j) = \frac{1}{2\pi i} \int_{\Gamma_j} \frac{\ell(x) f(t)}{\ell(t)\,(x - t)}\, \mathrm{d}t.$$

So, provided $x \notin \bigcup_j \Gamma_j$, and f is analytic inside all the Γ_j's,

$$p(x) = \frac{1}{2\pi i} \sum_{j=0}^{n} \int_{\Gamma_j} \frac{\ell(x)\, f(t)}{\ell(t)\,(x-t)}\, \mathrm{d}t.$$

Clearly, if Γ is a contour enclosing all x_j's but not x, then

$$p(x) = \frac{1}{2\pi i} \int_{\Gamma} \frac{\ell(x)\, f(t)}{\ell(t)\,(x-t)}\, \mathrm{d}t,$$

provided f is suitably analytic.

Now, near x, the integrand has a pole at $t = x$, with residue $-f(x)$. Thus, if we expand our contour to include x, calling this new contour $\tilde{\Gamma}$, then

$$p(x) - f(x) = \frac{1}{2\pi i} \int_{\tilde{\Gamma}} \frac{\ell(x)\, f(t)}{\ell(t)\,(x-t)}\, \mathrm{d}t.$$

Also, clearly

$$p(x) = \frac{1}{2\pi i} \int_{\tilde{\Gamma}} \frac{(\ell(x) - \ell(t))\, f(t)}{\ell(t)\,(x-t)}\, \mathrm{d}t.$$

The first equation is called the Hermite integral formula. While they are not necessarily helpful in practice for computing p, they are very useful for understanding the errors in approximation. To wit,

$$|p(x) - f(x)| \leq \underbrace{\max_{t \in \tilde{\Gamma}} \left| \frac{\ell(x)}{\ell(t)} \right|}_{T_1} \cdot \underbrace{\frac{1}{2\pi} \int_{\tilde{\Gamma}} \frac{|f(t)|}{|t-x|}\, \mathrm{d}t}_{T_2}.$$

Typically one then argues that T_1 decays rapidly in n, while T_2, which is independent of n, remains bounded. Of course this depends on the distribution of points. Define

$$\gamma_n(x,t) = \left| \frac{\ell(t)}{\ell(x)} \right|^{1/(n+1)}$$

and

$$\alpha_n = \min_{x \in X,\, t \in \Gamma} \gamma_n(x,t).$$

If $\alpha_n \geq \alpha > 1$, then we get the bound

$$\|p - f\| \in \mathcal{O}(\alpha^{-n}).$$

The Numerical Implementation of Lagrange Interpolation

So far we have been focused primarily on the theoretical implications of Lagrange interpolation. We now turn our attention to practical matters: how do we do it quickly and stably on the computer. Let's start with speed.

For the naïve algorithm,

- each denominator can be formed in precomputation (once per set of points, not once per x). This requires $\mathcal{O}(n^2)$ floating point operations,
- evaluating ℓ_j requires $\mathcal{O}(n)$ operations, and there are $n+1$ of them, so evaluating all of them is $\mathcal{O}(n^2)$ operations. This must be done for *each new* x.

A first improvement

Given

$$w_j = \frac{1}{\prod_{i \neq j}(x_j - x_i)},$$

we observe that if $\ell(x) = (x - x_0) \cdots (x - x_n)$, then

$$\ell_j(x) = w_j \frac{\ell(x)}{x - x_j)}.$$

For each new x, ℓ can be computed in $2n+2$ floating point operations (flops), and ℓ_j can be computed from ℓ in 3 flops. So, we have improved the evaluation time per x to $\mathcal{O}(n)$. Note also that the "barycentric weights" are independent of both x *and* f. It is also easy to modify this procedure to give a fast update if only a few of the x_i are changed.

We can make this look prettier in the following way. By interpolating the function 1, we see that

$$1 = \sum_{j=0}^{n} \ell_j(x) = \sum_{j=0}^{n} w_j \frac{\ell(x)}{(x - x_j)} = \ell(x) \sum_{j=0}^{n} \frac{w_j}{x - x_j}.$$

Similarly, if p_f is our Lagrange interpolant,

$$p_f(x) = \sum_{j=0}^{n} \ell_j(x) f_j = \ell(x) \sum_{j=0}^{n} \frac{w_j f_j}{x - x_j}.$$

Taking the ratio,

$$p_f(x) = \frac{\sum_{j=0}^{n} \frac{w_j f_j}{x - x_j}}{\sum_{j=0}^{n} \frac{w_j}{x - x_j}}.$$

This is called the barycentric interpolation formula.

Remark 10. *This can be evaluated in $\mathcal{O}(n)$ flops after $\mathcal{O}(n^2)$ flops in precomputation. The formula is quite striking - it represents a polynomial as the ratio of two rational approximations!*

Remark 11. *In principle one can compute the weights w_j approximately in $\mathcal{O}(n \log \epsilon)$, where ϵ is the error tolerance. In practice this is seldom done.*

What about accuracy?

There seems like an awful lot of subtraction going on, and one might get concerned, for example, about evaluations at x's near an x_j. Our next result gives us some reassurance on this front.

Theorem 24 (Higham (2004))**.** *Suppose $\hat{p}$ is the polynomial one actually computes and ϵ is machine precision. Then*

$$\frac{|p(x) - \hat{p}(x)|}{|p(x)|} \leq (3n+4)\epsilon C_{x,f} + (3n+2)\epsilon C_{x,1} + \mathcal{O}(\epsilon^2),$$

where

$$C_{x,f} = \frac{\sum_{j=0}^{n} \left| \frac{f_j w_j}{x - x_j} \right|}{\left| \sum_{j=0}^{n} \frac{f_j w_j}{x - x_j} \right|}.$$

Note, in particular, that $C_{x,1} = \lambda(x) \leq \Lambda$, where λ is the Lebesgue function and Λ the Lebesgue constant.

proof sketch. Let $\oplus, \ominus, \oslash$ and $\otimes$ denote the floating point operation of $+, -, /$, and $\times$. Then, for any floating point numbers a, b

$$(a \oplus b) = (a + b)(1 + \delta),$$

for some $|\delta| \leq \epsilon$. The same goes for $\ominus, \oplus$ and $\oslash$.

Let ϕ_j denote the floating point result of computing $1/w_j$. Then

$$\begin{aligned}
\phi_j &= (x_j \ominus x_0) \otimes \cdots \otimes (x_j \ominus x_n) \\
&= ((x_j - x_0)(1 + \delta_0)) \otimes \cdots \otimes ((x_j - x_n)(1 + \delta_n)) \\
&= (x_j - x_0)(x_j - x_1)(1 + \delta_0)(1 + \delta_1)(1 + \eta_0) \otimes \cdots ((x_j - x_n)(1 + \delta_n)) \\
&= \frac{1}{w_j} \prod_{i \neq j} (1 + \delta_i) \prod_{i \neq j, i < n-1} (1 + \eta_i).
\end{aligned}$$

Here $|\delta_i|, |\eta_i| \leq \epsilon$.

Thus, the computation of w_j in floating point, which we denote by $\hat{w}_j$ is given by

$$\hat{w}_j = w_j(1 + \xi) \prod_{i \neq j} (1 + \delta_i)^{-1} \prod_{i \neq j, i < n-1} (1 + \eta_i)^{-1},$$

for some $|\xi| \leq \epsilon$ and so

$$|\hat{w}_j - w_j| = |w_j|(1 + \mathcal{O}(n\epsilon) + \mathcal{O}(\epsilon^2).$$

□

For the first barycentric formula

$$p_f(x) = \ell(x) \sum_{j=0}^{n} \frac{w_j}{x - x_j} f_j$$

one can prove the following theorem.

Theorem 25 (Higham (2004))**.**

$$\frac{|p_f(x) - \hat{p}(x)|}{|p_f(x)|} \leq \frac{(5n+5)\epsilon}{1-(5n+5)\epsilon} C_{x,f}.$$

The proof can be found in the paper *The numerical stability of barycentric Lagrange interpolation* by Nicholas Higham in the IMA Journal of Numerical Analysis (2004).

Hermite interpolation

Frequently we are also interested in the case in which we not only have the values of a function at a collection of points, but also its derivative, or derivatives. In the linear algebraic picture of interpolation this poses no great trouble. Indeed, if our interpolating functions $\{\phi_j\}$ are differentiable and we are given information about the derivative of f at a point x_k then we can simply add an extra row to $\phi_j(x_\ell)$ consisting of $\phi_j'(x_k)$, $j = 0, \ldots, n-1$. For monomials this would give a linear system which looks like

$$\begin{pmatrix} 1 & x_0 & \cdots & x_0^{n-1} \\ 1 & x_1 & \cdots & x_1^{n-1} \\ \vdots & & \ddots & \vdots \\ 1 & x_{n-2} & \cdots & x_{n-2}^{n-1} \\ 0 & 1 & \cdots & (n-1)\, x_j^{n-2} \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_{n-2} \\ \alpha_{n-1} \end{pmatrix} = \begin{pmatrix} f(x_0) \\ f(x_1) \\ \vdots \\ f(x_{n-2}) \\ f'(x_j) \end{pmatrix},$$

where $\alpha_0, \ldots, \alpha_{n-1}$ are the coefficients of our approximant in the monomial basis.

This is fine, insofar as it is relatively easy to show that it is easy to show that the matrix on the right-hand side is invertible, and it is straightforward to see how to generalize the approach to add more derivative information (i.e. derivative information at more points and/or higher derivatives). Each new piece of information allows us to fit an extra function.

For notational convenience, we show that derivative information at x_j is included by repeating x_j twice when we list our points. Extending this, if we have information about $f(x_j), \ldots, f^{(k)}(x_j)$ then x_j would appear $k+1$ times in our list of nodes.

Example 8. *Fitting the n-term truncated Taylor series of f at a point x_j would correspond to the interpolation problem with nodes $x_j, x_j, \ldots, x_j$ where x_j appears n times in the list.*

This gives us a convenient way of keeping track of which derivatives to include. One can then create the interpolation matrix as above and solve for corresponding coefficients. This approach is a little unsatisfying for the following reason. When all n points are

distinct and relatively far away, the 'coefficients to values' matrix $V(x_0, \dots, x_{n-1})$ is invertible. As two points, x_j and x_{j+1} approach each other, the two corresponding rows become more and more parallel, and the condition number of V goes to infinity. When the two points are exactly equal, then we replace one by the derivative, and the system is (relatively) well-conditioned again. Thus, our interpolation problem is discontinuous in the location of the nodes $(x_0, \dots, x_{n-1})$ as a vector in $\mathbb{R}^n$.

In order to fix this situation, we start with the following definition.

Definition 10. *Given $v \in C^k$, the* divided difference of order j, $j \leq k$, *is the symmetric function defined inductively by the relation*

$$v[x_0, \dots, x_j] = \begin{cases} \frac{v[x_1,\dots,x_j]-v[x_0,\dots,x_{j-1}]}{x_j-x_0} & x_j \neq x_0, \\ \frac{1}{j!}v^{(j)}(x_0) & x_0 = x_1 = \cdots = x_j. \end{cases}$$

The following theorem then gives a solution to the general interpolation problem.

Theorem 26. *If $p \in P_n$ and $p[x_0, \dots, x_n]$ denotes the divided difference, then*

$$p(x) = p[x_0] + p[x_0, x_1](x - x_0) + \cdots + p[x_0, \dots, x_n](x - x_0) \cdots (x - x_{n-1}).$$

In particular, we have the following obvious corollary.

Corollary 5. *For any $x_0, \dots, x_n$, the Hermite interpolation problem associated with the monomials $1, x, \cdots, x^{n-1}$ is always solvable. In particular, for any set of real numbers $q_0, \dots, q_{n-1}$, there exists a polynomial p such that $p(x_j) = q_j$, where once again repetition of a point x_j means that p should be replaced by an appropriate derivative evaluated at x_j.*

This property can be generalized, and extends the notion of a Haar space.

Definition 11. *A space is called an* extended Chebyshev space *if any Hermite interpolation problem has a unique solution.*

As for Haar subspaces, one can formulate many different characterizations. For example, we have the following.

Lemma 7. *An n-dimensional space H is an extended Chebyshev space if and only if any non-zero element of H vanishes at most $n - 1$ times, including multiplicities.*

The following proposition also follows straightforwardly from the definition.

Proposition 5. *Let H be an extended Chebyshev system with basis $v_0, \dots, v_n$. For any collection of points $x_0, \dots, x_n$, (allowing for repetitions) the matrix*

$$V_{i,j} = \sum_{\ell=0}^{j} v_i[x_0, \dots, x_\ell]$$

is invertible. Here $v_i[\cdot]$ denote the divided differences.

Additional exercises

Exercise 21. *In this problem we will play around with interpolation in theory and practice.*

1. *Determine what happens to the Hermite integral formula when two points coincide, i.e. suppose one uses the points $x_0, x_0, x_2, x_3, \dots, x_n$ in the Hermite integral formula. What expression does this correspond to for the interpolant p? Does it still make sense? Hint: start with*

$$p(x) = \frac{1}{2\pi i} \int_\Gamma \frac{f(t)\,(\ell(t) - \ell(x))}{\ell(t)\,(t-x)}\,\mathrm{d}t$$

   and go backwards through the derivation of the Hermite integral formula.

2. *Confirm your answer to part (a) numerically for $f(x) = e^{-0.3x}$. That is, use the Lagrange-type formula you derived to compute $p(x)$ and then compute it by directly integrating*

$$p(x) = \frac{1}{2\pi i} \int_\Gamma \frac{f(t)\,(\ell(t) - \ell(x))}{\ell(t)\,(t-x)}\,\mathrm{d}t.$$

   For Γ choose a circle of radius 1.5 and perform the integration using left-hand Riemann sum (why?). For points, use a 2 point Chebyshev rule with each node repeated twice (to give a total of 4 points - two sets of two identical points). How does the error at $x = 1/3$ change as you add more points. Compare with the unrepeated Chebyshev rule.
   Note: *you can use either Chebyshev points of the first or second kind - whichever you prefer (either $\cos(1/(2n) + j/(n+1)$, $j = 0, \dots, n$ or $\cos(j\pi/n)$, $j = 0, \dots, n$, the second type are more common).*

3. *More generally, given a set of distinct points $x_1, \dots, x_n$, let α_n be defined by*

$$\alpha_n = \min_{x \in [-1,1],\, t \in \Gamma} \frac{\left(\prod_{j=1}^n |t - x_j|\right)^{1/n}}{\left(\prod_{j=1}^n |x - x_j|\right)^{1/n}}.$$

   Now, consider the doubled-version with each node repeated twice $[x_1, x_1, \dots, x_n, x_n]$. Assuming that $\alpha_n > 0$ find a bound for the error in terms of α_n, f, and Γ.

4. *Implement the barycentric interpolation formula for* 5 *Chebyshev nodes on* $[-1, 1]$ *and* $f(x) = e^{-0.3x}$. *Investigate what happens as the error approaches one of the nodes.*

Integration

We now turn our attention to integration, a task intimately related to interpolation. Indeed, suppose f is well-approximated (say in L^∞) by a set of basis functions $\phi_1, \ldots, \phi_n$. Moreover, suppose we are given a set of points $x_1, \ldots, x_n$ such that the Vandermonde matrix $V_{i,j} = \phi_j(x_i)$ is well conditioned.

Roughly speaking, if $f \approx \sum_{i=1}^n \alpha_i \phi_i(x)$ for some coefficients $\{\alpha_i\}$, then

$$\int_a^b f(x)\,\mathrm{d}x \approx \int_a^b \sum_{i=1}^n \alpha_i \phi_i(x)\,\mathrm{d}x = \sum_{i=1}^n \alpha_i \int_a^b \phi_i(x)\,\mathrm{d}x = \sum_{i=1}^n \alpha_i s_i,$$

where $s_i = \int_a^b \phi_i(x)\,\mathrm{d}x$. We can represent the right-most sum as a dot product $\vec{a} \cdot \vec{s}$. Now,

$$\alpha_i \approx \sum_{j=1}^n (V^{-1})_{i,j} f_j$$

and hence

$$\int_a^b f(x)\,\mathrm{d}x \approx \sum_{i=1}^n \sum_{j=1}^n (V^{-1})_{i,j} f_j s_i = \sum_{j=1}^n \left(\sum_{i=1}^n (V^{-1})_{i,j} s_i \right) f_j = \sum_{j=1}^n w_j f_j,$$

where $\vec{w} = (s^T V^{-1})^T$. The x_j are called *quadrature nodes,* and the w_j are called *quadrature weights*. Together they give a *quadrature rule.*

Let us make this a little more precise.

Theorem 27 (Martinsson,Rokhlin,Tygert (2011))**.** *Suppose S is a measure space, w is a non-negative real-valued integrable function on S, n is a positive integer, $f_1, \cdots, f_n$ are bounded complex-valued integrable functions on S, and $\epsilon \leq 1$ is a positive real number. Then, there exists n complex numbers $w_1, \ldots, w_n$, and n points $x_1, \ldots, x_n \in S$ such that*

$$|w_k| \leq (1+\epsilon) \int w(x)\,\mathrm{d}x, \quad k = 1, \ldots, n,$$

and

$$\int_S f(x)\, w(x)\,\mathrm{d}x = \sum_{k=1}^n w_k f(x_k)$$

for any f given by $f(x) = \sum_{j=1}^n c_j f_j(x)$ for some coefficients $c_1, \cdots, c_n$.

Generalized Gaussian quadrature

For most practical purposes, the result of the previous section is sufficient: n points to integrate n functions. But, counting degrees of freedom, we get to choose n locations/ points and n quadrature weights. So, we have $2n$ degrees of freedom to integrate n functions. A natural question is whether or not we can do better. Below we give a useful partial answer to this question.

Before formulating the theorem, we recall that an extended Chebyshev space is a space in which the "Hermite interpolation problem" is always solvable. A collection of functions $\phi_1, \cdots, \phi_n \in C^n[a,b]$ is called an extended Chebyshev system if they form a basis of an n-dimensional Chebyshev spaace.

The following theorem shows how this (quite strong) structure gives (quite powerful) control on quadrature. It is a simplified form of a theorem by Bojanov, Braess and Dyn (1986) though similar results to this one can be found in papers by Markov and the book by Karlin and Studden.

Theorem 28. *Let H be a Haar subspace of $C[a,b]$, spanned by an extended Chebyshev system $v_1, \cdots, v_n$. Moreover, suppose $\mathrm{d}\mu(x) = w(x)\,\mathrm{d}x$ with a positive weight function $w \in C([a,b])$. Then, if $n = 2m$ is even, there exists a unique set of points $a = x_0 < x_1 < \cdots < x_m < x_{m+1} = b$, such that*

$$\int_a^b u \,\mathrm{d}\mu = \sum_{i=1}^{m} a_i u(x_i), \quad \text{for all } u \in H.$$

Moreover, the quadrature weights a_i are positive.

Proof. The proof is a fun topological argument hinging upon the Borsuk antipodality theorem:

> *Let Ω be a bounded, open, symmetric neighborhood of 0 in $\mathbb{R}^{n+1}$ and suppose $T : \partial\Omega \to \mathbb{R}^n$ is an odd, continuous map. Then there exists some $x \in \partial\Omega$ for which $T(x) = 0$.*

Set

$$S = \left\{ (y_0, \cdots, y_m) \mid \sum_{i=0}^{m} |y_i| = b - a \right\}.$$

In particular, S can be thought of the set of vectors of "differences". For $y \in S$ we define the vector $x(y) = (x_0(y), \cdots, x_{m+1}(y))$ by

$$x(y) = \{a, a + |y_0|, a + |y_0| + |y_1|, \cdots, b\}.$$

As before, for $v \in C^k$, we let $v[x_0, \cdots, x_j]$ denote the divided difference of order j.

For any $y \in S$ define the functional L_y on H by

$$L_y(u) := \sum_{i=0}^{m} \operatorname{sgn}(y_i) \int_{x_i(y)}^{x_{i+1}(y)} u(x)\,\mathrm{d}\mu - \sum_{j=1}^{n} b_j(y) u(z_1, \cdots, z_i),$$

where

$$z = (x_1, \cdots, x_m, x_m \cdots, x_1),$$

and the b_j are chosen so that

$$L_y(v_j) = 0, \quad j = 1, \cdots, n.$$

Note that from the previous chapter we know that the required matrix is invertible, so that the b_j are guaranteed to exist for any y. Since the matrix is invertible and continuous for any $y \in S$, and the first term in the definition of L_y is continuous, we also see that all the b_j's are continuous in y.

Moreover, if we define the map $T : S \to \mathbb{R}^n$, by

$$T(y) = (b_n(y), \cdots, b_{n+1-m}(y)),$$

then it follows from the properties of b_j that T is continuous and odd. Thus, there exists a y^* such that $T(y^*) = 0$. So, setting $s(x) = \operatorname{sgn}(y_j^*)$,

$$\int_a^b u(x)\, s(x)\,\mathrm{d}\mu = \sum_{j=1}^{m} b_j(y^*) u(x_1(y^*), \cdots, x_j(x^*)).$$

Let ℓ denote the number of distinct x_j and, for each j, let k_j denote multiplicity of the j^{th} point. Then there are coefficients c_j^i such that

$$\int_a^b u(x)\, s(x)\,\mathrm{d}\mu = \sum_{j=1}^{\ell} \sum_{i=1}^{k_j} c_j^i u^{(i-1)}(x_j).$$

Let u be a function such that $u^{(i)}(x_j) = 0$ and $u(x)s(x) \geq 0$. If $\ell < m$, or if s is not strictly positive, then enforcing positivity requires less than $2m$ conditions and so one can always find such a u. Counting, there are m values or derivatives which must vanish, and $\ell < m$ points at which the solution might change sign. Add extra conditions on vanishing of higher derivatives at these points until the function is guaranteed positive. This gives a contradiction if $\ell < m$, since by construction the left-hand side is positive, while the right-hand side is zero. Thus, $\ell = m$ and $k_1 = \cdots = k_m = 1$.

Showing the positivity of the coefficients $c_1^1, \cdots, c_m^1$ is left as an exercise. □

Remark 12. *This is a specialized and simplified version of a more general result, the proof of which can be found in* Nonlinear Approximation Theory *by Braess.*

In conclusion, for a general class of subspaces, one can integrate $2n$ functions with n (unique) points and n positive quadrature weights. The positivity of the quadrature weights helps avoid catastrophic cancellations. Analogous results hold for spaces of odd dimension. Frequently, even when the system is not extended Chebyshev, one can exactly integrate n functions with $< n$ quadrature points. Finding them can be difficult. See Ma, Rokhlin, Wandzura (1996) for an optimization based approach.

Quadrature rules of this type are called *Generalized Gaussian quadrature* (GGQ) rules.

Gauss-Legendre quadrature and orthogonal polynomials

We now focus on the case of polynomials P_n on $[-1, 1]$. Here, for simplicity, we assume that n is even. Similar results hold for odd n, though the notation is clunkier.

Suppose we want a quadrature rule for integrating all polynomials in P_n, $n = 2m$. One could argue from the last section that an $(m+1)$-point quadrature rule exists which integrates all such polynomials exactly. Here we hope to obtain a more concrete understanding of the properties of this quadrature rule and how to construct it, at least for the special case of polynomials.

Remark 13. *There is an interesting connection to L^2 discretizations here. If $p \in P_n$ then it can be written as a linear combination of terms of the form q_1, q_2 where $q_1, q_2 \in P_m$. Integrating $p \in P_n$ is then equivalent to computing the sum of inner products accurately. An $(m+1)$-point quadrature rule for P_n induces a map $T : P_m \to \mathbb{R}^{m+1}$ defined by*

$$T(q) = \begin{pmatrix} q(x_0)\sqrt{w_0} \\ \cdots \\ q(x_m)\sqrt{w_m} \end{pmatrix}$$

which is an isometry from $P_m \subset L^2$ to $\ell^2(\mathbb{R}^{m+1})$. Moreover, an isometry of this form naturally gives an $(m+1)$-point quadrature rule for integrating functions in P_n.

The previous remark suggests a detour. Rather than considering quadrature, let us first try to write an orthogonal basis for $P_m \subset L^2$. In principle one could do this by applying Gram-Schmidt to P_m. In practice, there are better ways. In particular, running Gram-Schmidt in this context can lead to catastrophic cancellations.

Let us start by trying to think inductively. Suppose we have $p_0, \cdots, p_k$ with $\langle p_j, p_k \rangle = 0$, $i \neq j$, $p_j \in P_j$. Then, if $i < j - 1$,

$$\langle p_j x, p_i \rangle = \langle p_j, \underbrace{x p_i}_{\in P_{j-1}} \rangle = 0.$$

Set $a_j = \langle p_j x, p_{j+1} \rangle$, and $b_j = \langle p_j x, p_j \rangle$. By symmetry,

$$\int_{-1}^{1} x p_j^2 \, \mathrm{d}x = 0,$$

and so $b_j = 0$. Thus,

$$(xp_j - a_{j-1}p_{j-1}) \perp p_0, \cdots, p_j$$

and so $p_{j+1} = A_{j+1}(xp_j - a_{j-1}p_j)$, for some constant A_j. Putting this together, we see that for $j > 0$,

$$xp_j = \alpha_j p_{j+1} + \beta_j p_{j-1}$$

for some sequences α_j, β_j. for some constants. Deducing the exact values of these sequences requires some extra work, and there is some flexibility, since we only ask that $p_0, \cdots, p_{j+1}$ be orthogonal, not orthonormal. It is tradition to set $p_j(1) = 1$, in which case

$$\alpha_j = (j+1)/(2j+1), \quad \beta_j = j/(2j+1)$$

and

$$(j+1)p_{j+1}(x) = (2j+1)xp_j(x) - jp_{j-1}(x),$$

with $p_0 = 1$ and $p_1 = x$.

These are called *Legendre polynomials.* They have a wide variety of interesting and useful properties and appear in a number of contexts, particularly when rotational symmetry is invoked. Their integrals arise in the construction of higher order finite element methods.

With the above scaling, it can be shown that

$$\int_{-1}^{1} p_n p_m \, \mathrm{d}x = \frac{2}{2n+1} \delta_{n,m}$$

and so $\|p_n\|_{L^2([-1,1])} = \sqrt{2/(2n+1)}$.

Now that we have found a nice basis, let's return to our task of finding good quadrature formulae for P_n, $n = 2m$. Given $qinP_{2n}$, we can always write it as

$$q(x) = p(x)p_{m+1}(x) \, + r(x)$$

where $p \in P_{m-1}$, $r \in P_m$, and p_{m+1} is the degree $(m+1)$ Legendre polynomial. It has $m+1$ roots $x_0, \cdots, x_m$, and so

$$q(x_i) = \underbrace{p(x_i)p_{m+1}(x_i)}_{=0} + r(x_i).$$

Also, since $p \in P_{m-1}$ and $p_{m+1} \perp P_m$,

$$\int_{-1}^{1} p(x) \, p_{m+1}(x) \, \mathrm{d}x = 0$$

and so

$$\int_{-1}^{1} q(x)\,\mathrm{d}x = \int_{-1}^{1} r(x)\,\mathrm{d}x.$$

Now, since $r \in P_m$, there exist constants $c_0, \cdots, c_m$ such that

$$r(x) = \sum_{j=0}^{m} c_j p_j(x).$$

Then, $q(x_i) = \sum_{j=0}^{m} c_j p_j(x_i)$, $i = 0, \cdots, m$. Setting $V_{ji} = p_j(x_i)$, and

$$\vec{w} = V^{-1} \begin{pmatrix} 2 \\ 0 \\ \vdots \\ 0 \end{pmatrix},$$

then

$$\int_{-1}^{1} p_j(x)\,\mathrm{d}x = 2\delta_{j,0} = \sum_{i=0}^{m} p_j(x_i) w_i, \quad j = 0, \cdots, m.$$

This is just "interpolation based quadrature" from before, applied to $p_0, \cdots, p_m$. Now, if $q \in P_m$,

$$\int_{-1}^{1} q(x)\,\mathrm{d}x = \int_{-1}^{1} p(x)\, p_{m+1}(x)\,\mathrm{d}x + \int_{-1}^{1} r(x)\,\mathrm{d}x = \underbrace{\int_{-1}^{1} r(x)\,\mathrm{d}x = \sum_{i=0}^{m} r(x_i) w_i}_{\text{since } r \in P_m} = \sum_{i=0}^{m} [p(x_i) p_{m+1}(x_i) + r(x_i)\, w_i.$$

Thus

$$\int_{-1}^{1} q(x)\,\mathrm{d}x = \sum_{i=0}^{m} q(x_i) w_i,$$

as required and we have attained a quadrature rule with nodes $(x_0, \cdots, x_m)$ and weights $(w_0, \cdots, w_m)$ which integrates every polynomial in P_n exactly. These quadrature rules are called *Gauss-Legendre* (or just Legendre or Gaussian) quadrature.

Remark 14. *In the above, we have assumed that p_{m+1} has $m+1$ distinct real roots on the interval $[-1, 1]$. The proof follows similar lines as the proofs of analogous results for extended Chebyshev systems. In the same way, we can also probe that all the weights are positive. We leave this as an exercise.*

Projections

Given that our polynomials $p_0, p_1, \cdots$ form an orthogonal basis of $L^2([-1, 1])$, the projection operator S_n onto the span of the first $n+1$ polynomials is a convenient and frequently-encountered object. Naïvely, it requires $n+1$ integrals. THis is practically annoying, and theoretically cumbersome. Luckily, there is so much structure in this problem that we can find a slick formula.

We start by recalling that

$$(j+1)p_{j+1}(x) = (2j+1)xp_j(x) - jp_{j-1}(x).$$

Then

$$(j+1)[p_{j+1}(x)p_j(t) - p_{j+1}(t)p_j(x)] = (2j-1)(x-t)p_j(x)p_j(t) - j[p_{j-1}(x)p_j(t) - p_{j-1}(t)p_j(x)].$$

Setting $q_j = (j+1)[p_{j+1}(x)p_j(t) - p_{j+1}(t)p_j(x)]$, then

$$q_j - q_{j-1} = 2\frac{(x-t)}{\|p_j\|^2_{L^2([-1,1])}} p_j(x)p_j(t),$$

where we have used the fact that $\|p_j\|^2_{L^2([-1,1])} = 2/(2j+1)$. Summing from $j = 1$ to n, we obtain

$$2(x-t)\sum_{j=1}^{n} \frac{p_j(x)p_j(t)}{\|p_j\|^2_{L^2([-1,1])}} = q_n(x,t) - q_0(x,t).$$

Now, $q_0(x,t) = (x-t) = 2(x-t)p_0(x)p_0(t)/\|p_0\|^2$. So,

$$\sum_{j=0}^{n} \frac{p_j(x)p_j(t)}{\|p_j\|^2_{L^2([-1,1])}} = \frac{q_n(x,t)}{2(x-t)} =: k_n(x,t).$$

Then,

$$\begin{aligned} S_n[f](x) &= \int_{-1}^{1} \sum_{j=0}^{n} \frac{p_j(x)p_j(t)}{\|p_j\|^2_{L^2([-1,1])}} f(t)\,\mathrm{d}t \\ &= \int_{-1}^{1} \frac{(n+1)}{2(x-t)}[p_{n+1}(x)p_n(t) - p_{n+1}(t)p_n(x)]\,f(t)\,\mathrm{d}t \\ &= \int_{-1}^{1} k_n(x,t)\,f(t)\,\mathrm{d}t. \end{aligned}$$

This is called the *Christoffel-Darboux* formula.

Remark 15. *These results generalize naturally to positive weight functions w, i.e.*

$$\int_a^b \tilde{p}_j(x)\tilde{p}_k(x)\,w(x)\,\mathrm{d}x = c_j\delta_{j,k}, \quad \tilde{p}_j \in P_j.$$

In particular, they give "Gaussian" type quadrature rules (2m functions with m points), three-term recurrences, Christoffel-Darboux formulae, etc. For more information, seet Abramowitz and Stegun, NIST, or Orthogonal Polynomials *by Szegö, for example.*

Common weight functions include:

- Chebyshev polynomials (1st kind): $w(x) = (1-x^2)^{-1/2}$ on $[-1,1]$
- Chebyshev polynomials (2nd kind): $w(x) = (1-x^2)^{1/2}$ on $[-1,1]$

- Gegenbauer polynomials: $w(x) = (1-x^2)^{\alpha-1/2}$ on $[-1,1]$, $\alpha > -1/2$,
- Hermite polynomials: $w(x) = e^{-x^2}$ on $(-\infty,\infty)$, sometimes with a different exponent
- Jacobi polynomials: $w(x) = (1-x)^\alpha(1+x)^\beta$ on $(-1,1)$,
- Laguerre polynomials: $w(x) = e^{-x}$ on $[0,\infty)$,
- generalized Laguerre polynomials: $w(x) = x^k e^{-x}$ on $[0,\infty)$.

Further reading

For more information, see also Carothers, Chapters 8 and 9.

Additional Exercises

Exercise 22. *Discretizing and diagonalizing integral operators. Consider the integral operator $T : L^2[-1,1] \to L_2[-1,1]$ defined by*

$$T[f](x) = \int_{-1}^{1} e^{-(x-y)^2} f(y)\,\mathrm{d}y, \quad x \in [-1,1].$$

1. *Prove that $T[f]$ is continuous if $f \in L_2[-1,1]$.*
2. *Using a Gauss-Legendre quadrature rule, write a code that discretizes the integral using a 40 point Gauss-Legendre quadrature and evaluates it at arbitrary points $x \in [-1,1]$. You may assume that f is continuous. Plot the output for $f \equiv 1$ and $f \equiv x$. Then, increase the number of nodes to 80 and compare the output with the 40 point rule.*
3. *Construct the matrix that takes f sampled at an n point Gauss-Legendre rule and maps it to $T[f]$ evaluated at the same points, i.e. K maps $(f(x_1),\dots,f(x_n))$ (approximately) to $(T[f](x_1),\dots,T[f](x_n))$. Diagonalize K with $n = 40$ and plot all the eigenvalues and the first 4 eigenfunctions. Now, set $n = 80$ and repeat. Compare the eigenvalues for $n = 40$ and $n = 80$. What does this say about the original integral operator T? You don't need to be very precise here.*

Exercise 23. *In this problem we will play around with polynomial root finding. In the following suppose that $q_n, n = 0,1,2,\dots$ is a sequence of polynomials which satisfies a three-term recurrence*

$$q_{n+1}(x) = (\alpha_n x + \beta_n)q_n(x) + \gamma_n q_{n-1}(x), \quad n > 0,$$

where α_n, β_n and γ_n are real numbers and the α_n are bounded away from 0. Also, suppose $q_1(x) = (a_0 x + b_0)q_0(x)$. Suppose p is a polynomial with

$$p(x) = \sum_{j=0}^{n} c_j q_j(x),$$

for some coefficients $c_0, \ldots, c_n$ with $c_n \neq 0$. Hint: if you get stuck, look at Trefethen's book Approximation Theory and Approximation Practice, *Chapter 18, but try not to!*

1. *Find a linear map which sends the vector*

$$v = [q_0(x), q_1(x), \ldots, q_{n-1}(x)]^T$$

to

$$[xq_0(x), xq_1(x), \ldots, q_{n-2}(x), xq_{n-1}(x) - q_n(x)/\alpha_{n-1}]^T$$

for all $x \in [-1, 1]$. Your matrix should not depend on x. Is this map unique (assuming the independence of x)?

2. *Show that x_* is a root of p if and only if $q_n(x_*) = -\frac{1}{c_n}\sum_{j=0}^{n-1} c_j q_j(x_*)$.*

3. *If M is the matrix you found in part (a), consider the matrix C defined by $C = M + L$ where*

$$L = -\frac{1}{\alpha_{n-1}c_n}\begin{bmatrix} & & & \\ & & & \\ & & & \\ c_0 & c_1 & \ldots & c_{n-1} \end{bmatrix}.$$

Show that if p has distinct roots, then λ is an eigenvalue of L if and only if $p(\lambda) = 0$. Thus, diagonalizing C is the same as finding the roots of p.

4. *Specialize your construction to the case where: a) the q_n are monomials, b) the q_n are Chebyshev polynomials. Use the former to compute the roots of $p = x^2 - 5x + 2$, and the latter to compute the roots of $p = T_0 + 2T_1 + 4T_2$.*

Exercise 24. *More with projection operators. For $n \geq 0$ and $f \in L^2[-1, 1]$, define*

$$S_n[f](x) = \sum_{j=0}^{n} \frac{p_j(x)}{\|p_j\|_2^2} \int_{-1}^{1} p_j(t) f(t) \mathrm{d}t, \tag{1}$$

the projection onto the span of the first $n+1$ Legendre polynomials $p_0, p_1, \ldots, p_n$.

1. *Show that $S_n : L^2[-1, 1] \to L^2[-1, 1]$ is self-adjoint and of finite rank.*

2. *What are the eigenvalues and corresponding eigenfunctions of S_n?*

3. *Repeat part (a) for the operator $T_n := S_n H + H S_n$, where $H[f](x) = H(x)f(x)$, with H the Heaviside step function.*

4. *Calculate* Tr T_n. Hint: the trace of a trace-class integral operator $K[f](x) = \int k(x, y) f(y) \mathrm{d}y$ is given by $\int k(x, x) \mathrm{d}x$. In part (c), you proved that T_n is trace-class.

5. *Using a Gauss-Legendre quadrature rule, construct the matrix $\tilde{T}_n$ that takes f sampled at an N point Gauss-Legendre rule and maps it to $T_n[f]$ evaluated at the same points, i.e. $\tilde{T}_n$ maps $(f(x_1), \ldots, f(x_N))$ to $(T_n[f](x_1), \ldots, T_n[f](x_N))$. Diagonalize $\tilde{T}_n$ with $n = 3$ and $N = 80$, and plot the eigenfunctions corresponding to non-zero eigenvalues. Verify your answer to part (d).*

Polynomials in Pieces

So far, we have focused on 'global' polynomial representations. We have seen that if the function in question is smooth enough, then Chebyshev interpolation is a convenient way to form rapidly converging approximants. Gauss-Legendre quadratures give an efficient method for integrating polynomials, or functions which are close enough to polynomials. There are many contexts where this approach works extremely well, or there is no other choice. On the other hand, if the function has singularities, or small regions with rapid oscillations, then convergence of polynomial approximation can be exceedingly slow. In this chapter, we briefly highlight a few ways in which piecewise polynomial approximations can be constructed and used. We also give a brief flavor for the generalization of these methods to a more general class of approximation approaches.

Splines

Suppose we have reason to believe that our function is not very smooth (or analytic) and we are only given values of the function at a certain collection of preset points $x_0, \cdots, x_n$ (i.e. the locations in parameter space of experimental measurements). Most of the methods we have discussed so far are designed to take advantage of smoothness. Without it, they can perform just as poorly, if not worse, than a lower order method. Splines are local polynomial approximations that are used in a wide variety of contexts. The idea is to represent the function between each pair of adjacent data points by a polynomial of some degree p.

Let's do some bookkeeping. If we use a piecewise polynomial approximation of degree p, then this gives us $(p+1)n$ degrees of freedom. Demanding the curve is continuous and passes through our $n+1$ data points gives $2(n-1)+2$ constraints. How should we leverage our surplus degrees of freedom? One natural thing to do is enforce smoothness. We could ask for the derivative to be continuous, which would give $n-1$ more constraints. Each additional derivative gives us $n-1$ more constraints. So, with piecewise poly-

nomials we could fit the data and obtain an interpolant with $p-1$ continuous derivatives.

In this way, we obtain $(n-1)(p-1)+2n$ equations.

$$(p+1)n - [(n-1)(p-1)+2n] = p-1.$$

We still have $(p-1)$ left-over degrees of freedom. This makes sense, since the values at the endpoints are arbitrary (it is easiest to see this by considering the quadratic case). The space in which these approximations live is

$$S_p := \{s \in C^{p-1} \mid s|_{[x_{i-1},x_i]} \in P_p,\ 1 \leq i \leq n-1\}.$$

This is an $n+p$ dimensional space.

To get a unique interpolant, we get to impose $p-1$ additional constraints. There are many choices. We will focus on the case $p=3$. In that case, it is 'natural' to require that the second derivatives of the approximant vanish at x_0 and x_n. These are called *natural* cubic splines and live in

$$S_3^N := \{s \in S_3 \,|\, s''(x_0) = 0,\ s''(x_n) = 0\}.$$

If the spline passes through all the data points, then it is called interpolating. When it comes to finding a spline approximation to a given function, we can play a similar trick as for Lagrange interpolation. We can form $\phi_i \in S_3^N$, with $\phi_i(x_j) = \delta_{i,j}$. By linearity, $\sum_i \phi_i(x) f_i$ is the spline we are looking for.

Due to the structure of the problem, we can actually do a little better. Consider an interval $[x_i, x_{i+1}]$. On this interval, the interpolating cubic spline is of the form

$$s(x) = A_i + B_i(x-x_i) + C_i(x-x_i)^2 + D_i(x-x_i)^3$$

for some coefficients a_i, b_i, c_i, and d_i. Evaluating s and its derivatives at x_i and x_{i+1}, we obtain

$$\begin{aligned}
s(x_i) &= A_i \\
s(x_{i+1}) &= A_i + B_i\Delta_i + C_i\Delta_i^2 + D_i\Delta_i^3 \\
s'(x_i) &= B_i \\
s'(x_{i+1}) &= B_i + 2C_i\Delta_i + 3D_i\Delta_i^2 \\
s''(x_i) &= 2C_i \\
s''(x_{i+1}) &= 2C_i + 6D_i\Delta_i,
\end{aligned}$$

where $\Delta_i = x_{i+1} - x_i$. Set $\delta_i = f_{i+1} - f_i$. We now solve for A_i, B_i, C_i, and D_i in terms of the data values f_i, f_{i+1} and the values of s' at the

endpoints, which we denote by $v_i := s'(x_i)$ and $v_{i+1} := s'(x_{i+1})$. Using the data, $s(x_i) = A_i = f_i$ and so

$$s(x_{i+1}) = f_i + v_i\Delta_i + C_i\Delta_i^2 + D_i\Delta_i^3 = f_{i+1}.$$

The equation for $s'(x_{i+1})$ gives

$$v_{i+1} = v_i + 2C_i\Delta_i + 3D_i\Delta_i^2,$$

from which it follows that

$$\Delta_i^2 C_i = 3\delta_i - 3\Delta_i v_i - \Delta_i(v_{i+1} - v_i) = 3\delta_i - 2\Delta_i v_i - \Delta_i v_{i+1}$$

and $\Delta_i^3 D_i = -2\delta_i + \Delta_i v_i + \Delta_i v_{i+1}$.

The continuity of the second derivative implies that

$$2C_i + 6D_i\Delta_i = 2C_{i+1}.$$

Thus

$$\frac{2}{\Delta_i^2}\left[\Delta_i v_i + 2\Delta_i v_{i+1} - 3\delta_i\right] = \frac{2}{\Delta_{i+1}^2}[3\delta_{i+1} - 2\Delta_{i+1}v_{i+1} - \Delta_{i+1}v_{i+2}].$$

Rearranging, gives

$$\Delta_{i+1}v_i + 2(\Delta_{i+1} + \Delta_i)v_{i+1} + \Delta_{i+1}v_{i+2} = 3\left(\delta_{i+1}\frac{\Delta_i}{\Delta_{i+1}} + \delta_i\frac{\Delta_{i+1}}{\Delta_i}\right).$$

At the leftmost point, $s''(x_0) = 0$ which implies that $C_0 = 0$ and hence

$$v_0 + 2v_1 = \frac{3\delta_0}{\Delta_0}.$$

Similarly, at the rightmost point, $s''(x_n) = 0$ and so

$$2C_{n-1} + 3\Delta_{n-1}D_{n-1} = 0.$$

Plugging in the formulas for C_{n-1} and D_{n-1}, we obtain

$$2v_{n-2} + v_{n-1} = \frac{3\delta_{n-1}}{\Delta_{n-1}}.$$

Collecting our equations, we get the following linear system for the v_i's

$$\begin{bmatrix} 2 & 1 & & & & \\ \alpha_1 & 2\beta_1 & \gamma_1 & & & \\ & \alpha_2 & 2\beta_2 & \gamma_2 & & \\ & & \ddots & \ddots & \ddots & \\ & & & \alpha_{n-1} & 2\beta_{n-1} & \gamma_{n-1} \\ & & & & 1 & 2 \end{bmatrix} \begin{bmatrix} v_0 \\ v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} = \begin{bmatrix} 3\delta_0/\Delta_0 \\ 3\delta_2\Delta_0/\Delta_1 + \delta_1\Delta_1/\Delta_0 \\ \vdots \\ 3\delta_{n-1}\Delta_{n-2}/\Delta_{n-1} + \delta_{n-2}\Delta_{n-1}/\Delta_{n-2} \\ 3\delta_{n-1}/\Delta_{n-1} \end{bmatrix}$$

with $\alpha_i = \Delta_i$, $\beta_i = (\Delta_{i-1} + \Delta_i)$, and $\gamma_i = \Delta_{i-1}$. This is a tridiagonal system and so can be solved *very* quickly. Once we have found the v_i's, we can use our formulas for the A_i, B_i, C_i, and D_i's to obtain the local representations of s.

Some remarks are in order.

Remark 16. *Note that we get, for free, from the previous equation that the system is invertible. Thus, there is a unique spline in S_3^N passing through our data points.*

Remark 17. *Some texts define natural cubic splines on a larger interval $[a, b]$ and demand that the spline be linear on $[a, x_0]$ and $[x_n, b]$. It is easy to show uniqueness for this characterization. Since, by continuity, a spline defined in this way has a vanishing second derivative at x_0 and x_n, by the uniqueness property we just showed, it follows that the definitions are equivalent.*

It is quite nice that there are two different ways of viewing S_3^N, but we still must contend with the fact that there are many other splines in S_3 which interpolate at $x_0, \cdots, x_n$ and so far the justification of our choice is rather thin. Let us address this now.

Theorem 29. *Define the Sobolev space $H^2([a, b])$ as the completion of $C^2([a, b])$ with respect to the norm*

$$\|f\|_{H^2} := \left(\|f\|_{L^2}^2 + \|f'\|_{L^2}^2 + \|f''\|_{L^2}^2\right)^{1/2}.$$

Given $f \in H^2([x_0, x_n])$, and $f_i = f(x_i)$, if s is the natural cubic interpolant, then

$$\langle f'' - s'', s'' \rangle = 0.$$

Proof. We start by observing that s'' is linear on each interval. Integrating by parts we see

$$\begin{aligned}\int_{x_i}^{x_{i+1}} (f'' - s'')s'' \,\mathrm{d}x &= -\int_{x_i}^{x_{i+1}} (f' - s')s''' \,\mathrm{d}x + (f' - s')s''\big|_{x_i}^{x_{i+1}} \\ &= \int_{x_i}^{x_{i+1}} (f - s)\underbrace{s^{(4)}}_{=0} \,\mathrm{d}x + (f' - s')s''\big|_{x_i}^{x_{i+1}} - (f - s)s'''\big|_{x_i}^{x_{i+1}}.\end{aligned}$$

The last term on the right vanishes because $(f - s)(x_i) = 0$. For the first term, note that the continuity of s'' means that the contribution from the right endpoint will be killed off by the contribution from the left endpoint of the interval $[x_{i+1}, x_{i+2}]$. The only terms which survive are then those corresponding to x_0 and x_n. Here we use the naturalness of s, from which it follows that these also vanish. □

Corollary 6. *Let s be the natural cubic interpolant passing through the data points (x_i, f_i), $i = 0, \cdots, n$. For any $g \in H^2([x_0, x_n])$, such that $g(x_i) = f_i$, $i = 0, \cdots, n$,*

$$\|g''\|_{L^2}^2 = \|g'' - s''\|_{L^2}^2 + \|s''\|_{L^2}^2.$$

In particular, s is the unique function in H^2 with $s(x_i) = f_i$, $i = 0, \cdots, n$, which minimizes the semi-norm $|\cdot|_2$ where $|u|_2 := \|u''\|_{L^2}$.

Proof. For any such g, we see that s is also a natural cubic interpolant of it. Thus the previous theorem applies. THen

$$\begin{aligned}\langle g'', g'' \rangle &= \langle g'' - s'', g'' \rangle + \langle s'', g'' \rangle \\ &= \langle g'' - s'', g'' - s'' \rangle + \langle g'' - s'', s'' \rangle + \langle s'', g'' - s'' \rangle + \langle s'', s'' \rangle \\ &= \|g'' - s''\|_{L^2}^2 + \|s''\|_{L^2}^2.\end{aligned}$$

□

Let's play around with our representation. Clearly,

$$s(x) = \sum_{j=0}^{n-1} \alpha_j (x - x_j)_+^3 + \sum_{j=0}^{2} \beta_j x^j,$$

where

$$(x-\alpha)_+^3 := \begin{cases} (x-\alpha)^3, & \text{if } (x-\alpha)^3 > 0, \\ 0, & \text{if } (x-\alpha)^3 \leq 0. \end{cases}$$

Naturalness requires that $s''(x_0)$ and $s''(x_n) = 0$. Thus, $\beta_2 = 0$, and

$$\sum_{j=0}^{n-1} \alpha_j (x_n - x_j) = 0.$$

For notational convenience, we set

$$\alpha_n = -\sum_{j=0}^{n-1} \alpha_j.$$

Then, this and our previous condition give

$$\sum_{j=0}^{n-1} \alpha_j = 0, \quad \text{and} \quad \sum_{j=0}^{n} x_j \alpha_j = 0.$$

Using the identity, $x_+^3 = \frac{|x|^3 + x^3}{2}$,

$$\begin{aligned} s(x) &= \sum_{j=0}^{n} \frac{\alpha_j}{2} |x - x_j|^3 + \sum_{j=0}^{n} \frac{\alpha_j}{2} (x - x_j)^3 + \beta_0 + x\beta_1 \\ &= \underbrace{\sum_{j=0}^{n-1} \frac{\alpha_j}{2} |x - x_j|^3}_{\sum_{j=0}^{n} \tilde{\alpha}_j \phi(|x - x_j|)} + \sum_{\ell=0}^{3} \binom{3}{\ell} (-1)^{3-\ell} \left(\sum_{j=0}^{n} \alpha_j x_j^{3-\ell} \right) x^\ell + \beta_0 + \beta_1 x. \end{aligned}$$

Our two conditions on the α's imply that the $\ell = 2, 3$ terms of the above sum vanish, and the last three terms are thus in P_1. So, interpolating cubic splines can be written in the form

$$s(x) = \sum_{j=0}^{n} \tilde{\alpha}_j \phi(|x - x_j|) + p, \quad p \in P_1.$$

This style of representation generalizes much more broadly to other approximation spaces and higher dimensions, as we will see shortly. Before doing so, we briefly touch on some other interesting properties of splines, though our treatment is by no means complete or exhaustive.

The following proposition gives us some characterization of the geometry of the space of natural splines.

Proposition 6. *For $\phi(r) = r^3$, suppose that $s = \sum_{j=0}^{n} \alpha_j \phi(|x - x_j|) + p$ and $\tilde{s} = \sum_{j=0}^{m} \beta_j \phi(|x - y_j|) + \tilde{p}$ where $p, \tilde{p} \in P_1$ and $s, \tilde{s}$ are natural cubic splines on $[a, b]$. Then*

$$\langle s'', \tilde{s}'' \rangle = 12 \sum_{j=0}^{n} \sum_{\ell=0}^{m} \alpha_j \beta_\ell \phi(|x_j - y_\ell|).$$

Here we adopt the convention that the cubic spline s is continued linearly outside of $[x_0, x_n]$ and, similarly, $\tilde{s}$ is continued linearly outside of $[y_1, y_n]$.

The previous proposition invites the following definition.

Definition 12. *Set*

$$F_\phi[a,b] = \left\{ \sum_{j=0}^{n} \alpha_j \phi(|\cdot - x_j|) \,|\, n \in \mathbb{N} \cup \{0\},\ \alpha \in \mathbb{R}^n,\ X = \{x_j\} \subset [a,b], \text{ with } \sum_{j=0}^{n} \alpha_j p(x_j) = 0, \quad \forall p \in P_1 \right\}.$$

We equip $F_\phi[a, b]$ with the inner product

$$\left\langle \sum_{j=0}^{n} \alpha_j \phi(|\cdot - x_j|),\ \sum_{\ell=0}^{m} \beta_\ell \phi(|\cdot - x_\ell|),\ \right\rangle := \sum_{j=0}^{n} \sum_{\ell=0}^{m} \alpha_j \beta_\ell \phi(|x_j - x_\ell|).$$

The following proposition tells us that the set of natural splines on $[a, b]$, $F_\phi[a, b]$, is dense in H^2.

Proposition 7. $\overline{F_\phi} + P_1 = H^2$, *where the closure is with respect to the inner product on F_ϕ.*

Finally, we conclude with a result on the accuracy of these interpolations.

Theorem 30. *There exists a constant $c > 0$ such that for all $f \in H^2$,*

$$\|f - s\|_{L^\infty} \leq C h_x^{3/2} \|f''\|_{L^2},$$

where s is a natural interpolating spline and h_x denotes the maximum separation of the 'knots' of s.

Summary

Splines are a flexible way of producing continuous, differentiable, etc. approximations to a function. They are particularly useful for

relatively rough functions with lots of data points. They can be written as a linear combination of functions of the form $\phi(|\cdot - x_j|)$, plus degree one polynomials. Moreover, they have nice (functional) geometric properties with a natural inner product. This flavor of approximation can be extended to more general classes of functions and higher dimensions, and is related to *radial basis functions* and *reproducing kernel Hilbert spaces*.

Additional Exercises

Exercise 25. *Let $x_0 < \cdots < x_N$ be equispaced points on $[-1, 1]$ with $x_0 = -1$ and $x_N = 1$. Suppose we are given data $\{(x_j, y_j) : 0 \leq j \leq N\}$, where $y_j = x_j^3$.*

1. *What is the natural interpolating cubic spline, s_N, for the data when $N = 3$?*
2. *Write a code for computing s_N for arbitrary N. Plot s_N for $N = 3, 5, 7$.*
3. *Compare s_N with the function $f(x) = x^3$. For which $x \in [-1, 1]$ is $|s_N(x) - f(x)|$ maximized? Why?*
4. *(Open ended) Can you come up with an extension of 'natural' splines to higher-order? Do they satisfy an orthogonality condition like natural cubic splines? Can you write them in a 'radial basis function' type format?*

Applications to Linear Algebra

Our goal in this chapter is to solve the following linear system

$$Ax = b,$$

where A is an $n \times n$ matrix, and b is a vector of length n. In particular, we will focus on iterative solutions; producing a set of approximations $x_0, x_1, \cdots$ with residuals $r_0 = b - Ax_0$, $r_1 = b - Ax_1, \cdots$. We would like to quantify

$$\frac{\|r_n\|}{\|r_0\|}.$$

Krylov subspaces

Suppose we have an initial guess x_0. We define the residual $r_0 = b - Ax_0$ and the error as $e_0 = A^{-1}r_0$. The problem reduces to finding e_0. We now define the family of subspaces $\mathcal{K}_n$, by

$$\mathcal{K}_\ell(A, b) = \text{span}\{b, Ab, \cdots, A^{\ell-1}b\}.$$

If $\dim \mathcal{K}_\ell(A, r_0) < \ell$ then $r_0, A_0 r_0, \cdots, A^{\ell-1}r_0$ are linearly dependent and there exist constants $c_0, \cdots, c_{\ell-1}$ such that

$$c_0 r_0 + c_1 A r_0 + \cdots + c_{\ell-1} A^{\ell-1} r_0 = 0.$$

Moreover, if A is invertible, we can choose the c's so that $c_0 \neq 0$. Thus

$$r_0 = A \underbrace{\left(-\frac{1}{c_0} \sum_{j=1}^{\ell-1} c_j A^{j-1} r_0 \right)}_{=e_0}.$$

There is a nice connection to polynomial approximations:

$$\mathcal{K}_\ell(A, b) = \{p(A)b \mid p \in P_{\ell-1}\}.$$

Conjugate Gradient

As a specific example, let us assume that A is Hermitian and positive definite.

We wish to solve the problem $Ax = b$. Starting with an initial guess x_0 we construct a sequence of approximations. At each step, we move in some direction q_n. How far should we go? Ideally, we would go far enough so that if $x_{n+1} = x_n + \delta q_n$,

$$\langle x - (x_n + \delta_n q_n), q_n \rangle = 0.$$

Unfortunately, this requires knowing x (which defeats the purpose of constructing an algorithm to find it!).

The solution is to change the problem. Rather than focus on the error vector $x - x_n$ we focus on the residual $Ax - Ax_n$. We demand that q_n be 'A-orthogonal' to $(x - x_{n+1})$, i.e.

$$\langle x - x_{n+1}, q_n \rangle_A := \langle x - x_{n+1}, Aq_n \rangle = 0.$$

Using the relation $x_{n+1} = x_n + \delta_n q_n$, we find

$$\delta_n = \frac{\langle r_n, d_n \rangle}{\langle d_n, Ad_n \rangle}.$$

What search directions should we choose? A natural choice would be to pick the q_n so that they are A-orthogonal as well. How do we find them? Suppose for now that we are given a set of vectors $v_0, \cdots, v_{n-1}$, from which to construct our $q_0, \cdots, q_n$. We could run a (weighted) version of Gram-Schmidt as follows.

$$q_0 = v_0$$
$$q_i = v_i + \sum_{k=0}^{i-1} \beta_{i,k} q_k$$

with

$$\beta_{i,k} = -\frac{\langle v_i, q_j \rangle_A}{\langle q_j, q_j \rangle_A}.$$

This choice guarantees that $\langle q_i, q_j \rangle_A = 0$ if $i \neq j$. Thus, given a collection of vectors we can construct a sequence of A-orthogonal search directions $q_0, q_1, \cdots$. We will return to the question of which v_i's to pick later. For now, we will leave the choice as arbitrary.

By the nature of our iterations, if $e_i = x - x_i$, then $e_i = e_0 + \sum_{j=0}^{i-1} \alpha_j q_j$, for some coefficients α_j. To see this, note that

$$e_i = x - x_i = x - x_0 - \delta_1 Aq_1 - \cdots - \delta_{i-1} Aq_{i-1}.$$

In addition, since the d_j, $j = 0, cdots, n-1$, form a basis of $\mathbb{R}^n$, for some coefficients $\{\sigma_j\}$, we have

$$e_0 = \sum_{j=0}^{n-1} \sigma_j q_j.$$

Comparing the two expansions, and using the orthogonality of e_i to $q_0, \cdots, q_{i-1}$, it is clear that $\sigma_j = -\alpha_j$, and hence

$$e_i = \sum_{j=i}^{n-1} \alpha_j q_j.$$

We get a nice optimality result from this. For $v \in \text{span}\{q_0, \cdots, q_{i-1}\}$ then

$$\begin{aligned}\|v - e_0\|_A^2 &= \langle v - e_0, v - e_0\rangle_A \\ &= \sum_{j=0}^{i-1} (v_j - \sigma_j)^2 \langle q_j, q_j\rangle_A + \sum_{j=i}^{n-1} \sigma_j^2 \langle q_j, q_j\rangle_A \\ &\geq \sum_{j=i}^{n-1} \sigma_j^2 \langle q_j, q_j\rangle_A = \|e_i\|_A^2.\end{aligned}$$

So $\sum_{j=0}^{i-1} \alpha_j q_j$ is the best approximation to e_0 from this space!

Now, there is some flexibility that we have yet to exploit - the choice of $q_0, \cdots, q_{n-1}$. This is good because, as it stands, this algorithm is not particularly useful - we have to do a lit of work to calculate each new q_k and we have to store the big coefficient matrix $\{\beta_{i,k}\}$.

One natural choice (which gives the *Conjugate gradient method*) is to choose $v_i = r_i$. It is easy to show that with this choice

$$\langle r_i, r_j\rangle = 0, \quad i \neq j.$$

Indeed, as we have seen above,

$$\langle q_j, r_i\rangle = \langle q_j, Ae_i\rangle = 0, \quad j < i.$$

by construction,

$$\langle r_j, q_i\rangle = \langle r_j, q_i\rangle + \sum_{k=0}^{i-1} \beta_{i,k} \langle r_j, q_k\rangle$$

which, using the previous equations, implies that $\langle v_i, r_j\rangle = 0$ if $i < j$. Since now the v_i are chosen equal to r_i, the result follows.

Also, since $x_{i+1} = x_i + \delta_i q_i$, we obtain

$$r_{i+1} = A(x - x_{i+1}) = A(x - x_i - \delta_i q_i) = r_i - \delta_i A d_i.$$

With this choice,

$$q_i = r_i + \sum_{j=0}^{i-1} \beta_{i,j} q_j, \quad \beta_{i,j} = -\frac{\langle r_i, d_j\rangle_A}{\langle d_j, d_j\rangle_A}.$$

Also,

$$0 = \langle r_j, r_{i+1}\rangle = \langle r_j, r_i\rangle - \delta_i \langle r_j, q_j\rangle_A$$

which gives

$$\langle r_j, d_i \rangle_A = \frac{1}{\delta_i} \left[\langle r_j, r_i \rangle - \langle r_j, r_{i+1} \rangle \right].$$

Thus

$$\langle r_j, d_i \rangle_A = \begin{cases} \frac{1}{\delta_i} \langle r_i, r_i \rangle & \text{if } j = i, \\ \frac{1}{\delta_{j-1}} \langle r_j, r_j \rangle & \text{if } j = i+1, \\ 0 & \text{else.} \end{cases}$$

So,

$$\beta_{i,j} = \begin{cases} \frac{1}{\delta_{i-1}} \frac{\langle r_i, r_i \rangle}{\langle q_{i-1}, q_{i-1} \rangle_A}, & \text{if } i = j+1 \\ 0 & \text{else.} \end{cases}$$

Set $\beta_i = \beta_{i,i-1}$, the one non-zero coefficient per row.

By construction,

$$\delta_i = \frac{\langle r_i, q_i \rangle}{\langle q_i, q_i \rangle_A}$$

from which it follows that

$$\beta_i = \frac{\langle r_i, r_i \rangle}{\langle r_{i-1}, q_{i-1} \rangle} = \frac{\langle r_i, r_i \rangle}{\langle r_{i-1}, r_{i-1} \rangle}$$

where the last equality holds since $q_i \perp r_j$, $i < j$, and using the construction of q_j.

Thus, we arrive at the algorithm,

$$\begin{aligned} d_0 &= r_0 = b - Ax_0 \\ \delta_i &= \frac{\langle r_i, r_i \rangle}{\langle q_i, q_i \rangle_A} \\ x_{i+1} &= x_i + \delta_i q_i \\ r_{i+1} &= r_i - \delta_i A q_i \\ \beta_{i+1} &= \frac{\langle r_{i+1}, r_{i+1} \rangle}{\langle r_i, r_i \rangle} \\ q_{i+1} &= r_{i+1} + \beta_{i+1} q_i. \end{aligned}$$

Polynomials and Conjugate gradient

Let us now recast this in more familiar language. At each stage we form a new approximant x_i which is an ith degree polynomial in A, $p_i(A)$, applied to r_0. Rather than compute $p_i(A)r_0$ each time, we have a recurrence relation that allows us to compute $p_{i+1}(A)r_0$ recursively from x_i, r_i, and q_i.

To analyze, we look at the eigenvectors. This is a classic trick - turning linear algebra into simple (one-dimensional) algebra. Indeed,

because we only ever take linear combinations, we can study how our approximations work on each eigenvector separately. Note, however, that the coefficients are *nonlinear* in r_0, and so we have to 'freeze' our coefficients first. That is to say, fix the β_i, δ_i.

Let u_j denote the eigenvectors of A, and λ_j the corresponding eigenvalues. Then, we can expand e_0 in this basis, $e_0 = \sum_{j=1}^n \xi_j u_j$. Similarly, by linearity,

$$e_i = \sum_{j=1}^n p_i(\lambda_j)\xi_j v_j,$$

and

$$Ae_i = \sum_{j=1}^n \lambda_i p_i(\lambda_j)\xi_j v_j,$$

from which it follows that

$$\|e_i\|_A^2 = \sum_{j=1}^n \xi_j^2 [p_i(\lambda_j)]^2 \lambda_j.$$

Note that by our earlier optimality result, the conjugate gradient polynomial will be the best possible over all polynomials $p \in P_i$ with $p_i(0) = 1$.

If we wish to find the relative error in the worst possible case then we should maximize over all ξ with $\|\xi\|_2 = 1$, which gives

$$\|e_i\|_A^2 \leq \min_{p\in P_i, p(0)=1} \max_{\lambda\in\Lambda(A)} |p(\lambda)|^2 \|e_0\|_A^2.$$

where $\Lambda(A)$ is the set of eigenvalues of A.

To obtain a more tractable upper bound, we enlarge the interval over which λ can be chosen, to be $[\lambda_{\min}, \lambda_{\max}]$. Thus, discarding the prefactor $\|e_0\|_A^2$, we wish to bound the error in

$$\min_{p\in P_i} \max_{\lambda\in[\lambda_{\min},\lambda_{\max}} \frac{|p(\lambda)|}{|p(0)|}.$$

Let's standardize this by mapping it into the interval $[-1, 1]$. Set

$$s = 1 - 2\left(\frac{\lambda - \lambda_{\min}}{\lambda_{\max} - \lambda_{\min}}\right)$$

in which case

$$s(0) = \frac{\lambda_{\max} + \lambda_{\min}}{\lambda_{\max} - \lambda_{\min}} =: s_*.$$

Our previous problem reduces to

$$\min_{p\in P_i} \max_{s\in[-1,1]} \frac{|p_i(s)|}{|p_i(s_*)|}.$$

Noting that $s_* > 1$, it is clear now that our goal is to find a polynomial which is small on $[-1, 1]$ but grows as fast as possible away

from the interval. This now feels like quite a classical approximation problem, and indeed it is!

Intuitively, we would expect that this mystery polynomial should have all of its zeros inside $[-1,1]$ and that the local maxima and minima should be approximately equal in absolute value (otherwise you could lower $\|p\|_{L^\infty([-1,1])}$ by shifting the roots). This hints at Chebtshev, or something close to Chebyshev at the very least. To show this we will play some familiar games.

Suppose p is optimal and consider

$$q(s) = \frac{p(s)}{|p(s_*)|} - \frac{T_i(s)}{|T_i(s_*)|}.$$

Since all the extremal values of T_i are the same,

$$\left| \frac{p(s_j)}{|p(s_*)|} \right| \leq \left| \frac{T_i(s_j)}{|T_i(s_*)|} \right|, \quad j = 0, \cdots, i$$

where the s_j are the points where T_i attains its maximum (in absolute value) on the interval $[-1,1]$.

Thus, q changes signs $i+1$ times on the interval $[-1,1]$ and so has i roots in $[-1,1]$. But... $q(s_*) = 0$ by construction. Hence $q \equiv 0$. So the Chebyshev polynomials are optimal.

Thus,

$$\|e_i\|_A \leq |T_i(s_*)|^{-1} \|e_0\|.$$

Note that $s_* = (\kappa+1)/(\kappa-1)$, where κ is the condition number of A. Then

$$\|e_i\|_A \leq T_i\left(\frac{\kappa+1}{\kappa-1}\right)^{-1} \|e_0\|_A = \cos\left(i \arccos \frac{\kappa+1}{\kappa-1}\right) \|e_0\|_A.$$

After a few trigonometric identities we arrive at the bound

$$\|e_i\|_A \leq 2\left(\frac{\sqrt{\kappa}+1}{\sqrt{\kappa}-1}\right)^{-i} \|e_0\|_A.$$

Remark 18. *For a particular matrix this bound might not be sharp, particularly if the eigenvalues are clustered (i.e. not evenly distributed).*

General analysis

We now give a brief, and necessarily superficial, discussion of the general theory. Our goal is to find an approximate solution $z \in \mathcal{K}_{\ell-1}$ for the problem

$$r_0 \approx Az.$$

Using our characrterization of $\mathcal{K}_\ell$, this amounts to finding a $q \in P_{\ell-2}$ such that $r_0 - Aq(A)r_0$ is as small as possible. Clearly, this simplifies

to the task of finding a $p \in P_{\ell-1}$ with $p(0) = 1$ such that $p(A)r_0$ is as small as possible.

Let S (a compact set in $\mathbb{C}$) be an approximation to the spectrum of A and assume $0 \notin S$. Then $p(A)r_0$ will be small if $\|p\|_S = \max_{z\in S} |p(z)|$ is small. So, we care about the decay of $E_n(S) = \min_{p\in P_n,\, p(0)=1} \|p\|_S$.

If $\rho = \lim_{n\to\infty}(E_n(S))^{1/n} \leq 1$, then we expect $\|r_n\|/\|r_0\| \approx C\rho^n$.

How do we estimate ρ? We begin by observing

$$|\rho(z)| = \prod_{k=1}^{n} |z - z_k| \implies \log|p(z)| = \sum_{k=1}^{n} \log|z - z_k|.$$

We want to minimize the maximum of $|p(z)|/|p(0)|$ on S. By analyticity, it suffices to minimize the maximum on ∂S. This can be interpreted as finding locations of negative "charges" $z_1, \cdots, z_n$ to minimize the maximum electric potential on ∂S.

Set

$$g_n(z) = \frac{1}{n}\sum_{i=1}^{n} \log|z - z_i| + C.$$

Taking the limit as $n \to \infty$ we can approximate this by an integral

$$g(z) = \int \log|z - z_0|\, \mathrm{d}\mu(z_0) + C,$$

where μ is a probability measure over which we wish to optimize.

Our intuition here is that the minimum will occur when g is constant on ∂S. This will occur when all the charge is on the boundary. This has the following physical meaning. Inject 1 unit of negative charge into the system and let it reach equilibrium. The potential $g(z)$ will be constant. Add C so that this constant is 0. Then $\rho = e^{-g(0)}$.

More precisely, g is the Green's function associated to S, $g : \mathbb{C} \setminus S$,

$$\begin{cases} \nabla^2 g = 0, & \mathbb{C} \setminus S, \\ g(z) \to 0, & z \to \partial S, \\ g(z) \sim \log|z| \to C, & |z| \to \infty. \end{cases}$$

C is *Robin's constant* and e^{-C} is the logarithmic capacity of S.

Theorem 31. *Let g be the Green's function for S. Then $\rho = e^{-g(0)}$ and for all n and all $p \in P_n$,*

$$\|p\|_S \geq \rho^n.$$

References

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- GMRES: *From Potential Theory to Matrix Iterations in Six Steps* by Tobin A. Driscoll, Kim-Chuan Toh, Lloyd N. Trefethen

Trigonometric polynomials

We now turn our attention away from polynomial approximation, picking up where we left in the introductory chaper with trigonometric functions. As we will see though, there are many interesting and deep connections between these representations and polynomials. Since this subject is covered in detail in many other books and courses, our tour will be brief, incomplete, and focused on questions of approximation.

A *trigonometric polynomial* is a function of the form

$$a_0 + \sum_{k=1}^{n} \left[a_k \cos(kx) + b_k \sin(kx) \right]. \tag{2}$$

Its *degree* is the highest "frequency" appearing in the sum (here it is n if either a_n or b_n is non-zero). We will denote the set of all *real* trigonometric polynomials of degree at most n by $\mathcal{T}_n$. Our goal is to understand which functions can be approximated well by things in $\mathcal{T}_n$. Along the way, we will come up with other interesting and useful ways of representing functions in $\mathcal{T}_n$.

The most obvious thing to do is expand the sines and cosines, which gives a sum of the form

$$\sum_{k=-n}^{n} c_k e^{ikx}. \tag{3}$$

It is clear that if complex coefficients are allowed then anything of the form (2) can be written in the form (3), and vice versa. What about if we insist that the a_i and b_i are real? What does this imply about the c_k?

Suppose that $f = \sum_{k=-n}^{n} c_k e^{ikx}$ is real. Then

$$\bar{f} = \sum_{k=-n}^{n} \overline{c_k} e^{-ikx} = \sum_{k=-n}^{n} \overline{c_{-k}} e^{ikx} = f.$$

Comparing coefficients of the various complex exponentials we see that $c_k = \overline{c_{-k}}$ is a necessary and sufficient condition. Here we have tacitly used the linear independence of complex exponentials.

Let us now turn to a slightly less standard representation. We saw when discussing Chebyshev polynomials that $\cos(kx)$ can be written as a polynomial in $\cos(x)$, with the recurrence relation

$$\cos(kx) + \cos((k-2)x) = 2\cos((k-1)x)\cos(x).$$

Similarly, one can show that

$$\sin((k+1)x) - \sin((k-1)x) = 2\cos(kx)\sin(x).$$

Exercise 26. *Verify these identities.*

Thus we see that $\sin((k+1)x) = Q_k(\cos(x))\sin(x)$ where $Q_k \in P_k$ and its leading coefficient is 2^k. Thus, (2) can be written in the form

$$p(\cos(x)) + q(\cos(x))\ \sin(x), \tag{4}$$

where $p \in P_n$ and $q \in P_{n-1}$. By dimension counting it is clear that everything of the form (4) can also be written in the form (2) and vice versa. This last representation suggests a natural approach to proving a Weierstrass-type approximation result: convert trigonometric polynomial approximation to a polynomial approximation and use the original Weierstrass theorem. Modulo a few tweaks, that will be our strategy.

We start by defining the space of functions which we wish to approximate. Since everything in $\mathcal{T}_n$ is 2π-periodic, it is natural to restrict our attention to 2π-periodic continuous functions. We denote this space by $C^{2\pi}$. Note that it is a subspace of $C(\mathbb{R})$. We can also think of it as the space of real continuous functions on the unit circle in the complex plane. For $f \in C^{2\pi}$ we define the norm

$$\|f\| = \max_{x\in\mathbb{R}} |f(x)| = \max_{0\le x<2\pi} |f(x)|.$$

We are now ready to state our first approximation result.

Theorem 32. *Suppose $f \in C^{2\pi}$ and let $\epsilon > 0$ be given. Then, there is a trigonometric polynomial T such that $\|f - T\| < \epsilon$.*

de la Vallée Poussin's version of Lebesgue's proof of Weierstrass's second theorem. Our proof consists of two parts.

1. We start by assuming that $f \in C^{2\pi}$ is even, and show that it can be approximated by even trigonometric polynomials.
   If f is even then it suffices to find an even approximation to f on the interval $[0, \pi]$. In particular, we look for an n and a $p \in P_n$ such that $f \approx p(\cos(x))$ on $[0, \pi]$. Why? Restricting to $[0, \pi]$ allows us to change variables $y = \cos(x)$ and map the problem to a polynomial approximation problem. Indeed,

$$|f(x) - p(\cos(x))| < \epsilon,\ \forall x \in [0,\pi] \iff |\underbrace{f(\arccos(y))}_{\tilde{f}(y)} - p(y)| < \epsilon,\ \forall y \in [-1,1]$$

Since $\tilde{f}$ is continuous, such a polynomial always exists by Weierstrass's theorem.

2. Approximate $f(x)\sin^2(x)$ and $f(x) = \cos^2(x)$.

   (a) For $f(x)\sin(x)^2$, we split f into an even part, $f_e(x) = (f(x) + f(-x))/2$, and n odd part $f_o(x) = (f(x) - f(-x))/2$. We observe that $f_e(x)\sin^2(x)$ is even and so can be approximated by a trigonometric polynomial T_1 by the previous part. Additionally, $f_o(x)\sin(x)$ is even so we can approximate it, to arbitrary accuracy, by a trigonometric polynomial T_2. Thus, for some T_1 and T_2,

   $$|T_1(x)\sin^2(x) + T_2(x)\sin(x) - f(x)\sin^2(x)| < 2\epsilon.$$

   (b) For $\tilde{f}(x) = f(x)\cos^2(x)$, we observe that $\tilde{f}(x - \pi/2) = f(x - \pi/2)\sin^2(x)$. So, there exists a trigonometric polynomial T_3 such that

   $$|\tilde{f}(x-\pi/2) - T_3(x)| < \epsilon \ \forall x \in [0, 2\pi] \iff |\tilde{f}(x) - T_3(x+\pi/2)| < \epsilon \ \forall x \in [0, 2\pi].$$

   But $T_3(x + \pi/2)$ is a trigonometric polynomial if T_3 is.

□

Best approximations and trigonometric polynomials

Following the same course as we did for polynomials, now that we know that trigonometric polynomials can represent continuous, periodic functions, we set out to try to characterize the best approximations. Here again we find a lot of commonality with the case of polynomials.

Theorem 33. *Trigonometric polynomials form a Haar subspace of $C^{2\pi}$ of dimension $2n + 1$.*

Proof. Using (3), the interpolation matrix is

$$\underbrace{\begin{bmatrix} e^{-inx_0} & \dots & e^{inx_0} \\ \vdots & & \vdots \\ e^{-inx_{2n}} & \dots & e^{inx_{2n}} \end{bmatrix}}_{U} \begin{bmatrix} c_{-n} \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} y_0 \\ \vdots \\ y_{2n} \end{bmatrix}$$

Now,

$$\begin{aligned} \det U &= e^{-in(x_0+\cdots+x_{2n})} \begin{vmatrix} 1 & \dots & e^{2inx_0} \\ 1 & & e^{2inx_1} \\ \vdots & & \vdots \\ 1 & \dots & e^{2inx_{2n}} \end{vmatrix} \\ &= e^{-in(x_0+\cdots+x_{2n})} \prod_{0 \le j < j \le 2n} (e^{ix_k} - e^{-ix_j}). \end{aligned}$$

□

By our *General equioscillation theorems*, we see immediately that the trigonometric polynomials have the equioscillation property, etc. In particular, we have the following corollary, which we leave as an exercise (there is a little work to do to argue that our results apply in the periodic case).

Corollary 7. *For all $f \in C^{2\pi}$, f has a unique best approximation $T^* \in \mathcal{T}_n$. The error, $f - t^*$ has an alternating set containing $(2n+2)$ points in $[0, 2\pi)$. Moreover, if $T \in \mathcal{T}_n$ has an alternating set containing $(2n+2)$ points then $T = T^*$.*

The Fourier series

We now consider what happens when the number of terms in our expansions goes to infinity. Given f (2π periodic, bounded, integrable) its Fourier series is given by

$$\frac{a_0}{2} + \sum_{k=1}^{\infty} a_k \cos(kx) + b_k \sin(kx)$$

where

$$a_k = \frac{1}{\pi}\int_{-\pi}^{\pi} \cos(kt)\, f(t)\, \mathrm{d}t, \quad b_k = \frac{1}{\pi}\int_{-\pi}^{\pi} f(t)\, \sin(t)\, \mathrm{d}t.$$

Alternatively, we can write

$$\sum_{k=-\infty}^{\infty}, \quad c_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-ikt} f(t)\, \mathrm{d}t.$$

Clearly, $\frac{|a_k|}{2}, \frac{|b_k|}{2}, |c_k| \leq \|f\|_\infty$ if $f \in C^{2\pi}$. We define the n^{th} *partial sum* by

$$s_n(f)(x) = \frac{a_0}{2} + \sum_{k=1}^{n} (a_k \cos(kx) + b_k \sin(kx)).$$

Proposition 8. *The functions*

$$\frac{1}{\sqrt{2\pi}}, \frac{1}{\sqrt{\pi}}\cos(x), \frac{1}{\sqrt{\pi}}\sin(x) \frac{1}{\sqrt{\pi}}\cos(2x), \frac{1}{\sqrt{\pi}}\sin(2x), \cdots$$

are orthonormal on $[0, 2\pi)$ with respect to the standard L^2 inner product. In particular,

$$\begin{aligned} s_n(1)(x) &= 1 \\ s_n(\cos(kx))(x) &= \cos(kx) \\ s_n(\sin(kx))(x) &= \sin(kx), \end{aligned}$$

and so $s_n(T)(x) = T(x)$ for all $T \in \mathcal{T}_n$.

We leave the proof as an exercise.

Remark 19. *The last proposition shows that $s_n^2(f) = s_n(f)$ and so s_n is a projection from $C^{2\pi}$ to $\mathcal{T}_n$. In fact it is an orthogonal projection with respect to the standard L^2 inner product on $[0, 2\pi)$.*

We have a few useful corollaries.

Corollary 8. *If $f \in C^{2\pi}$, and $a_k, b_k = 0$ for all k, then $f \equiv 0$.*

Proof. Given the assumptions on f,

$$\int_{-\pi}^{\pi} Tf \, \mathrm{d}x = 0,$$

for any trigonometric polynomial. By Weierstrass, there exists a trigonometric polynomial $\tilde{T}$ with $\|f - \tilde{T}\| < \epsilon$. Then

$$\int_{-\pi}^{\pi} f^2(x) \, \mathrm{d}x \leq \int_{-\pi}^{\pi} \tilde{T}f \, \mathrm{d}x + \epsilon \int_{-\pi}^{\pi} |f| \, \mathrm{d}x = \epsilon \int_{-\pi}^{\pi} |f| \, \mathrm{d}x.$$

Thus,

$$\int_{-\pi}^{\pi} f^2(x) \, \mathrm{d}x = 0 \implies f \equiv 0,$$

since f is continuous. □

Corollary 9.

$$\frac{1}{\pi} \int_{-\pi}^{\pi} [s_n(f)(x)]^2 \mathrm{d}x = \frac{a_0^2}{2} + \sum_{k=1}^{n} (a_k^2 + b_k)^2 \leq \frac{1}{\pi} \int_{-\pi}^{\pi} f^2(x) \, \mathrm{d}x.$$

In particular, the coefficients are square summable.

Corollary 10. *For any $f \in C^{2\pi}$,*

$$\lim_{n \to \infty} s_n(f) = f$$

in an L^2 sense.

Proof. For any $\epsilon > 0$, there exists a trigonometric polynomial T such that $\|f - T\|_\infty < \epsilon$. Then

$$\|f - s_n(f)\|_2 \leq \|f - T\|_2 + \|s_n(f - T)\|_2$$

for n large enough. Since $\|s_n\|_{2 \to 2} = 1$, we arrive at

$$\|f - s_n(f)\|_2 \leq 2\|f - T\|_2 \leq 2\sqrt{2\pi}\epsilon.$$

□

A detour and an important example

In many cases we want to represent functions which are only piecewise continuous. Let's see what happens. Consider $f(x) = \operatorname{sgn}(x)$ on $[-\pi, \pi)$. Then $a_k = 0$ for all k. Moreover,

$$b_k = \frac{1}{\pi} \int_{-pi}^{\pi} \sin(kt) \operatorname{sgn}(t) \, \mathrm{d}t = \frac{2}{\pi k}[1 - (-1)^k].$$

So,

$$s_{2n}(f) = \sum_{k=1}^{n} \frac{4}{(2k-1)\pi} \sin((2k-1)x).$$

Generically, we might expect $s_n(f) \to f$ in L^2. But what about in C? Let's check one point $\pi/(2n)$.

$$\begin{aligned}
s_n(f)\left(\frac{\pi}{2n}\right) &= \frac{4}{\pi}\left(\sin\left(\frac{\pi}{2n}\right) + \frac{1}{3}\sin\left(\frac{3\pi}{2n}\right) + \cdots + \frac{1}{2n-1}\sin\left(\frac{(2n-1)\pi}{2n}\right)\right) \\
&= \frac{4}{\pi}\frac{\pi}{2n}\left(\frac{1}{\frac{\pi}{2n}}\sin\left(\frac{\pi}{2n}\right) + \frac{1}{\frac{3\pi}{2n}}\sin\left(\frac{3\pi}{2n}\right) + \cdots + \frac{1}{\frac{(2n-1)\pi}{2n}}\sin\left(\frac{(2n-1)\pi}{2n}\right)\right) \\
&\approx \frac{2}{\pi}\int_0^{\pi} \frac{\sin(t)}{t}\,\mathrm{d}t \\
&= 1 + 2(0.0894898722\ldots).
\end{aligned}$$

Also,

$$s_{2n}(f)\left(\frac{-\pi}{2n}\right) = -1 - 2(\underbrace{0.0894898722\ldots}_{\text{Wilbraham}-\text{Gibbs constant}}).$$

This phenomenon (oscillations near discontinuities) is called *Gibbs phenomenon* and is ubiquitous in signal processing where it is associated with "ringing".

Properties of the projection s_n

We now examine the projection operator in a little more detail. We recall the definition

$$s_n(f)(x) = \sum_{k=-n}^{n} e^{ikx} c_k, \quad c_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-iky} f(y)\,\mathrm{d}y.$$

So,

$$\begin{aligned}
s_n(f)(x) &= \sum_{k=-n}^{n} \frac{e^{ikx}}{2\pi}\int_{-\pi}^{\pi} e^{-iky} f(y)\,\mathrm{d}y \\
&= \frac{1}{2\pi}\int_{-\pi}^{\pi}\left(\sum_{k=-n}^{n} e^{-ik(x-y)}\right) f(y)\,\mathrm{d}y \\
&= \frac{1}{\pi}\int_{-\pi}^{\pi}\left[\Re\left(\sum_{k=0}^{n} e^{-ik(x-y)}\right) - \frac{1}{2}\right] f(y)\,\mathrm{d}y \\
&= \frac{1}{\pi}\int_{-\pi}^{\pi}\left[\Re\left(\frac{1-e^{i(n+1)(x-y)}}{1-e^{i(x-y)}}\right) - \frac{1}{2}\right] f(y)\,\mathrm{d}y \\
&= \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{\sin((x-y)(n+1/2))}{\sin((x-y)/2)} f(y)\,\mathrm{d}y.
\end{aligned}$$

We call the kernel in the above integral the *Dirichlet kernel* $D_n(x-y)$, defined by

$$D_n(t) = \frac{\sin(t(n+1/2))}{\sin(t/2)}.$$

Proposition 9. *Let D_n be defined as above.*

1. *D_n is continuous and $\lim_{t\to 0} D_n(t) = (2n+1)$. It is also even.*

2. $$\frac{1}{2\pi}\int_{-\pi}^{\pi} D_n(t)\,\mathrm{d}t = 1.$$

3. $$\frac{\left|\sin\left(\left(n+\frac{1}{2}\right)t\right)\right|}{\frac{|t|}{2}} \leq |D_n(t)| \leq \frac{\pi}{|t|}, \quad -\pi < t < \pi.$$

4. $$\frac{8}{\pi}\log(n) \leq \|D_n\|_1 \leq 6\pi + \pi\log(n).$$

Proof. 1. An application of l'Hôpital's rule

2. Observe that $s_n(1)(0) = 1$.

3. This follows from standard properties of the sine function.

4. We use a standard splitting here:

$$\begin{aligned}\frac{1}{2}\|D_n\|_1 &\leq \int_0^{1/n}(2n+1)\,\mathrm{d}t + \int_{1/n}^{\pi}\frac{\pi}{|t|}\,\mathrm{d}t\\ &\leq 2 + 1/n + \log(n)\pi + \log(\pi)\pi\\ &\leq 3\pi + \log(n)\pi.\end{aligned}$$

To prove the lower bound, we write

$$\frac{1}{2}\|D_n\|_1 = \sum_{j=0}^{n-1}\int_{\frac{j\pi}{n+1/2}}^{\frac{(j+1)\pi}{n+1/2}} |D_n(t)|\,\mathrm{d}t + \int_{\frac{n\pi}{n+1/2}}^{\pi}|D_n(t)|\mathrm{d}t.$$

We drop the second term, and denote the bounds in the integrands in the first term by a_j and b_j.

Thus,

$$\begin{aligned}\frac{1}{2}\|D_n\|_1 &\geq 2\sum_{j=0}^{n-1}\int_{a_j}^{b_j}\frac{|\sin(n+1/2)t|}{t}\,\mathrm{d}t\\ &\geq \sum_{j=0}^{n-1}\frac{2(n+1/2)}{(j+1)\pi}\int_{a_j}^{b_j}\sin((n+1/2)t)(-1)^j\,\mathrm{d}t\\ &= \sum_{j=1}^{n}\frac{4}{j\pi} \geq \frac{4}{\pi}\int_1^n\frac{1}{t}\,\mathrm{d}t = \ frac4\pi\log(n).\end{aligned}$$

□

Remark 20. *Note that P defined by*

$$P(f)(x) = \frac{1}{2\pi}\int_{-\pi}^{\pi} D_n(x-y)\,f(y)\,\mathrm{d}y$$

projects real *functions to $\mathcal{T}_n$ and is an orthogonal projector with respect to the real inner product.*

Corollary 11. *There exists an $f \in C^{2\pi}$ for which $\|s_n(f)\|$ is unbounded (in n).*

Proof. $s_n : C^{2\pi} \to C^{2\pi}$ are continuous for every n. If

$$\sup_n \|s_n(f)\| < \infty, \quad \forall f \in C^{2\pi} \implies \sup_n \|s_n\| < \infty,$$

by the principle of uniform boundedness. Now, $\|s_n\| = \|D_n\|_1 \to \infty$. Rather than equality, all we need is to show that the L^1 norm is a lower bound, which is easier and all that we require. □

We have the following theorem, bounding the error in the truncated Fourier series in terms of the error in the best trigonometric polynomial approximation.

Theorem 34. *Fiven $f \in C^{2\pi}$ let T^* denote the best approximation to f from $\mathcal{T}_n$. Let $\tilde{T}$ denote the truncated Fourier series up to order n (also in $\mathcal{T}_n$). Then*

$$\|f - \tilde{T}\|_\infty \leq (1 + \|D_n\|_1)\|f - T\|_\infty,$$

where $\|\cdot\|_\infty$ denotes the infinity norm.

Proof. We leave it as an exercise. Hint: look at the general theory for inner product projections in a Banach space. □

Let's play around with D_n a bit more and see if we can't get some more intuition. Recall the definition of the convolution

$$(f \times g)(x) = \int_{-\pi}^{\pi} f(x-y)g(y)\,\mathrm{d}y = \int_{-\pi}^{\pi} f(y)g(x-y)\,\mathrm{d}y.$$

Then

$$\begin{aligned}\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-ikx}(f \star g)(x)\,\mathrm{d}x &= \frac{1}{2\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} e^{-ikx} f(y)g(x-y)\,\mathrm{d}y\,\mathrm{d}x \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-iky} f(y)\,\mathrm{d}y \int_{-\pi}^{\pi} e^{-ikz} g(z)\,\mathrm{d}z \\ &= 2\pi \underbrace{c_k(f)}_{\hat{f}_n}\underbrace{c_k(g)}_{\hat{g}_k}.\end{aligned}$$

Thus,

$$\widehat{(f \star g)}_n = 2\pi \hat{f}_n \hat{g}_n.$$

Now,

$$s_n(f) = \frac{1}{2\pi}(D_n \star f) \quad \text{and so} \quad \widehat{s_n(f)}_k = (\hat{D}_n)_k \hat{f}_k.$$

Now, by construction, $(\widehat{D_n})_k$ is constant for $|k| \leq n$ and drops abruptly to zero. Thus, in "frequency" space, $\widehat{D_n}$ drops abruptly to zero. Perhaps by sacrificing the projection requirement for s_n we

can get mappings from $c^{2\pi} \to \mathcal{T}_n$ which converge better. More precisely, we want a set of operators $\sigma_n : C^{2\pi} \to \mathcal{T}_n$ such that $\sigma_n(f) \to f$ in $C^{2\pi}$ for all $f \in C^{2\pi}$.

Our idea: choose a filter (kernel) which is smoother in frequency space. In particular, let's choose a K_n with $\widehat{K_n}_0 = 1$, and is linearly decreasing to zero at $\pm n$. In real space this has a nice interpretation. Convolving with K_n is equivalent to applying σ_n defined by

$$\sigma_n(f) = \frac{1}{n}\left(s_0(f) + \cdots + s_{n-1}(f)\right),$$

i.e. it is the *average* of the first n partial sums. Note that

$$\sigma_n(e^{ikx}) = \begin{cases} 0 & \text{if } |k| \geq n \\ \left(1 - \frac{|k|}{n}\right) e^{ikx} & \text{if } |k| < n. \end{cases}$$

So $\sigma_n(e^{ikx}) \to e^{ikx}$.

Remark 21. *This trick of replacing partial sums by averages of partial sums is called Cesàro summation, and is frequently used to assign values to infinite sums which do not converge in the traditional sense. For example*

$$1 - 1 + 1 - 1 + \cdots$$

then $s_n = (1 + (-1)^n)/2$. On the other hand, $\sigma_n = 1/2$ if n is even and $1/2 - 1/n$ if n is odd. Thus σ_n converges.

Returning to the matter at hand, we see that

$$\begin{aligned}
\sigma_n(f)(x) &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{1}{n}\sum_{k=0}^{n-1} D_k(x-y) f(y)\,\mathrm{d}y \\
&= \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{1}{n\sin\left(\frac{x-y}{2}\right)} \sum_{k=0}^{n-1} \sin\left(\left(k+\frac{1}{2}\right)(x-y)\right) f(y)\,\mathrm{d}y \\
&= \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{1}{n\sin\left(\frac{x-y}{2}\right)} \sum_{k=0}^{n-1} \frac{\cos(k(x-y)) - \cos((k+1)(x-y))}{2\sin\left(\frac{x-y}{2}\right)} f(y)\,\mathrm{d}y \\
&= \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{1}{n\sin\left(\frac{x-y}{2}\right)} \frac{1-\cos(n(x-y))}{2\sin\left(\frac{x-y}{2}\right)} f(y)\,\mathrm{d}y \\
&= \frac{1}{2\pi}\int_{-\pi}^{\pi} \underbrace{\frac{\sin^2\left(\frac{n(x-y)}{2}\right)}{n\sin^2\left(\frac{x-y}{2}\right)}}_{K_n} f(y)\,\mathrm{d}y.
\end{aligned}$$

The function K_n is called the Fejér kernel.

Remark 22. *Note that σ_n is* not *a projection.*

Lemma 8. *K_n is non-negative, continuous, even, and $\frac{1}{2\pi}\int_{-\pi}^{\pi} K_n(t)\,\mathrm{d}t = 1$. In particular, $\|K_n\|_1 = 2\pi$. Moreover, for $\delta > 0$ fixed,*

$$\int_{\delta \le |t| < \pi} K_n(t)\,\mathrm{d}t \to 0 \quad \text{as} \quad n \to \infty.$$

Proof. We leave the proofs as an exercise. □

Theorem 35. *If $f \in C^{2\pi}$ then $\sigma_n(f)$ converges uniformly to f as $n \to \infty$.*

Proof. We summarize the necessary relevant facts about K_n.

1. $K_n \ge 0$
2. $K_n \in C^{2\pi}$
3. $\frac{1}{2\pi}\int_{-\pi}^{\pi} K_n(t)\,\mathrm{d}t = 1$
4. $\int_{\delta < |t| < \pi} K_n(t)\,\mathrm{d}t \to 0$, for any $\delta > 0$.

These properties make it an *approximate identity*. This is enough for the result to hold.
Fix $\epsilon > 0$. There is a $\delta > 0$ such that for all x, $|f(x) - f(x+t)| < \epsilon$ for all $|t| < \delta$. Then

$$\begin{aligned}
\left| f(x) - \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x+t)K_n(t)\,\mathrm{d}t \right| &= \frac{1}{2\pi}\left| \int_{-\pi}^{\pi} (f(x) - f(x+t))k_n(t)\,\mathrm{d}t \right| \\
&\le \frac{1}{2\pi}\int_{-\pi}^{\pi} |f(x) - f(x+t)| K_n(t)\,\mathrm{d}t \\
&\le \frac{\epsilon}{2\pi}\underbrace{\int_{|t|<\delta} K_n(t)\,\mathrm{d}t}_{\le 1} + \frac{2\|f\|_\infty}{2\pi}\underbrace{\int_{\delta<|t|<\pi} K_n(t)\,\mathrm{d}t}_{\to 0,\text{ as } n\to\infty}.
\end{aligned}$$

□

Additional Exercises

Exercise 27. *Let $\mathbb{T}$ denote the one-dimensional torus, i.e. the interval $[-\pi, \pi)$ with periodic boundary conditions. Let $\|\cdot\|$ denote the L^2 norm on $\mathbb{T}$, and $f^{(j)}$ the jth derivative of f. Prove the following inequalities:*

1. *For all $f \in C^\infty(\mathbb{T})$ and $j \in \mathbb{N}$, $\|f^{(j)}\| \le \|f^{(j+1)}\|^{\frac{j}{j+1}}\|f\|^{\frac{1}{j+1}}$.*
   Hint: use induction, integration by parts, and Holder.
2. *Fix $k \in \mathbb{N}$. Then for all $f \in C^\infty(\mathbb{T})$ and $j \in \{0, 1, \ldots, k\}$, $\|f^{(j)}\| \le \|f^{(k)}\|^{\frac{j}{k}}\|f\|^{\frac{k-j}{k}}$.*
3. *Challenge: let j, k, m be non-negative integers satisfying $j + k \le m$. Then for all $f \in C^\infty(\mathbb{T}^2)$,*

$$\|\partial_x^j \partial_y^k f\| \le \|\partial_x^m f\|^{\frac{j}{m}}\|\partial_y^m f\|^{\frac{k}{m}}\|f\|^{1-\frac{j+k}{m}}.$$

Exercise 28. *1. Suppose $f \in C^j(\mathbb{T})$, $j > 0$. Let $\hat{f}_k$ denote its Fourier coefficients. Show that*

$$|\hat{f}_k| \leq \frac{1}{2\pi|k|^j}\|f^{(j)}\|_1.$$

2. For $n \in \mathbb{N}$, set $x_k = 2\pi k/n$, $k = 0, \ldots, (n-1)$. Consider the quadrature rule with nodes x_k, and corresponding weights $w_k = 2\pi/n$ (they are all the same). What answer do you get from using this quadrature rule on the functions e_j defined by

$$e_j(x) = e^{2\pi ijx}.$$

Give your answer as a function of n and j.

3. Suppose you use the quadrature in (b) to compute the Fourier series coefficients of f, i.e. $\hat{f}_k$ by approximating the integral

$$\hat{f}_k = \frac{1}{2\pi}\int_0^{2\pi} f(x)e^{-ikx}\,\mathrm{d}x.$$

What value does your quadrature formula give? Give your answer as a function of n, k, and the Fourier coefficients of f. Simplify as much as possible. Bound the error as a function of k and n assuming $f \in C^j(\mathbb{T})$.

4. Assuming $f \in C^j(\mathbb{T})$, bound the L^2 error in your approximation, if you set

$$f(x) \approx \sum_{k=-(n-1)}^{(n-1)} \tilde{f}_k e^{ikx},$$

where $\tilde{f}_k$ are the coefficients you computed in part (c).

Exercise 29. *In this problem, we will explore more on Gibbs phenomenon.*

1. Write the Fourier series of the function $f(x) = \mathrm{sgn}(x)(\pi - |x|)$ on $(-\pi, \pi]$. Analyze its partial sums and deduce whether or not there is Gibbs phenomenon. If there is, then quantify what the maximum error (in the L^∞ norm) is in the limit as $n \to \infty$. Here n is the degree of the truncated Fourier approximation. Plot the series for $n = 1, 10, 20, \ldots, 100$ sampled at 1000 equispaced points on $(-\pi, \pi]$.

2. Repeat part (a) for $f(x) = |x|(1 + \cos(x))$.

3. Based on these experiments, and the discussion in class, what do you expect the convergence of the Fourier series will look like near a point x_* for which

$$\lim_{x \to x_*^+} f(x) - \lim_{x \to x_*^-} f(x) = a?$$

Back up your guess with a numerical experiment. Note: you may assume that $\lim_{x \to x_*^\pm} f'(x)$ exist and are bounded.

4. *Redo the analysis in class for $f(x) = \operatorname{sgn}(x)$ and find the locations of the maxima and minima of the truncated Fourier series, as well as their amplitudes (at least in the limit as $n \to \infty$). It is ok to leave your answer in terms of integrals but try to come up with an upper and lower bound.*

The Fourier Transform

So far, except for a passing mention of Hermite polynomials, we have been focused primarily on approximations over finite intervals. In this chapter we consider representation of functions defined on all of $\mathbb{R}$ in terms of complex exponentials.

Smoothness and Decay

Remark 23. *There are many different normalizations and scalings that one encounters in the literature. Caveat lector!*

Suppose for now that $f \in L^1$. Then, for any $\xi \in \mathbb{R}$, we can define

$$\tilde{f}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\xi x} f(x)\, \mathrm{d}x.$$

This is called the *Fourier transform* of f.

Theorem 36 (Fourier inversion theorem)**.** *Suppose both f and $\tilde{f}$ are in L^1. Then*

$$f(x) = \frac{1}{\sqrt{2\pi}} \int \tilde{f}(\xi) e^{i\xi x}\, \mathrm{d}x.$$

Remark 24. *The previous theorem, in essence, says that f can be "synthesized" out of complex exponentials, with coefficients given by $\tilde{f}$.*

Proof. We assume here that f and $\tilde{f}$ are also continuous. The result can be extended to L^1 by standard density arguments.
We begin with a formal argument.

$$\begin{aligned}
\frac{1}{\sqrt{2\pi}} \int \tilde{f}(\xi) e^{i\xi x}\, \mathrm{d}\xi &= \frac{1}{2\pi} \int \int e^{i\xi(x-y)} f(y)\, \mathrm{d}y\, \mathrm{d}\xi \\
&= \int f(y) \underbrace{\left(\int \frac{e^{i\xi(x-y)}}{2\pi}\, \mathrm{d}\xi \right)}_{\approx \delta(x-y)?}\, \mathrm{d}y \\
&= f(x).
\end{aligned}$$

Let's make this more rigorous. We use a classic trick. Consider instead, the integral

$$I_\epsilon = \frac{1}{\sqrt{2\pi}} \int \tilde{f}(\xi)\, e^{-\xi^2 \epsilon} e^{i\xi x}\, \mathrm{d}\xi.$$

Making the appropriate sacrifices to Fubini (DCT and all that),

$$\begin{aligned} I_\epsilon &= \frac{1}{2\pi}\int\int f(y)e^{i\xi(x-y)}e^{-\xi^2\epsilon}\,\mathrm{d}\xi\mathrm{d}y \\ &= \frac{1}{2\pi}\int f(y)\underbrace{\left(\int e^{-\xi^2\epsilon}e^{-\xi(x-y)}\mathrm{d}\xi\right)}_{=\frac{\sqrt{\pi}}{\sqrt{\epsilon}}e^{-(x-y)^2/4\epsilon}}\,\mathrm{d}y \\ &= \frac{1}{\sqrt{4\pi\epsilon}}\int f(y)e^{-(x-y)^2/4\epsilon}\,\mathrm{d}y. \end{aligned}$$

This is a convolution of f with a continuous positive function integrating to 1 with $\int_{|y|>\delta} e^{-y^2/4\epsilon}/\sqrt{4\pi\epsilon}\,\mathrm{d}y = 0$ for any $\delta > 0$. Since f is continuous this converges to f in the limit. □

Actually, we can say a little more.

Lemma 9. *If $f \in L^1$, then $\tilde{f} \in C$.*

Proof.

$$\tilde{f}(\xi) - \tilde{f}(\xi_0) = \int f(x)(e^{-i\xi x} - e^{-i\xi_0 x})\,\mathrm{d}x.$$

By dominated convergence theorem, $\tilde{f}(\xi) \to \tilde{f}(\xi_0)$ as $\xi \to \xi_0$. □

In fact, we can say something stronger.

Lemma 10 (Riemann-Lebesgue lemma)**.** *Suppose $f \in L^1$. Then $\tilde{f}$ is a continuous function such that $|\tilde{f}(\xi)| \to 0$ as $\xi t \pm \infty$.*

Proof. If $f \in L^1$ then it can be approximated arbitrarily well (in an L^1 sense) by a continuous, compactly supported function. Let f_ϵ be such a function with $\|f - f_\epsilon\|_1 < \epsilon$. For $\xi \neq 0$,

$$\begin{aligned} \sqrt{2\pi}\tilde{f}(\xi) &= \int e^{-i\xi x}f_\epsilon(x)\,\mathrm{d}x = \int e^{-i\xi(x+\pi/\xi)}f_\epsilon\left(x+\frac{\pi}{\xi}\right)\,\mathrm{d}x \\ &= e^{-i\pi}\int e^{-i\xi}f_\epsilon\left(x+\frac{\pi}{\xi}\right)\,\mathrm{d}x \\ &= -\int e^{-i\xi(x+\pi/\xi)}f_\epsilon\left(x+\frac{\pi}{\xi}\right)\,\mathrm{d}x. \end{aligned}$$

Thus

$$\tilde{f}(\xi) = \frac{1}{2\sqrt{2\pi}}\int e^{-i\xi x}(f_\epsilon(x) - f_\epsilon(x+\pi/\xi))\,\mathrm{d}\xi,$$

from which it follows that

$$|\tilde{f}_\epsilon(\xi)| \leq \frac{1}{2\sqrt{2\pi}}\int |(f_\epsilon(x) - f_\epsilon(x+\pi/\xi))|\,\mathrm{d}\xi$$

which goes to zero as $\xi \to \pm\infty$ by the dominated convergence theorem. So,

$$|\tilde{f}(\xi) - \tilde{f}_\epsilon(\xi)| < \epsilon \implies \limsup_{\xi\to\pm\infty}|\tilde{f}(\xi)| < \epsilon.$$

□

As we have seen numerous times before, if we assume more regularity we can get faster decay of the Fourier transform.

Proposition 10. *Suppose j is a positive integer and f has j integrable derivatives. Then there exists a constant C such that*

$$|\tilde{f}(\xi)| \leq \frac{C}{(1+|\xi|^2)^{j/2}}.$$

Conversely, if $|\tilde{f}(\xi)|$ decays like $|\xi|^{-(j+1+\epsilon)}$ for some $\epsilon > 0$ then f is continuous and has j continuous derivatives.

Proof. We begin by proving the first part. Integrating by parts,

$$\int e^{-i\xi x} f(x)\,\mathrm{d}x = \frac{1}{i\xi}\int e^{-i\xi x} f'(x)\,\mathrm{d}x.$$

It follows that $\tilde{f}(\xi) = (i\xi)^{-1}\widetilde{f'}(\xi)$. Iterating this identity proves the result.

To prove the second part, we use the Fourier inversion theorem,

$$f(x) = \frac{1}{2\pi}\int e^{i\xi x}\tilde{f}(\xi)\,\mathrm{d}\xi.$$

Differentiating the right-hand side ℓ times yields

$$f^{(\ell)}(x) = \frac{1}{2\pi}\int e^{i\xi x}(i\xi)^{\ell}\tilde{f}(\xi)\,\mathrm{d}\xi.$$

The above integral converges for all $\ell \leq j$. □

What about if f is compactly supported? Then, for some Ω,

$$\tilde{f}(\xi) = \frac{1}{\sqrt{2\pi}}\int_{-\Omega}^{\Omega} f(x)e^{-i\xi x}\,\mathrm{d}x, \quad f \in L^2.$$

Clearly then, if f is compactly supported, $\int_{-\Omega}^{\Omega}(i\xi)^{\ell}f(x)e^{-i\xi x}\,\mathrm{d}x$ is well-defined for any $k \geq 0$ and $\xi \in \mathbb{C}$. In particular, $\tilde{f}$ is an entire function. This is sometimes known as the Paley-Wiener theorem (though there are several!).

As an aside, we record here the following useful result, called the *Kramers-Kronig relation*, which appears frequently in physics.

Theorem 37. *If $\chi(\xi)$ is analytic in the closed upper half plane, and $|\chi(\xi)\xi| \to 0$ as $|\xi| \to \infty$ in the closed upper half plane then*

$$\Re(\chi(\xi)) = \frac{1}{\pi}\mathrm{p.v.}\int_{-\infty}^{\infty}\frac{\Im(\chi(\xi'))}{\xi - \xi'}\,\mathrm{d}\xi'.$$

There is much more that can be said about for which spaces the Fourier transform can be defined, and how. Here we content ourselves with one extension, to $L^2(\mathbb{R}$. See almost any book on harmonic analysis or Fourier analysis for more properties of the Fourier transforms and the spaces on which they are defined.

A brief summary of some L^2 properties of Fourier transforms

We begin with the question of how to define the Fourier transform on L^2.

Theorem 38. *If $f \in L^2 \cap L^1$, then*

$$\int_{-\infty}^{\infty} |f(x)|^2 \, \mathrm{d}x = \int_{-\infty}^{\infty} |\tilde{f}|^2 \, \mathrm{d}\xi,$$

sometimes called Parseval's theorem.

Proof. Here we give a formal proof. See the proof of the Fourier inversion theorem for an idea of how to make this rigorous. Using the definitions,

$$\begin{aligned} \int |\tilde{f}(\xi)|^2 \, \mathrm{d}\xi &= \int\int\int \frac{f(x)\overline{f}(y)}{2\pi} e^{-i\xi x} e^{i\xi y} \, \mathrm{d}y \, \mathrm{d}x \, \mathrm{d}\xi \\ &= \int\int \delta(x-y) f(x)\overline{f}(y) \, \mathrm{d}x \, \mathrm{d}y = \int |f(x)|^2 \, \mathrm{d}x. \end{aligned}$$

□

For $f \in L^2$ we set $\tilde{f}_R(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-R}^{R} e^{-i\xi x} f(x) \, \mathrm{d}x$. The previous theorem guarantees that

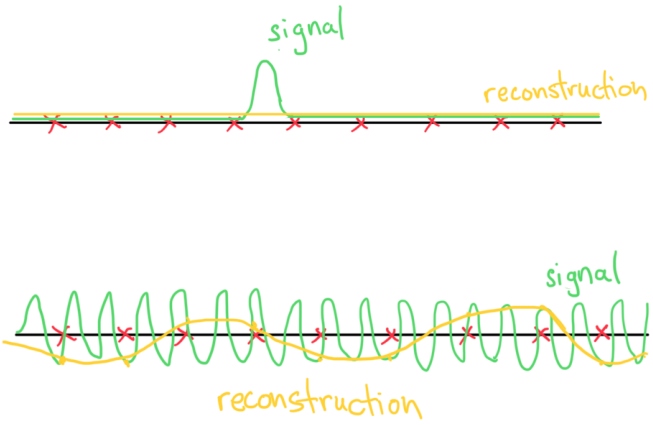
$$\tilde{f} = \lim_{R\to\infty} \tilde{f}_R$$

exists in an L^2 sense.

Some basic signal processing

Now, let us return to approximation. We imagine that we have a time dependent signal which we can sample at some collection of points. What properties of signal and sampling allow us to recover the signal with a given accuracy?

Example 9. *Consider the following two reconstructions from the equispaced points marked in red.*



These examples suggest that the 'sampling rate' (the spacing between samples) should scale with the frequency content of the signal.

To be a bit more precise, suppose the function f is bandlimited with bandlimit Ω – i.e. the support of the Fourier transform of f is contained within $[-\Omega, \Omega]$. Furthermore, suppose we can evaluate f at equispaced times $t_j = j\tau$, $j \in \mathbb{Z}$. This is an old question, typically associated with Claude Shannon and Harry Nyquist, though E.T. Whittaker analyzed it in a 1915 paper.

Theorem 39 (Shannon-Nyquist)**.** *If* $f \in L^1(\mathbb{R})$ *and* $\operatorname{supp}(\tilde{f}) \subseteq [\Omega, \Omega]$ *then*

$$f(t) = \sum_{n \in \mathbb{Z}} f\left(\frac{n\pi}{\Omega}\right) \operatorname{sinc}(\Omega t - n\pi),$$

where the equality holds in L^2.

Remark 25. *The previous theorem says that f can be written as a linear combination of translations of the* sinc *function. This is quite magical: we can recover a function solely from equispaced samples of a fixed spacing! Moreover, recovery is just taking linear combinations of translations of a single function! Note: there is no 'convergence' here - it is exact provided that $\tau \leq \pi/\Omega$.*

Before proving Shannon-Nyquist we first need to prove a few preliminary results (which are interesting in their own right).

Theorem 40. *Suppose*

$$\sum_n \tilde{f}(\xi + 2\Omega n) \in L^2[0, 2\Omega]$$

with $f, \tilde{f} \in L^1$. Then

$$\sum_n \tilde{f}(\xi + 2\Omega n) = \frac{\sqrt{2\pi}}{2\Omega} \sum_n f\left(\frac{n\pi}{\Omega}\right) e^{-2\pi i \xi n/2\Omega}.$$

Proof. Set $\phi(\xi) = \sum_n \tilde{f}(\xi + 2\Omega n)$. Then ϕ is periodic and in $L^2[0, 2\Omega]$. Thus we can represent it by a Fourier series

$$\phi(\xi) = \sum_n c_n e^{-2\pi i \xi n/2\Omega}, \quad c_n = \frac{1}{2\Omega} \int_0^{2\Omega} e^{2\pi i \xi n/2\Omega} \phi(\xi)\, \mathrm{d}\xi.$$

Turning to the Fourier coefficients, c_n,

$$\begin{aligned} c_n &= \frac{1}{2\Omega} \int_0^{2\Omega} e^{2\pi i \xi n/2\Omega} \sum_n \tilde{f}(\xi + 2\Omega n)\, \mathrm{d}\xi, \\ &= \frac{1}{2\Omega} \sum_n \int_{2\Omega n}^{2\Omega(n+1)} e^{2\pi i \xi n/2\Omega} \tilde{f}(\xi)\, \mathrm{d}\xi, \\ &= \frac{\sqrt{2\pi}}{2\Omega} f\left(\frac{n\pi}{\Omega}\right). \end{aligned}$$

□

Theorem 41. *Suppose additionally that* $\operatorname{supp} \tilde{f} \subseteq [-\Omega, \Omega]$. *Then*

$$f(x) = \sum_n f\left(\frac{n\pi}{\Omega}\right) \operatorname{sinc}(\Omega x - n\pi).$$

Proof. If $\operatorname{supp}(\tilde{f}) \subseteq [-\Omega, \Omega]$ then $\sum_n \tilde{f}(\xi + 2\Omega) = \tilde{f}(\xi)$, $\xi \in [-\Omega, \Omega]$. Thus,

$$\tilde{f}(\xi) = \chi_{[-\Omega,\Omega]}(\xi) \sum_n \tilde{f}(\xi + 2\Omega),$$

where χ denotes the indicator function. Then

$$\begin{aligned} f(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\xi x} \tilde{f}(\xi)\, \mathrm{d}\xi, \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\Omega}^{\Omega} e^{i\xi x} \sum_n \tilde{f}(\xi + 2\Omega)\, \mathrm{d}\xi, \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\Omega}^{\Omega} e^{i\xi x} \frac{\sqrt{2\pi}}{2\Omega} \sum_n f\left(\frac{n\pi}{\Omega}\right) e^{-2\pi i \xi n/2\Omega} \mathrm{d}\xi, \\ &= \frac{1}{2\Omega} \sum_n f\left(\frac{n\pi}{\Omega}\right) \int_{-\Omega}^{\Omega} e^{i\xi x - 2\pi i \xi n/2\Omega}\, \mathrm{d}\xi, \\ &= \sum_n f\left(\frac{n\pi}{\Omega}\right) \frac{2}{2\Omega} \frac{\sin(\Omega x - \pi n)}{x - \pi n/\Omega}. \end{aligned}$$

□

And with that, we have proved the Shannon-Nyquist theorem. The following is a nice result about approximation with bandlimited functions.

Proposition 11. *For $f \in L^1$ and $\Omega > 0$, then the Ω-bandlimited function which is closest to f in L^2 is*

$$f_* = \mathcal{F}^{-1}(\tilde{f}\chi_{[-\Omega,\Omega]}).$$

Note that the right-hand side is a projection.

Proof. If h is Ω-bandlimited,

$$\|h - f\|_2^2 = \|\tilde{f} - \tilde{h}\|_2^2 = \int_{|\xi|\leq\Omega} |\tilde{f} - \tilde{h}|^2 \mathrm{d}\xi + \int_{|\xi|>\Omega} |tildef|^2 \mathrm{d}\xi.$$

Clearly then,

$$\|h - f\|_2^2 \geq \int_{|\xi|>\Omega} |\tilde{f}|^2 \mathrm{d}\xi = \|\tilde{f}_* - \tilde{f}\|_2^2 = \|f - f_*\|^2.$$

□

Replacing f by f_* before subsampling is called anti-aliasing.

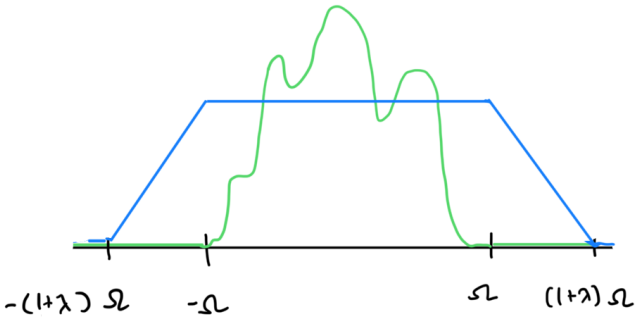
This is all very well and good, but there are still some issues with this representation. In particular, f is represented as a linear combination of sinc functions. These 'elementary building blocks' are not very local and neither are they absolutely integrable. This has implications for the number of terms required which in turn affects computational efficiency, and (potentially) accuracy due to rounding errors. It also means that one 'bad' point will contaminate recovery relatively far away.

What if we oversample? Can we avoid this?

To understand the question, let's think about why we ended up with sinc to begin with. It arose as the inverse Fourier transform of

the indicator function. Since the indicator function is discontinuous, this leads to slow decay. So, if we can replace the indicator by something smoother, then our issues might be alleviated. But how?

Suppose we sample at a rate of $(1+\lambda)$ times Nyquist. Then, redoing the above arguments with $(1+\lambda)\Omega$ instead of Ω, we see that when it comes time to multiply by the indicator function, we can replace it by any function which is one on $\mathrm{supp}(\tilde{f})$ and zero for $|\xi| > (1+\lambda)\Omega$. For example,



Our reconstruction formula becomes

$$f(x) = \sum_n \left(\frac{n\pi}{\Omega(1+\lambda)}\right) G_\lambda\left(x - \frac{n\pi}{\Omega(1+\lambda)}\right)$$

where

$$G_\lambda(x) = \frac{2\sin(x\Omega(1+\lambda/2))\sin(x\Omega\lambda/2)}{\lambda\Omega^2(1+\lambda)x^2}.$$

In principle, one can make G_λ decay faster for large x by making our filter smoother. In practice, the decay will be heavily dependent on λ. Indeed, one might expect it to scale like $C_N\lambda/(|x|\Omega\lambda)^{N+1}$ where C_N depends on N but not on Ω or λ (although this depends on the filter - it is certainly possible to do worse!).

Getting precise about uncertainty

In the following, to avoid getting bogged down in technicalities of regularity, let's freely assume that every function decays fast enough, and has enough derivatives, for everything to be well-defined. The 'space chasing' we leave as an exercise.

Given a function $f \in L^2$, $\|f\|_2 = 1$, we define its *positional uncertainty* Δx by

$$(\Delta x)^2 = \int_{-\infty}^{\infty} x^2|f(x)|^2\,\mathrm{d}x - \left(x|f(x)|^2\,\mathrm{d}x\right)^2$$

and its *momentum/frequency uncertainty* Δp by

$$(\Delta p)^2 = \int_{-\infty}^{\infty} \xi^2|\tilde{f}(\xi)|^2\,\mathrm{d}\xi - \left(\xi|\tilde{f}(\xi)|^2\,\mathrm{d}\xi\right)^2.$$

A natural question is whether Δx and Δp can both be small. To explore this further, we note that we can replace f by

$$f_c(x) := e^{-ip_0 x} f(x + x_0),$$

which has the same Δx and δp, but with

$$\int_{-\infty}^{\infty} x|f_c(x)|^2 \, \mathrm{d}x = 0 = \int_{-\infty}^{\infty} \xi |\tilde{f}_c(\xi)|^2 \, \mathrm{d}\xi.$$

Without loss of generality then, and by a slight abuse of notation, we write f instead of f_c. Set $u = xf$ and $v = \frac{\mathrm{d}}{\mathrm{d}x} f$ so that $\tilde{v} = i\xi \tilde{f}$. Then

$$\int_{-\infty}^{\infty} |u(x)|^2 \, \mathrm{d}x = (\Delta x)^2,$$
$$\int_{-\infty}^{\infty} |v(x)|^2 \, \mathrm{d}x = (\Delta p)^2.$$

Then,

$$\begin{aligned}
\Re \int_{-\infty}^{\infty} u^*(x) v(x) \, \mathrm{d}x &= \frac{1}{2} \int_{-\infty}^{\infty} \left[x f^*(x) f'(x) + (f^*)'(x) x f(x) \right] \, \mathrm{d}x \\
&= \frac{1}{2} \int_{-\infty}^{\infty} \left[x f^*(x) f'(x) - (f^*)(x)(x f(x))' \right] \, \mathrm{d}x \\
&= \frac{1}{2} \int_{-\infty}^{\infty} f^*(x) \left[x, \frac{\mathrm{d}}{\mathrm{d}x} \right] f(x) \, \mathrm{d}x \\
&= -\frac{1}{2} \int_{-\infty}^{\infty} |f(x)|^2 \, \mathrm{d}x = -1/2.
\end{aligned}$$

Also,

$$\left| \Re \int_{-\infty}^{\infty} u^*(x) v(x) \, \mathrm{d}x \right| \leq \|u\|_{L^2} \|v\|_{L^2} = (\Delta x)\,(\Delta p).$$

Putting it together we find

$$\frac{1}{2} \leq (\Delta x)\,(\Delta p).$$

Let's try to make this a bit more quantitative. Let Q_T be the *time-limiting* operator defined by

$$(Q_T f)(x) = \begin{cases} f(x), & |x| \leq T, \\ 0, & \text{else}, \end{cases}$$

and P_Ω be the *bandlimiting* operator defined by

$$(\widetilde{P_\Omega f})(\xi) = \begin{cases} \tilde{f}(\xi), & |\xi| \leq \Omega, \\ 0, & \text{else}. \end{cases}$$

Then, $P_\Omega Q_T f$ time limits and then bandlimits. Since P_Ω and Q_Ω are both orthogonal projections, f is bandlimited and time-limited if

and only if $P_\Omega Q_T f = f$. Now, since $\|P_\Omega Q_T\| \leq \|P_\Omega\| \, \|Q_T\| \leq 1$, simultaneous bandlimiting and time-limiting is only possible if $P_\Omega Q_T$ contains an eigenvalue of modulus one. The uncertainty principle shows that this is generally impossible. In fact, since f is time-limited this implies that $\tilde{f}$ is analytic and hence if $\tilde{f}$ is compactly supported, $\tilde{f} = 0$. But, can we get close?

We measure the failure of f to be bandlimited and time-limited by

$$\frac{\|P_\Omega Q_T\|^2}{\|f\|^2} = \frac{\langle Q_T P_\Omega Q_T f, f \rangle}{\|f\|^2},$$

which is clearly bounded in absolute value by the spectral radius of $Q_T P_\Omega Q_T$. In order to understand this operator a bit better, we note that it is an integral operator with kernel

$$\begin{aligned}
(Q_T P_\Omega Q_T)(f)(x) &= \frac{1}{2\pi} \int_{-\Omega}^{\Omega} e^{i\xi x} \int_{-T}^{T} e^{-i\xi t} f(t) \, \mathrm{d}t \mathrm{d}\xi, \quad |x| \leq T, \\
&= \frac{1}{2\pi} \int_{-T}^{T} \frac{2\sin(\Omega(x-t))}{x-t} f(t) \, \mathrm{d}t, \quad |x| < T, \\
&= \frac{\Omega}{\pi} \int_{-T}^{T} \sin(\Omega(x-t)) f(t) \, \mathrm{d}t, \\
&= \lambda \int_{-\pi}^{\pi} \mathrm{sinc}(\lambda(x-t)) f(tT/\pi) \mathrm{d}t, \quad \lambda = \frac{\Omega T}{\pi}.
\end{aligned}$$

In particular, $Q_T P_\Omega Q_T$ is compact, and its eigenvalues depend only on $T\Omega$ (which is proportional to the area in phase space).

One can say more though. As it turns out, a miracle occurs. $Q_T P_\Omega Q_T$ commutes with the operator $\mathcal{L}$, defined by

$$(\mathcal{L} f)(x) = \frac{\mathrm{d}}{\mathrm{d}x}(T^2 - x^2) \, \mathrm{d}f \mathrm{d}x - \frac{\Omega^2}{\pi^2} x^2 f,$$

a fact frequently referred to as Slepian's miracle. Using this, one can find the eigenfunctions of $Q_T P_\Omega Q_T$ and thence defuce many interesting facts about its eigenvalues. In particular, for any $\epsilon > 0$, there exists a C_ϵ such that

$$\begin{aligned}
|\{n \,|\, \lambda_n \geq 1 - \epsilon\}| &\leq 2\lambda - C_\epsilon \log(\lambda) \\
|\{n \,|\, 1 - \epsilon \geq \lambda_n \geq \epsilon\}| &\geq 2C_\epsilon \log(\lambda).
\end{aligned}$$

Reproducing Kernel Hilbert Spaces

In the previous chapter we discussed several interesting properties of bandlimiting operators. In this chapter we discuss a more general class of function spaces which share many nice properties with the space of bandlimited functions.

Bandlimited functions again

Consider the set

$$B_\Omega := \{f \in L^2(\mathbb{R}) \,|\, \mathrm{supp}\tilde{f} \subseteq [-\Omega, \Omega]\}.$$

Clearly this is a closed subspace in L^2. From before, we know that if $f \in B_\Omega$, then f extends to an entire function on $\mathbb{C}$ which is of *exponential type*, i.e.

$$|f(z)| \leq \frac{1}{\sqrt{2\pi}} \|\tilde{f}\|_{L^2} e^{\Omega|\Im z|}.$$

Thus, B_Ω is a Hilbert space of entire functions.

Now, for any $f \in B_\Omega$, if $f \in L^1(\mathbb{R})$,

$$\begin{aligned} f(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\Omega}^{\Omega} e^{i\xi x} \tilde{f}(\xi)\, \mathrm{d}\xi \\ &= \frac{1}{2\pi} \int_{-\Omega}^{\Omega} e^{i\xi x} \int_{-\infty}^{\infty} e^{-i\xi y} f(y)\, \mathrm{d}y\, \mathrm{d}\xi \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) \frac{2\sin(\Omega(x-y))}{x-y}\, \mathrm{d}y \\ &= \int_{-\infty}^{\infty} \frac{\sin(\Omega(x-y))}{\pi(x-y)} f(y)\, \mathrm{d}y. \end{aligned}$$

This can be extended to general $f \in B_\Omega$ using standard arguments.

Setting $e_x(y) = \sin(\Omega(x-y))/(\pi(x-y))$ we obtain

$$f(x) = \langle e_x, f \rangle.$$

Thus, e_x acts like the δ function. But there is a major difference– $e_x \in B_\Omega$!

Setting $K(x,y) = e_x(y)$ we also see that

$$f(x) = \int_{-\infty}^{\infty} K(x,y)\, f(y)\, \mathrm{d}y.$$

K is the kernel of an integral operator whose action "reproduces" f. Moreover, for all x, $K(x,\cdot) \in B_\Omega$. Hilbert spaces which have such K are called *reproducing kernel Hilbert spaces* and such K are called *reproducing kernels*.

Reproducing Kernel Hilbert spaces

Given a set X, let H be a Hilbert space of functions on X. H is a reproducing kernel Hilbert space if for all $x \in X$ there exists an $\ell_x \in H^*$ ($\|\ell_x\| < \infty$) such that

$$\ell_x(f) = f(x), \quad \forall f \in H.$$

Remark 26. *Reproducing kernel Hilbert spaces were first introduced in 1907 by Zaremba for considering boundary value problems for harmonic functions. Mercer also looked at similar structures when considering integral equations.*

Our first example is a non-example.

Example 10. *The space $L^2([-1,1])$ is* not *a reproducing kernel Hilbert space. In particular, pointwise evaluation is not even well-defined.*

Example 11 (Hardy spaces)**.** *Consider all functions which are analytic inside the unit disk D such that*

$$\sup_{0\le r<1} \left(\frac{1}{2\pi} \int_0^{2\pi} |f(re^{i\theta})|^2 \, \mathrm{d}\theta \right)^{1/2} < \infty.$$

Thus, for any f in this space, $F(\theta) = \lim_{r\to 1^-} f(re^{i\theta})$ exists for almost every $\theta \in [0, 2\pi)$.
This space is called the Hardy space $H^2(D)$*, and has inner product*

$$\langle f, g \rangle_{H^2(D)} := \frac{1}{2\pi} \int_0^{2\pi} F(\theta)\overline{G}(\theta)\, \mathrm{d}\theta.$$

Let's see whether or not this is a reproducing kernel Hilbert space. To that end, fix $w \in D$. Then, we require

$$e_w \in H^2(D), \quad \text{and} \quad \frac{1}{2\pi} \int_0^{2\pi} \overline{E_w}(\theta)\, F(\theta)\, \mathrm{d}\theta = f(w),$$

for all $f \in H^2(D)$. Representing E_w as a Fourier series, $\sum_{n=0}^{\infty} a_n^w e^{in\theta}$, we find that

$$\begin{aligned} w^j &= \frac{1}{2\pi} \int_0^{2\pi} \sum_{n=0}^{\infty} \overline{(a_n^w)} e^{-in\theta} e^{ij\theta}\, \mathrm{d}\theta \\ &= \overline{(a_j^w)}. \end{aligned}$$

Thus, $a_j^w = \overline{w}^j$. We find $e_w(z)$ by summing, to obtain

$$e_w(z) = \sum_{n=0}^{\infty} \overline{w}^n z^n = \frac{1}{1-\overline{w}z}$$

which is clearly in $H^2(D)$.

Example 12 (Sobolev spaces)**.** *The Sobolev space $H_0^1([0,1])$ defined by*

$$H_0^1([0,1]) := \{f \in L^2([0,1]) \mid f' \in L^2,\ f(0) = f(1) = 0\}$$

together with the inner product

$$\langle f, g\rangle_{H^1} := \int_0^1 f(x)\,\bar{g}(x)\,\mathrm{d}x + \int_0^1 f'(x)\,\bar{g}'(x)\,\mathrm{d}x.$$

We leave the construction of e_x (and the proof that it is in H_0^1) as an exercise.

Continuous wavelet transforms

We continue our tour of reproducing kernel Hilbert space with another important class of examples. Before getting into the details, we need some preliminaries first. Suppose we are given a function $\psi \in L^2(\mathbb{R})$ with

$$C_\psi = 2\pi \int |\xi|^{-1} |\tilde{\psi}(\xi)|^2\,\mathrm{d}\xi < \infty.$$

Note that if $\psi \in L^1$ then $\tilde{\psi}$ is continuous and $\tilde{\psi}(0) = 0$ implies $\int \psi\,\mathrm{d}x = 0$.

Consider the family of functions

$$\psi^{a,b}(x) = |a|^{1/2}\psi\left(\frac{x-b}{a}\right), \quad a, b \in \mathbb{R},\ a \neq 0.$$

In the following, we normalize ψ so that $\|\psi\| = 1$.

Definition 13. *The continuous wavelet transform with respect to the family $\psi^{a,b}$ is defined by*

$$(T^{\mathrm{wav}} f)(a,b) = \langle f, \psi^{a,b}\rangle = \int f(x)|a|^{-1/2}\overline{\psi\left(\frac{x-b}{a}\right)}\,\mathrm{d}x.$$

Note that $|(T^{\mathrm{wav}} f)(a,b)| \leq \|f\|$.

Proposition 12. *For all $f, g \in L^2$,*

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} (T^{\mathrm{wav}} f(a,b))\overline{(T^{\mathrm{wav}} g(a,b))}\,\frac{\mathrm{d}a\,\mathrm{d}b}{a^2} = C_\psi \langle f, g\rangle.$$

Proof.

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(T^{\text{wav}}f(a,b))\overline{(T^{\text{wav}}g(a,b))}\,\frac{\mathrm{d}a\,\mathrm{d}b}{a^2} = \int\int\left(\int\tilde{f}(\xi)|a|^{1/2}e^{-ib\xi}\overline{\tilde{\psi}(a\xi)}\,\mathrm{d}\xi\right)\left(\int\overline{\tilde{g}(\xi')}|a|^{1/2}e^{ib\xi'}\tilde{\psi}(a\xi)\,\mathrm{d}\xi\right)\frac{\mathrm{d}a\,\mathrm{d}b}{a^2}$$

$$= 2\pi\int\int\widetilde{F_a}(\zeta)\widetilde{\overline{G}_a}(\zeta)\,\mathrm{d}\zeta\frac{\mathrm{d}a}{a^2}$$

Setting $F_a(\xi) = |a|^{1/2}\tilde{f}(\xi)\overline{\tilde{\psi}(a\xi)}$ and $G_a(\xi) = |a|^{1/2}\tilde{g}(\xi)\overline{\tilde{\psi}(a\xi)}$

$$= 2\pi\int\int F_a(\xi)\overline{G}_a(\xi)\,\mathrm{d}\xi\frac{\mathrm{d}a}{a^2}$$

$$= 2\pi\int\tilde{f}(\xi)\overline{\tilde{g}}(\xi)\int|a|\,|\tilde{\psi}(a\xi)|^2\frac{\mathrm{d}a}{|a|^2}$$

Making a change of variables, setting $z = a\xi$ in the innermost integral

$$= 2\pi C_\psi\langle f,g\rangle.$$

□

Setting $g = f$ in the previous theorem, we see that

$$C_\psi^{-1}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}|(T^{\text{wav}}(a,b))|^2\,\frac{\mathrm{d}a\,\mathrm{d}b}{a^2} = \int|f(x)|^2\,\mathrm{d}x$$

and so T^{wav} is an isometry of $L^2(\mathbb{R})$ into $L^2(\mathbb{R}^2, C_\psi^{-1}a^{-2}\,\mathrm{d}a\,\mathrm{d}b)$. This latter space is a Hilbert space. We denote its norm by $\|\cdot\|_w$. It is also easy to show that the image of L^2 is a closed subspace of $L^2(\mathbb{R}^2, C_\psi^{-1}a^{-2}\,\mathrm{d}a\,\mathrm{d}b)$, and thus is a Hilbert space in its own right. We call it H.

For any $F \in H$, there is an $f \in L^2$ such that $F = T^{\text{wav}}f$. Then,

$$\begin{aligned}F(a,b) &= \langle f,\psi^{a,b}\rangle\\ &= \frac{1}{C_\psi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(T^{\text{wav}}f(a',b'))\overline{(T^{\text{wav}}\psi^{a,b}(a',b'))}\,\frac{\mathrm{d}a'\,\mathrm{d}b'}{(a')^2}\\ &= \frac{1}{C_\psi}\int_{-\infty}^{\infty}K(a,b,a',b')\frac{\mathrm{d}a'\,\mathrm{d}b'}{(a')^2}\end{aligned}$$

with $K(a,b,a',b') = \langle\psi^{a',b'},\psi^{a,b}\rangle$. Thus H is a reproducing kernel Hilbert space.

Radial basis functions

We conclude our list of examples of reproducing kernel Hilbert spaces with an important class of examples.

A continuous function $\phi : \mathbb{R}^d \to \mathbb{C}$ is called *positive semi-definite* if for all $N \in \mathbb{N}$ and all pairwise distinct points $X = \{x_1, \cdots, x_N\} \subset \mathbb{R}^d$ and all $\alpha \in \mathbb{C}^N$ the quadratic form

$$\sum_{j=1}^{N}\sum_{k=1}^{N}\alpha_j\overline{\alpha_k}\phi(x_j - x_k$$

is nonnegative. ϕ is positive definite if it is positive definite for all non-zero $\alpha \in \mathbb{C}^N$. More generally, we could consider functions of the form $\phi(x_j, x_k)$.

Given Ω, set

$$F_\phi = \text{span}\{\phi(\cdot, y) \,|\, y \in \Omega\}$$

with bilinear form

$$\left(\sum_{j=1}^{N} \alpha_j (\phi(\cdot, x_j)\,,\, \sum_{k=1}^{M} \beta_k (\phi(\cdot, y_k) \right)_\phi := \sum_{j=1}^{N} \sum_{k=1}^{N} \alpha_j \overline{\beta_k} \phi(x_j, y_k).$$

Theorem 42. *If ϕ is symmetric and positive definite then $(\cdot,\cdot)_\phi$ defines an inner product on the pre-Hilbert space F_ϕ. Moreover, ϕ is a reproducing kernel.*

Proof. The proof is more or less obvious.

$$(f, \phi(\cdot, y))_\phi = \left(\sum_{j=1}^{N} \alpha_j \phi(\cdot, x_j), \phi(\cdot, y) \right)_\phi = \sum_{j=1}^{N} \alpha_j \phi(y, x_j) = f(y).$$

□

With some technical work, we can extend this to the completion. Putting it together we have the following theorem.

Theorem 43 (Moore-Aronszajn)**.** *Let ϕ be symmetric and positive definite on X. Then there is a unique Hilbert space of functions on X for which ϕ is the reproducing kernel.*

Remark 27. *Note, conversely, that if K is a reproducing kernel, then for all $\alpha \in \mathbb{R}^n$, $x_j \in X$, distinct,*

$$\begin{aligned} 0 &\leq \left\langle \sum_{j=1}^{n} \alpha_j K(\cdot, x_j),\, \sum_{j=1}^{n} \alpha_j K(\cdot, x_j) \right\rangle \\ &= \sum_{j=1}^{n} \alpha_j \left\langle \sum_{k=1}^{n} \alpha_k K(\cdot, x_k), K(\cdot, x_j) \right\rangle \\ &= \sum_{j=1}^{n} \sum_{k=1}^{n} \alpha_j \alpha_k K(x_j, x_k). \end{aligned}$$

so K is positive semi-definite, and positive definite if all the point evaluation functionals are linearly independent.

Representer theorems

We conclude our discussion with a useful result related to optimization in reproducing kernel Hilbert spaces. For more information, see for example Wahba, Kimeldorf (1970,1971) or Wahba (1990,1992).

To start with a simple example, let H be a reproducing kernel Hilbert space, and consider the penalized least squares problem

$$\min_{f \in H} \left\{ \sum_{i=1}^{n} (y_i - f(x_i))^2 + \lambda J(f) \right\}. \tag{5}$$

Here, the pairs (x_i, y_i) can be thought of as data points, and J is a square semi-norm penalty. In particular, $J(f) = \|(I - P)f\|^2$ where P is an orthogonal projection.

Suppose further that $H_0 = \{f \,|J(f) = 0\}$ is finite dimensional. Decompose $H = H_0 \oplus H_1$. Let $\phi_1, \cdots, \phi_m$ be a basis for H_0 and K_1 be the kernel of H_1. Set $e_i(\cdot) = K_1(\cdot, x_i)$.

Theorem 44. *The solution to 5 is expressable in the form*

$$f_* = \sum_{j=1}^{m} \alpha_k \phi_j + \sum_{k=1}^{n} \beta_k e_k,$$

i.e. the only part of the infinite dimensional space H_1 we care about is the finite dimensional subspace spanned by $K(\cdot, x_i)$ where the x_i are the "sampling locations".

Proof. We begin by writing any $f \in H$ as

$$f = \sum_{j=1}^{m} a_j \phi_j + \sum_{k=1}^{n} b_k e_k + \psi,$$

where ψ is a residual which is orthogonal to all the e_k's and ϕ_j's. If F is our objective functional,

$$\begin{aligned} F(f) &= \sum_{j=1}^{n} (y_i - \langle e_i, f \rangle)^2 + \lambda \sum_{i=1}^{n} \sum_{j=1}^{n} b_i b_j K_1(x_i, x_j) + \lambda \|\psi\|^2 \\ &= \sum_{j=1}^{n} \left(y_i - \left(\sum_{j=1}^{m} a_j \phi_j + \sum_{k=1}^{n} b_k e_k \right) \right)^2 + \lambda \sum_{i=1}^{n} \sum_{j=1}^{n} b_i b_j K_1(x_i, x_j) + \lambda \|\psi\|^2. \end{aligned}$$

Clearly then, setting $\psi = 0$ reduces F. □

There are, of course, many possible generalizations. One due to Schölkopf, Herbrich, and Smola is as follows.

Theorem 45. *Let X be a set with reproducing kernel Hilbert space H_k and with corresponding kernel K. Suppose we are given samples (x_i, y_i), a strictly increasing real-valued function g, and an error function $E : (X \times \mathbb{R}^2)^n \to \mathbb{R} \cup \{\infty\}$. Consider the functional*

$$F(f) := E((x_1, y_1, f(x_1)), \cdots, (x_n, y_n, f(x_n))) + g(\|f\|).$$

Then any minimizer f_* of F is of the form

$$f_* = \sum_{i=1}^{n} \alpha_i e_i,$$

where $e_i = K(\cdot, x_i)$.

Proof. We write $f = \sum_{i=1}^{n} a_i e_i + \psi$. Then

$$f(x_i) = \langle e_i, f \rangle = \sum_{j=1}^{n} a_j e_j(x_i).$$

Moreover,

$$g(\|f\|) \geq g(\| \sum_{i=1}^{n} \alpha_i e_i \|).$$

□

Additional Exercises

Exercise 30. *Prove that H_0^1 is a reproducing kernel Hilbert space. Give an explicit construction of e_x and show that is satisfies the required properties.*

To be added

Proof of convergence of Legendre expansion (adaptive discretization homework exercise)

Bibliography

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