Packing, coding, and ground states

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Preface

In these lectures, we'll study simple models of materials from several different perspectives: geometry (packing problems), information theory (error-correcting codes), and physics (ground states of interacting particle systems). These perspectives each shed light on some of the same problems and phenomena, while highlighting different techniques and connections.

One noteworthy phenomenon is the exceptional symmetry that is found in certain special cases, and we'll examine when and why it occurs. The overall theme of the lectures is thus order vs. disorder. How much symmetry can we expect to see in optimal geometric structures?

The style of these lecture notes is deliberately brief and informal. See Conway and Sloane’s book *Sphere packing, lattices and groups* [26] for far more information about many of the mathematical objects we’ll discuss, as well as the references cited in the notes for omitted details.

I’ve included a dozen exercises for the reader, which cover things I think it’s most useful to do for oneself. The exercises vary in difficulty, from routine verifications to trickier computations. There’s no need to solve them if you are willing to take a few things on faith, but I highly recommend engaging actively with this material, and the exercises would be a good way to get started.

These notes are based on my PCMI lectures from 2014 and were written before Viazovska [80] found a remarkable solution to the sphere packing problem in \( \mathbb{R}^8 \) using linear programming bounds. The only updates to reflect this development are a few footnotes.

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1. Introduction

The sphere packing problem asks for the densest packing of congruent spheres in $\mathbb{R}^n$. In other words, how can we cover the greatest fraction of space using congruent balls that do not overlap (i.e., that have disjoint interiors)? The density is the fraction of space covered. Finding the densest sphere packing sounds simple, but it turns out to be a surprisingly deep and subtle problem.

Before we dive into the sphere packing problem, it’s worth thinking about how to write down a rigorous definition. Although pathological packings may not have well-defined densities, everything we could reasonably hope for is true: we can define the optimal density by taking a suitable limit, and there is a packing that achieves this density. Specifically, given a packing $\mathcal{P}$, a point $x \in \mathbb{R}^n$, and a positive real number $r$, let

$$\Delta_{r,x}(\mathcal{P}) = \frac{\text{vol}(B_r(x) \cap \mathcal{P})}{\text{vol} B_r(x)}$$

be the fraction of the ball $B_r(x)$ of radius $r$ centered at $x$ that is covered by $\mathcal{P}$. If we define the optimal packing density $\Delta_n$ in $\mathbb{R}^n$ by

$$\Delta_n = \limsup_{r \to \infty} \sup_{\mathcal{P}} \Delta_{r,0}(\mathcal{P}),$$

then there exists a single packing $\mathcal{P}$ for which

$$\lim_{r \to \infty} \Delta_{r,x}(\mathcal{P}) = \Delta_n$$

uniformly for all $x \in \mathbb{R}^n$. See [37] for a proof.

What are the optimal sphere packings in low dimensions? In one dimension, we have the interval packing problem on the line, which is trivial. In two dimensions, the answer is pretty clearly the hexagonal packing, with each disk surrounded by six others:

![Hexagonal Packing](image)

However, proving optimality takes a genuine idea. For example, one can show that the Voronoi cells (the sets of points closer to each sphere center than to the others) in the hexagonal packing are as small as possible in any packing. See [74] for the first proof of optimality, [63, 35] for subsequent proofs, and [38] for a particularly short proof.
In three dimensions, the sphere packing problem is much more difficult. There is a natural guess for the solution, namely stacking hexagonal layers as densely as possible, so that each is nestled into the gaps in the neighboring layers. Such a packing is known to be optimal, via an elaborate proof \[39\] that depends on computer calculations. The original proof was so long and complex that it was difficult to check carefully, but it has recently been verified at the level of formal logic \[40\].

In four or more dimensions, the optimal sphere packing density is not known, although there are upper and lower bounds.\[1\]

**Exercise 1.1.** How can hexagonal layers be stacked to form dense packings in \(\mathbb{R}^3\)? Show that there are an uncountable number of different ways to do so, even if you consider two packings the same when they are related by a rigid motion of space. Can you extend this analysis to \(\mathbb{R}^4\)? Which packings can you get by stacking optimal three-dimensional packings as densely as possible? How many can you find? How dense are they? What about \(\mathbb{R}^5\), \(\mathbb{R}^6\)? How high can you go?

Feel free to give up after four dimensions, but the further you go, the more interesting phenomena you’ll run into. By \(\mathbb{R}^{10}\), this iterated stacking process will no longer produce the densest possible sphere packings, but nobody knows whether it fails before that. See \[25\] for more details on what happens in dimensions two through ten.

### 2. Motivation

There are several reasons why we should care about sphere packing. One is that it’s a natural geometric problem: humanity ought to know the answer to such a simple and natural question.

Another reason is that the problem has interesting solutions. Sometimes it’s difficult to judge how interesting a problem is in the abstract, before taking a look at the phenomena that occur. Sphere packing is full of rich, intricate structures that are themselves of intrinsic interest, and this makes the problem far more appealing than it would have been if the answers had been less exciting.

A third reason to care about sphere packing is that it is a toy model of granular materials. Of course no real material consists of identical perfect spheres, and the sphere packing problem also neglects forces and dynamics. However, sphere packing is at least a first step towards understanding the density of an idealized material. (See \[52\] for a statistical physics perspective on packing.)

The most important practical reason to study sphere packing is also one of the most surprising reasons: high-dimensional sphere packings are essential for communication over noisy channels, as we’ll spend the rest of this section understanding. This is really an assertion about information theory, Claude Shannon’s great discovery from his famous 1948 paper *A mathematical theory of communication* \[70\]. Sphere packing per se again deals with an idealized scenario, but it illustrates some of the fundamental principles underlying information theory.

The setting works as follows. Suppose we are sending messages over some communication channel. We will represent the signals by points in a bounded subset of \(\mathbb{R}^n\), say the ball of radius \(R\) about the origin (the precise subset is not so

\[1\] Viazovska \[80\] has recently solved the sphere packing problem in \(\mathbb{R}^8\) using linear programming bounds.
In this model, each coordinate represents some measurement used to describe the signal. For example, for a radio signal we could measure the amplitude at different frequencies. There is no reason to expect the number of measurements to be small, and realistic channels can involve hundreds or even thousands of coordinates. Thus, the signal space for the channel will be high-dimensional. Note that this dimensionality has nothing to do with the physical space we are working in; instead, it simply represents the number of independent measurements we make on the signals.

Each signal will be an individual transmission over the channel at a given time, and we will send a stream of signals as time passes. Of course, the big difficulty with communication is noise: if we send a signal \( s \), then the received signal \( r \) at the other end will generally not be exactly equal to \( s \). Instead, it will have been perturbed by channel noise. In a useful channel, the noise level will be fairly low, and we can expect that \( |r - s| < \varepsilon \) for some fixed \( \varepsilon \) (the noise level of the channel).

Thus, we can imagine an open error ball of radius \( \varepsilon \) about each signal sent, which shows how it could be received after adding noise:

This is a simplistic model of noise, since we assume that the noise has no directionality or structure, and that every perturbation up to radius \( \varepsilon \) could plausibly occur but nothing beyond that limit. In practice, engineers use more sophisticated noise models; for example, cell phones have to take into account all sorts of other phenomena, such as interference from reflected signals. However, our basic noise model is a good illustration of the essential principles.

How can we arrange our communications so as to remove the effects of noise? We will build a vocabulary \( S \subseteq \mathbb{R}^n \) of signals and only send signals in \( S \). This is called an error-correcting code. If two distinct signals \( s_1, s_2 \in S \) satisfy \( |s_1 - s_2| < 2\varepsilon \), then the received signal could be ambiguous:

Therefore, we will keep all signals in \( S \) at least \( 2\varepsilon \) apart, so that the error balls are disjoint:

This is exactly the sphere packing problem. We want the signal set \( S \) to be as large as possible, since having more signals available increases the rate at which we can transmit information, but the \( \varepsilon \)-balls about the signals in \( S \) are not allowed
to overlap. How large can we make $S$ subject to this constraint? Recall that the only available subset of $\mathbb{R}^n$ in our model is the ball of radius $R$. Thus, the question becomes how many $\varepsilon$-balls we can pack into a ball of radius $R + \varepsilon$. (The radius is $R + \varepsilon$, rather than $R$, because the error balls can stick out over the edge.) That’s a finite version of sphere packing, and we recover the usual version in all of $\mathbb{R}^n$ in the limit when $R$ is much larger than $\varepsilon$. That limit is exactly the situation we expect, since the channel is not very useful if $\varepsilon$ is on the same scale as $R$.

It is remarkable that although high-dimensional packing sounds utterly abstract and impractical, it turns out to be particularly important for applications. In these lectures we will focus on the theory behind sphere packing, rather than the applications, but it is helpful to keep in mind that a high-dimensional packing is a tool for communicating over a noisy channel.

3. Phenomena

Relatively little is understood about the sphere packing problem. One might hope for a systematic solution that works in every dimension, but that just doesn’t seem possible. Instead, each dimension has its own idiosyncrasies. Getting a feeling for how $\mathbb{R}^8$ differs from $\mathbb{R}^7$ or $\mathbb{R}^9$ is part of the charm of the subject, but these differences mean the packing problem is much more subtle than it sounds. In two or three dimensions, we can rely on our spatial intuition and summarize the procedure as “just do the obvious thing,” but there is no obvious thing to do in $\mathbb{R}^n$.

Good constructions are known in low dimensions, and there is little doubt that humanity has found the optimal density through at least the first eight dimensions. However, we have absolutely no idea what the best high-dimensional packings look like. For example, we do not know whether to expect them to be ordered and crystalline, or disordered and pseudorandom. Many researchers expect disorder, perhaps on the grounds that this is the default when there is no reason to expect order. However, we lack the theoretical tools to analyze this question.

All we know in general are upper and lower bounds for the optimal density, and these bounds are distressingly far apart. For example, in $\mathbb{R}^{36}$ (they differ by a multiplicative factor of 58: if you take the densest known packing in $\mathbb{R}^{36}$, then the best we can say is that you couldn’t fit in any more than 58 times as many spheres if you rearranged them. The ratio of the upper and lower bounds in $\mathbb{R}^n$ grows exponentially as $n \to \infty$.

At first, this gap sounds absurd. How could our bounds possibly be off by an exponential factor? One way to think about it is that volume scales exponentially in high dimensions, because the volume of a hypercube of side length $\ell$ in $\mathbb{R}^n$ is $\ell^n$, which is exponential in $n$. If you take a packing in $\mathbb{R}^n$ and move the sphere centers 1% further apart, then you lower the density by a factor of $1.01^n$. In low dimensions this factor is insignificant, but in high dimensions it is enormous. Thus, even a little bit of uncertainty in the sphere locations translates to an exponential uncertainty in the density.

On a scale from one to infinity, a million is small, but we know almost nothing about sphere packing in a million dimensions. The best we can say is that the optimal density is at least a little larger than $2^{-1000000}$. More generally, the following greedy argument gives a surprisingly easy lower bound of $2^{-n}$ in $\mathbb{R}^n$.

Consider a saturated packing in $\mathbb{R}^n$, i.e., a packing such that no further spheres can be added without overlap. Such packings certainly exist, because one can
obtain a saturated packing by iteratively adding spheres as close to the origin as possible. Alternatively, there are saturated packings on flat tori because there is room for only finitely many spheres, and unrolling such a packing yields a saturated periodic packing in Euclidean space.

**Proposition 3.1.** Every saturated sphere packing in $\mathbb{R}^n$ has density at least $2^{-n}$.

**Proof.** No point in $\mathbb{R}^n$ can have distance at least 2 from all the sphere centers in a saturated packing with unit spheres, because we could center a new sphere at such a point without creating any overlap (see Figure 1). In other words, doubling the radius of the spheres in a saturated packing would cover space completely. Doubling the radius increases the volume by a factor of $2^n$, and so the original spheres must occupy at least a $2^{-n}$ fraction of $\mathbb{R}^n$. Thus, every saturated packing has density at least $2^{-n}$. □

In $\mathbb{R}^1$ there are saturated packings with density arbitrarily close to 1/2, but that is the only case in which Proposition 3.1 is sharp, because the bound is sharp exactly when the double-radius balls can tile $\mathbb{R}^n$. One way to improve it is to prove a lower bound for how inefficient a sphere covering in $\mathbb{R}^n$ must be. For example, using the Coxeter-Few-Rogers theorem on sphere covering \[27\] improves the bound to $e^{-3/2}n \cdot 2^{-n}$ asymptotically.

At first $2^{-n}$ sounds like a rather weak bound, which must be far from the truth. However, nobody has been able to obtain any exponential improvement to it, and perhaps it is closer to the truth than one would guess. In any case, it is nearly all we know regarding density lower bounds in high dimensions. A long sequence of improvements ground to a halt with Ball’s bound of $2(n-1) \cdot 2^{-n}$ in 1992 \[7\], before progress began again nearly twenty years later. Vance proved a lower bound asymptotic to $6n/e \cdot 2^{-n}$ in 2011 \[77\], which improves on Ball’s bound because $e < 3$, and Venkatesh followed that with a much larger constant-factor improvement as well as a bound proportional to $n \log \log n \cdot 2^{-n}$ for a certain sparse sequence of dimensions \[78\]. This last bound is particularly exciting because it is the first superlinear improvement on $2^{-n}$, but on an exponential scale all of these improvements are small. For comparison, the best upper bound known is $2^{-\left(0.5990...+o(1)\right)n}$, due to Kabatiansky and Levenshtein \[41\] in 1978, with a constant-factor improvement by Cohn and Zhao \[23\] in 2014.

Note that the greedy argument is nonconstructive, and the same is true of the improvements mentioned above. For large $n$, all known bounds anywhere near $2^{-n}$
are nonconstructive, while every packing anyone has described explicitly is terrible in high dimensions. For example, one natural attempt is to center spheres of radius $1/2$ at the integer lattice points $\mathbb{Z}^n$. That yields a packing of density
\[
\frac{n^{n/2}}{(n/2)!2^n},
\]
and the factorial in the denominator ruins the density. (Note that when $n$ is odd, $(n/2)!$ means $\Gamma(n/2 + 1)$.)

There are some patterns in low dimensions, but they quickly stop working. For example, natural generalizations of the face-centered cubic packing from $\mathbb{R}^3$ work well in $\mathbb{R}^4$ and $\mathbb{R}^5$, but not in higher dimensions, as we will see in the next section. In $\mathbb{R}^{10}$, the best packing known is based on a periodic arrangement with 40 spheres in each fundamental cell [26, p. 140].

Crystalline packings work beautifully in low dimensions, but they become increasingly difficult to find in high dimensions. Perhaps they just aren’t optimal? It’s natural to speculate about amorphous packings, but nobody really knows. In high dimensions, we can analyze only random or typical packings, and we simply do not know how close they are to the very best.

One philosophical quandary is that too much structure seems to make high-dimensional packings bad, but the known lower bounds all rely on some sort of heavy structure. Vance’s and Venkatesh’s techniques give the best density, but they involve the most structure, namely lattices with nontrivial symmetry groups acting on them. The trade-off is that structure seemingly hurts density but helps in analyzing packings.

The most remarkable packings are the $E_8$ root lattice in $\mathbb{R}^8$ and the Leech lattice $\Lambda_{24}$ in $\mathbb{R}^{24}$. They are incredibly symmetrical and dense packings of spheres, and they must be optimal, although this has not yet been proved. What makes them exciting is that they turn out to be connected with many areas in mathematics and physics, such as string theory, hyperbolic geometry, and finite simple groups. See [26] and [32] for more information about these wonderful objects, as well as the next section for a construction of $E_8$.

4. Constructions

How can we form a sphere packing? The simplest structure we could use is a lattice, the integer span of $n$ linearly independent vectors in $\mathbb{R}^n$. In other words, given a basis $v_1, \ldots, v_n$, we center the spheres at the points
\[
\{a_1v_1 + a_2v_2 + \cdots + a_nv_n \mid a_1, \ldots, a_n \in \mathbb{Z}\}.
\]
The packing radius of a lattice is half the shortest nonzero vector length, since that is the largest radius for which the spheres do not overlap. Given a lattice basis $v_1, \ldots, v_n$, the corresponding fundamental cell is the parallelotope
\[
\{x_1v_1 + x_2v_2 + \cdots + x_nv_n \mid x_1, \ldots, x_n \in [0, 1)\}.
\]
The translates of the fundamental cell by lattice vectors tile space.

In a lattice packing, there is one sphere per translate of the fundamental cell, and the density is the volume ratio of the sphere and cell. More generally, we could form a periodic packing, which is the union of finitely many translates of a

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2 Until very recently in [80] for $n = 8$. 
lattice. Equivalently, there can be several spheres per cell, which are then translated throughout space by the lattice vectors. There is no reason to believe that one sphere per cell is the best choice, and indeed periodic packings offer considerably more flexibility.

One confusing issue is that physicists use the term “lattice” to mean periodic packing, while they call lattices “Bravais lattices.” We will stick with the standard mathematical terminology.

There is no reason to believe that periodic packings achieve the greatest possible density. This is an open question above three dimensions, and it is plausibly false in high dimensions. However, periodic packings always come arbitrarily close to the optimal density. To see why, consider an optimal packing, and imagine intersecting it with a large box. If we try to repeat the part in the box periodically through space, then the only place overlap could occur is along the boundary of the box. We can fix any problems by removing the spheres next to the boundary. Shaving the packing in this way produces a periodic packing without overlap, at the cost of slightly lowering the density. The decrease in density becomes arbitrarily small if we use a sufficiently large box, and thus periodic packings come arbitrarily close to the optimal packing density.

By contrast, lattices probably do not approach the optimal density in high dimensions. The problem is that unlike periodic packings, lattices have limited flexibility. A lattice is completely determined by a basis, and thus a lattice in \( \mathbb{R}^n \) can be specified by \( n^2 \) parameters (in fact, fewer if we take the quotient by rigid motions). Quadratically many parameters just don’t give enough flexibility to fill all the gaps in an exponential amount of space. It’s natural to guess that when \( n \) is large enough, no lattice packing in \( \mathbb{R}^n \) is ever saturated, but this conjecture remains out of reach.

The best sphere packings currently known are not always lattice packings (\( \mathbb{R}^{10} \) is the first case in which lattices seem to be suboptimal), but many good packings are. The simplest lattice is \( \mathbb{Z}^n \), but it is a lousy packing when \( n > 1 \), as discussed above. Instead, the “checkerboard” packing

\[
D_n = \{ (x_1, \ldots, x_n) \in \mathbb{Z}^n \mid x_1 + \cdots + x_n \text{ is even} \}
\]

is better for \( n \geq 3 \). In fact, \( D_3 \), \( D_4 \), and \( D_5 \) are the best packings known in their dimensions, and provably the best lattice packings (see [26] for more information). However, they are suboptimal for \( n \geq 6 \).

What goes wrong for \( n \geq 6 \) is that the holes in \( D_n \) grow larger and larger. A hole in a lattice \( \Lambda \) in \( \mathbb{R}^n \) is a point in \( \mathbb{R}^n \) that is a local maximum for distance from the nearest point in \( \Lambda \). There are two classes of holes in \( D_n \) for \( n \geq 3 \), represented by \( (1, 0, \ldots, 0) \), which is at distance 1 from \( D_n \), and \( (1/2, 1/2, \ldots, 1/2) \), which is at distance

\[
\sqrt{\left(\frac{1}{2}\right)^2 + \cdots + \left(\frac{1}{2}\right)^2} = \sqrt{\frac{n}{4}}.
\]

More generally, the translates of these points by \( D_n \) are also holes, as are the translates of \( (1/2, 1/2, \ldots, 1/2, -1/2) \).

When \( n > 4 \) we call \( (1, 0, \ldots, 0) \) a shallow hole in \( D_n \) and \( (1/2, \ldots, \pm 1/2) \) a deep hole, because \( \sqrt{n/4} > 1 \). When \( n \) is large, the depth \( \sqrt{n/4} \) of a deep hole is enormous. For comparison, note that the spheres in the \( D_n \) packing have radius
\(\sqrt{2}/2\), because the nearest lattice points are \\
\((0,0,\ldots,0)\) and \((1,1,0,\ldots,0)\), at distance \(\sqrt{2}\). When \(n\) is large, the holes are much larger than the spheres in the packing, and \(D_n\) is not even saturated, let alone an optimal packing.

This transition occurs at dimension eight, and something wonderful happens right at the transition point. When \(n = 8\), the radius \(\sqrt{n/4}\) of a deep hole equals the distance \(\sqrt{2}\) between adjacent lattice points. Thus, we can slip another copy of \(D_8\) into the holes, which doubles the packing density, and the new spheres fit perfectly into place. The resulting packing is called the \(E_8\) root lattice.

This construction of \(E_8\) appears asymmetric, with two different types of spheres, namely the original spheres and the ones that were added. However, they are indistinguishable, because \(E_8\) is a lattice and thus all the spheres are equivalent under translation.

**Exercise 4.1.** Check that \(E_8\) is in fact a lattice.

The \(E_6\) and \(E_7\) lattices are certain cross sections of \(E_8\). The \(E_6\), \(E_7\), and \(E_8\) lattices are the densest lattice packings in \(\mathbb{R}^6\) through \(\mathbb{R}^8\), and they are almost certainly the densest sphere packings.

The Leech lattice \(\Lambda_{24}\) in \(\mathbb{R}^{24}\) is similar in spirit, but with a more elaborate construction. See [32] for an elegant treatment of the Leech lattice, as well as the theory of root lattices.

The kissing number in \(\mathbb{R}^n\) is the greatest number of spheres that can touch a central sphere, if they all have the same size and cannot overlap except tangentially. It is known to be 6 in \(\mathbb{R}^2\), 12 in \(\mathbb{R}^3\), 24 in \(\mathbb{R}^4\), 240 in \(\mathbb{R}^8\), but is not known in any other dimensions. The case of \(\mathbb{R}^2\) is easy, but \(\mathbb{R}^3\) is not [60], and \(\mathbb{R}^4\) is yet more difficult [55]. Surprisingly, \(\mathbb{R}^8\) and \(\mathbb{R}^{24}\) are quite a bit simpler than \(\mathbb{R}^3\) or \(\mathbb{R}^4\) are [59, 50], and we will settle them in the fourth lecture.

**Exercise 4.2.** What are the shortest nonzero vectors in \(D_n\)? In \(E_8\)? This will give optimal kissing configurations in \(\mathbb{R}^3\), \(\mathbb{R}^4\), and \(\mathbb{R}^8\).

**Exercise 4.3.** The vertices of a cross polytope centered at the origin in \(\mathbb{R}^n\) consist of \(n\) pairs of orthogonal vectors of the same length (it’s a generalized octahedron). Show how to decompose the vertices of a hypercube in \(\mathbb{R}^4\) into two cross polytopes. Find a symmetry of the hypercube that interchanges them.

**Exercise 4.4.** Show how to decompose the minimal vectors in \(D_4\) into three disjoint cross polytopes, and find a symmetry of \(D_4\) that cyclically permutes these cross polytopes.

This symmetry is called triality, and it makes \(D_4\) more symmetrical than any of its siblings. When \(n \neq 4\), the symmetries of \(D_n\) are simply permutations and sign changes of the coordinates, while \(D_4\) has all those plus triality.

### 5. Difficulty of sphere packing

Why is the sphere packing problem hard? There are several reasons for this. One is that there are many local optima. For example, among lattices in \(\mathbb{R}^8\), there are 2408 local maxima for density [73]. This number seems to grow rapidly in high dimensions, and it means the structure of the space of packings is complicated.
There is lots of space to move in, with complicated geometrical configurations, and it is difficult to rule out implausible configurations rigorously.

To get a feeling for the difficulties, it is useful to think about the geometry of high dimensions. Let’s start by looking at the \( n \)-dimensional cube

\[
\{(x_1, \ldots, x_n) \mid |x_i| \leq 1 \text{ for all } i\}
\]

of side length 2. It has \( 2^n \) vertices \((\pm 1, \ldots, \pm 1)\), each at distance \( \sqrt{1^2 + \cdots + 1^2} = \sqrt{n} \) from the center. When \( n = 10^6 \), the number of vertices is absurdly large, and they are each 1000 units from the center, despite the fact that the side length is only 2. These facts are amazingly different from our intuition in low dimensions. I like to imagine the vertices as vast numbers of tiny fingers stretching out from the center of the cube. I find it difficult to imagine that the result is convex, but somehow a million dimensions has enough space to accommodate such a convex body. The reason why cubes pack much better than spheres is that the vertices stick out far enough to fill in all the gaps.

One of the most important insights in high-dimensional geometry is the following principle: almost all the volume of a high-dimensional body is concentrated near its boundary. To see why, imagine shrinking such a body by 1%, leaving just a thin fringe near the boundary. The volume of the shrunk copy is lower by a factor of \((99/100)^n\), which tends exponentially to zero as \( n \to \infty \). Thus, virtually all of the volume lies in that boundary fringe. There is of course nothing special about 1%. The appropriate shrinkage scale in \( \mathbb{R}^n \) to capture a constant fraction of the volume is on the order of \( 1/n \), because \((1 - c/n)^n\) converges to \( e^{-c} \).

Boundaries, where all the interaction takes place, become increasingly important as dimension rises. This helps explain the difficulty of sphere packing, because avoiding overlap is all about interaction along boundaries.

This principle reverses our intuition from low dimensions. We typically think of boundaries as small and exceptional, but in high dimensions there’s practically nothing but boundary, and this changes everything. For example, suppose we are analyzing a numerical algorithm that uses many variables and thus operates in a high-dimensional space. If it works efficiently throughout a certain region except near the boundary, then that sounds good until we realize that almost all the region is near the boundary.

### 6. Finding dense packings

In this section we’ll examine how record-setting sphere packings can be found. The high and low-dimensional cases are handled very differently in practice. First, we’ll look at the averaging techniques used in high dimensions, and then we’ll briefly discuss how computer searches can be used in low dimensions.

The key technique used in the most recent papers in high dimensions \cite{77, 78} is the Siegel mean value theorem \cite{72}, which lets us average suitable functions over the space of lattices. To carry out such an averaging we need a probability measure, and indeed there is a canonical probability measure on lattices with fixed determinant (i.e., fundamental cell volume). Specifically, it’s the unique \( SL_n(\mathbb{R}) \)-invariant probability measure on this space. The existence of an \( SL_n(\mathbb{R}) \)-invariant measure follows from general results on Haar measure \cite{56}, but it takes a calculation to show that it has finite volume and can thus be normalized to yield a probability measure.
Once we have this probability measure on lattices, we can ask various statistical questions. For example, what does the average pair correlation function look like? In other words, what can we say about the average number of neighbors at each distance in a random lattice? The Siegel mean value theorem says that these pair correlations are exactly the same as for a Poisson distribution (i.e., uniformly scattered points). More precisely, it says that for a sufficiently well-behaved function $f: \mathbb{R}^n \to \mathbb{R}$ with $n > 1$, the average of
\[ \sum_{x \in \Lambda \setminus \{0\}} f(x) \]
over all lattices $\Lambda$ of determinant 1 equals
\[ \int_{\mathbb{R}^n} f(x) \, dx. \]
Intuitively, averaging over a random lattice blurs the sum into an integral.

The reason why the Siegel mean value theorem holds is that there is enough symmetry to rule out any other possible answer. Specifically, by linearity the answer must be $\int f \, d\mu$ for some measure $\mu$ on $\mathbb{R}^n \setminus \{0\}$ that is invariant under $SL_n(\mathbb{R})$. There is only one such measure up to scaling when $n > 1$ (given a few mild hypotheses), and some consistency checks determine the constant of proportionality.

The meta principle here is that averaging over all possible structures is the same as having no structure at all. Of course this is not always true. It generally depends on invariance under the action of a large enough group, and $SL_n(\mathbb{R})$ is more than large enough.

It is not hard to deduce lower bounds for sphere packing density from the Siegel mean value theorem. The following proposition is far from the state of the art, but it illustrates the basic technique.

**Proposition 6.1.** The sphere packing density in $\mathbb{R}^n$ is at least $2 \cdot 2^{-n}$.

**Proof.** Let $B$ be a ball of volume 2 centered at the origin. For a random lattice of determinant 1, the expected number of nonzero lattice points in $B$ is $\text{vol}(B) = 2$, by applying the Siegel mean value theorem to the characteristic function of $B$. These lattice points come in pairs (negatives of each other), so the number is always even. Since the average number is 2 and some lattices have many, other lattices must have none. Such a lattice gives a packing with one copy of $B/2$ per unit volume and density
\[ \text{vol}(B/2) = \frac{\text{vol}(B)}{2^n} = 2 \cdot 2^{-n}, \]
as desired. \qed

Vance’s key idea [77] builds on the extra factor of 2 that arises because lattice vectors occur in pairs of the same length. What if we impose additional symmetry? The intuition is that the average number of neighbors remains the same, but now they occur in bigger clumps, and so the chances of no nearby neighbors go up. Vance used lattices with quaternion algebras acting on them, and Venkatesh [78] obtained even stronger results by using cyclotomic fields.

Is this the best we can do? Only certain symmetry groups work here: we need a big centralizer to get enough invariance for the Siegel mean value theorem proof, and only division algebras will do. Cyclotomic fields are the best division algebras
for this purpose. Other sorts of groups will distort the pair correlation function away from Poisson statistics, but that could be good or bad. The area is wide open, and it is unclear which sorts of constructions might help.

In low dimensions, one can obtain much better results through numerical searches by computer. Several recent papers have taken this approach and recovered the densest lattices known in up to 20 dimensions. So far the computer searches have not yielded anything new, but they seem to be on the threshold of doing so. Can we push the calculations further, to unknown territory? What about periodic packings?

7. Computational problems

Lattices may sound down to earth, but they are full of computational difficulties. For example, given a lattice basis it is hard to tell how dense the corresponding sphere packing is. The difficulty is that to compute the density, we need to know both the volume of a fundamental cell and the packing radius of the lattice. The former is just the absolute value of the determinant of a basis matrix, which is easy to compute, but computing the packing radius is not easy. We can see why as follows.

Recall that the packing radius is half the shortest nonzero vector length in the lattice. The problem is that the basis vectors may not be the shortest vectors in the lattice, because some linear combination of them could be much shorter. There are exponentially many linear combinations that could work, and there is no obvious way to search efficiently. In fact, computing the shortest vector length is NP-hard. In other words, many other search problems can be reduced to it. No proof is known that it cannot be solved efficiently (this is the famous problem of whether \( P = NP \)), but that is almost certainly the case.

There are good algorithms for “lattice basis reduction,” such as the LLL algorithm, and they produce pretty short vectors. These vectors are generally far from optimal, but they are short enough for some applications, particularly in relatively low dimensions.

Shortest vector problems and their relatives come up in a surprising range of topics. One beautiful application is cryptography. We’ll briefly discuss the Goldreich-Goldwasser-Halevi cryptosystem, which turns out to have weaknesses but is a good illustration of how lattice problems can be used to build cryptosystems. It’s a public key cryptosystem, in which the public key is a basis for a high-dimensional lattice, while the private key is a secret nearly orthogonal basis for the same lattice, which makes it easy to find the nearest lattice point to any given point in space (while this problem should be hard for anyone who does not know the secret basis). We encode messages as lattice points. Anyone can encrypt a message by adding a small random perturbation, thereby moving it off the lattice. Decryption requires finding the nearest lattice point, which has no obvious solution without the private key. As mentioned above, this system is not as secure as it was intended to be, but there are other, stronger lattice-based systems. See for a survey of recent work in this area.

Recognizing algebraic numbers is a rather different sort of application. The number

\[
\alpha = -7.82646099323767402929927644895
\]
is a 30-digit approximation to a root of a fifth-degree polynomial equation. Which equation is it? Of course there are infinitely many answers, but Occam’s razor suggests we should seek the simplest one. One interpretation of “simplest” is that the coefficients should be small.

For comparison, 

\[ 0.1345345345345345345345345345345 \]

is clearly an approximation to \( 1/10 + 345/9990 \), and no other answer is nearly as satisfying.

To identify the number \( \alpha \) given above, let \( C = 10^{20} \) (chosen based on the precision of \( \alpha \)), and look at the lattice generated by the vectors

\[
\begin{align*}
  v_0 &= (1, 0, 0, 0, 0, 0, C), \\
  v_1 &= (0, 1, 0, 0, 0, 0, C\alpha), \\
  v_2 &= (0, 0, 1, 0, 0, 0, C\alpha^2), \\
  v_3 &= (0, 0, 0, 1, 0, 0, C\alpha^3), \\
  v_4 &= (0, 0, 0, 0, 1, 0, C\alpha^4), \\
  v_5 &= (0, 0, 0, 0, 0, 1, C\alpha^5).
\end{align*}
\]

The lattice vectors are given by

\[
a_0v_0 + \cdots + a_5v_5 = \left( a_0, a_1, a_2, a_3, a_4, a_5, C\left( \sum_{i=0}^5 a_i\alpha^i \right) \right)
\]

with \( a_0, \ldots, a_5 \in \mathbb{Z} \). Such a vector is small when the coefficients \( a_i \) are small and the sum \( \sum_{i=0}^5 a_i\alpha^i \) is tiny, since \( C \) is huge. Thus, finding a short vector amounts to finding a polynomial \( \sum_{i=0}^5 a_i x^i \) with small coefficients such that \( \alpha \) is nearly a root.

If we search for a short vector using the LLL algorithm, we find

\[
(71, -5, 12, -19, 13, 2, 0.000004135 \ldots).
\]

This tells us that

\[
71 - 5\alpha + 12\alpha^2 - 19\alpha^3 + 13\alpha^4 + 2\alpha^5 \approx 0.
\]

(More precisely, it is about 0.000004135/C \( \approx 4 \cdot 10^{-26} \).) In fact, this is the equation I used to generate \( \alpha \).

More generally, we can use lattices to find integral linear relations between any real numbers, not just powers of \( \alpha \). I find it really remarkable that the same sort of mathematics arises in this problem as in communication over a noisy channel.
LECTURE 2

Symmetry and ground states

1. Introduction

One of the beautiful phenomena in sphere packing is the occurrence of spontaneous order. There seems to be no reason to expect that an optimal sphere packing should be highly structured, but this happens time and again, with the precise structure being difficult to predict a priori.

These questions of order vs. disorder fit into a broader context. Where do symmetry and structure come from? László Fejes Tóth played an important role in formulating and attracting attention to this question. He drew a distinction between the systematology of the regular figures, which amounts to classifying the possible symmetries that could occur, and the genetics of the regular figures, which studies when and why they do occur. He sought to explain the genetics of the regular figures via optimization principles, and he made considerable progress towards this goal. In his vision [34] p. x], “regular arrangements are generated from unarranged, chaotic sets by the ordering effect of an economy principle, in the widest sense of the word.”

Typically the optimization problem has certain symmetries, but it is far from obvious when its solutions will inherit these symmetries. Steiner trees are an attractive illustration of this issue. What is the minimal-length path connecting the vertices of a square? One obvious guess is an X, which inherits all the symmetries of the square:

However, the optimal solution turns out to look like this, or its rotation by 90°:

There is partial symmetry breaking, in that the set of all solutions is of course invariant under the full symmetry group of the square, but each individual solution is invariant under just a subgroup.

This behavior occurs generically for optimization problems. For example, in the sphere packing problem the full symmetry group of the optimization problem consists of all rigid motions of Euclidean space, while each optimal sphere packing...
will be invariant under a much smaller subgroup, consisting of just a discrete set of motions. The difficulty lies in predicting what that subgroup will be. Which materials crystallize beautifully, and which remain amorphous?

From this perspective, we would like to understand which optimization problems admit highly symmetrical solutions, such as lattices or regular polytopes. Can we explain why $E_8$ and the Leech lattice are so much more symmetrical than the best packing known in $\mathbb{R}^{10}$?

2. Potential energy minimization

There’s no hope of developing a comprehensive theory of symmetry in optimization problems, because optimization is just too broad a topic. If you choose an arbitrary function to optimize, then you can make literally anything happen to the optima. To make progress, we must restrict the class of functions under consideration. In this lecture we will take a look at point particles with pairwise forces acting on them.

Given a collection of particles interacting according to some potential function, what do they do? For example, the Thomson problem deals with charged particles on the surface of the unit sphere $S^2$ in $\mathbb{R}^3$. Each pair of particles at Euclidean distance $r$ has potential energy $1/r$, and the total potential energy is the sum over all the pairs.

The simplest question is what the ground states are. In other words, what are the minimal-energy configurations? They describe the behavior of the system at zero temperature. This is a simple question, but the ground states in the Thomson problem are far from obvious, and in fact not fully known in general.

More generally, we can ask about dynamics or the behavior at positive temperature. These questions are more subtle, and we will generally restrict our attention to ground states. After all, if we can’t even understand the ground states, then there is little hope of analyzing anything more involved than that.

Before we restrict our attention to ground states, though, it’s worth putting everything in the context of Gibbs measures. They are a canonical way of putting a probability measure on the states of a system based on nothing except their energies and the system’s temperature. Of course one can’t possibly capture the behavior of every system based on so little information, but Gibbs measures do a good job of describing a system that is in equilibrium with a heat bath (a neighboring system that is so much larger that its temperature is unaffected by the smaller system).

For simplicity, imagine that our system has only $n$ states, labeled 1 through $n$, where state $i$ has energy $E_i$. (To handle continuous systems we can simply replace sums over states with integrals.) If we are given the average energy $\overline{E}$ of the system, we determine the corresponding probability distribution on the states by finding probabilities $p_1, \ldots, p_n$ so that $\sum_i p_i E_i = \overline{E}$ and the entropy $\sum_i -p_i \log p_i$ is maximized, where we interpret $0 \log 0$ as 0. In other words, the system is as disordered as possible, subject to having a certain average energy.

It is not difficult to solve this optimization problem via Lagrange multipliers, and the result is that

$$\log(1/p_i) = \alpha + \beta E_i$$

for some constants $\alpha$ and $\beta$. Thus, we can write

$$p_i = \frac{e^{-\beta E_i}}{Z},$$
where the partition function $Z = \sum_i e^{-\beta E_i}$ ensures that $\sum_i p_i = 1$ (it is also $e^{\alpha}$).

Such a probability distribution is called a Gibbs distribution.

In physics terms, $\beta$ turns out to be proportional to the reciprocal of temperature. As the temperature tends to zero, $\beta$ tends to infinity and the Gibbs distribution becomes concentrated on the ground states. As the temperature tends to infinity, $\beta$ tends to zero and the Gibbs distribution becomes equidistributed among all the states.

One question we have not yet addressed is why $\sum_i -p_i \log p_i$ deserves the name entropy. In fact, it is an excellent measure of disorder, essentially because it measures how surprising the probability distribution is on average. Consider how surprised we should be by an event of probability $p$. Call this surprise function $S(p)$, and think of it as a measure of how much you learn from seeing this event happen.

(Information theory makes this intuition precise.)

Clearly $S$ should be a decreasing function: the higher the probability is, the less surprising it is and the less you learn from seeing it happen. Furthermore, we should have

$$S(pq) = S(p) + S(q).$$

In other words, the amount you learn from independent events is additive. This makes good sense intuitively: if you learn one bit of information from a coin flip, then you learn two bits from two independent coin flips.

These conditions uniquely determine the function $S$ up to a constant factor, as $S(p) = -\log p$. Now the entropy is $\sum_i p_i S(p_i)$, and this quantity measures disorder by telling us how surprised we’ll be on average by the outcome.

Part of the beauty of mathematics is that concepts are connected in ways we would never guess. Gibbs measures are not just a construction from statistical physics, but rather occur throughout mathematics. For example, Dyson recognized that they describe eigenvalues of random matrices, as follows.

Haar measure gives a canonical probability measure on the unitary group $U(n)$. What does a random $n \times n$ unitary matrix chosen from this distribution look like? It has $n$ eigenvalues $z_1, \ldots, z_n$ on the unit circle, and the Weyl integral formula tells us that the probability density function for these eigenvalues is proportional to

$$\prod_{i<j} |z_i - z_j|^2.$$

If we call the constant of proportionality $1/Z$, then we can rewrite this formula as

$$\frac{1}{Z} e^{-\frac{1}{2} \sum_{i<j} \log |z_i - z_j|^2}.$$

In other words, the eigenvalue distribution of a random unitary matrix is a Gibbs distribution for a certain potential function between the eigenvalues. Specifically, they repel each other according to the potential function $x \mapsto \log(1/|x|)$. This function is harmonic on $\mathbb{R}^2 \setminus \{(0, 0)\}$, just as the Coulomb potential $x \mapsto 1/|x|$ is harmonic on $\mathbb{R}^3 \setminus \{(0, 0, 0)\}$. Thus, the eigenvalues of a random unitary matrix literally repel each other via electrostatic interactions in two dimensions, with the 2 in the exponent specifying the temperature of this system.

3. Families and universal optimality

Given that we are going to study particles interacting via pairwise potential functions, what do we hope to learn from it? There are many possibilities:
We may care about the ground states for their own sake, as part of pure mathematics or physics (see [11] for many examples in physics).

We may seek a highly uniform point distribution so that we can discretize the ambient space.

We may wish to construct error-correcting codes by letting the codewords repel each other, so that they become well separated.

We may seek well-distributed sample points for numerical integration.

To account for these and other goals, we will have to look at a broad range of potential functions.

There are also many spaces we could work in, such as spheres, projective spaces, Grassmannians, Euclidean spaces, hyperbolic spaces, and even discrete spaces such as the Hamming cube \( \{0,1\}^n \). All of these possibilities are interesting, but in this lecture we will focus on spheres. (For comparison, [24] and [20] examine spaces that are rather different from spheres.)

Thus, we will focus on the question of what energy minima on spheres look like for a variety of potential functions. As we vary the potential function, how do the optimal configurations change? They vary in some family, and we would like to understand these families. Note that our perspective here is broader than is typical for physics, where the potential function is usually fixed in advance.

The simplest case is that the optimal configurations never vary, at least for reasonable potential functions, such as inverse power laws.\(^{1}\) For example, 4 points on \( S^2 \) always form a regular tetrahedron. Abhinav Kumar and I named this property universal optimality [17].

More generally, we can ask for a parameter count for the family, which is 0 for universal optima. As we vary the potential function (say, among all smooth functions), what is the dimension of the space of configurations attained as ground states? There is little hope of proving much about this quantity in general. However, we can try to estimate it from numerical data [8]. These parameter counts can be difficult to predict, because they take into account how well the number of points accommodates different sorts of symmetry. For example, 44 points on \( S^2 \) vary in a one-parameter family near the putative Coulomb minimizer when we perturb the potential function, while 43 points vary in a 21-parameter family. See Figure 1 for an illustration. What this means is that the 44-point configuration is nearly determined by symmetry, with just one degree of freedom remaining to be specified by the choice of potential function, while the 43-point configuration is far more complex.

To give a precise definition of universal optimality, we must specify the class of potential functions. For a finite subset \( C \subset S^{n-1} \) and a function \( f: (0,4] \to \mathbb{R} \), we define the energy of \( C \) with respect to the potential function \( f \) to be

\[
E_f(C) = \frac{1}{2} \sum_{\substack{x,y \in C \\quad x \neq y}} f(|x-y|^2).
\]

The factor of 1/2 simply corrects for counting each pair twice and is not important. The use of squared Euclidean distance similarly doesn’t matter in principle, since

---

\(^{1}\)Of course it is impossible for a configuration of more than one point to be a ground state for literally every potential function, since minimizing \( f \) is the same as maximizing \( -f \). We must restrict the class of potential functions at least somewhat.
the squaring could be incorporated into the potential function, but it turns out to be a surprisingly useful convention.

A function $f$ is completely monotonic if it is infinitely differentiable and

$(-1)^k f^{(k)} \geq 0$

for all $k \geq 0$ (i.e., its derivatives alternate in sign, as in inverse power laws). We say $C$ is universally optimal if it minimizes $E_f(C)$ for all completely monotonic $f$, compared with all $|C|$-point configurations on $S^{n-1}$.

It's not obvious that completely monotonic functions are the right class of functions to use, but they turn out to be. The fact that $f$ is decreasing means the force is repulsive, and convexity means the force grows stronger at short distances. Complete monotonicity is a natural generalization of these conditions, and the results and examples in [17] give evidence that it is the right generalization (see pages 101 and 107–108). Note in particular that inverse power laws are completely monotonic, so universal optima must minimize energy for all inverse power laws.

In the circle $S^1$, there is a universal optimum of each size, namely the regular polygon. This is not as straightforward to prove as it sounds, but it follows from Theorem 1.2 in [17], which we will state as Theorem 3.3 in the fourth lecture. In $S^2$, the complete list of universal optima with more than one point is as follows:

1. Two antipodal points (2 points)
2. Equilateral triangle on equator (3 points)
3. Regular tetrahedron (4 points)
4. Regular octahedron (6 points)
5. Regular icosahedron (12 points)

See Figure 2. Universal optimality again follows from Theorem 1.2 in [17] (after special cases were proved in [81, 44, 2, 45, 3]), while completeness follows from a theorem of Leech in [48].
The cube and regular dodecahedron are conspicuously missing from this list. The cube cannot be universally optimal, because rotating one face moves its corners further from those of the opposite face, and the dodecahedron fails similarly. Square and pentagonal faces are not particularly favorable shapes for energy minimization, although cubes and dodecahedra can occur for unusual potential functions \cite{19}.

Five points are the first case without universal optimality, and they are surprisingly subtle. There are two natural ways to arrange the particles: we could include the north and south poles together with an equilateral triangle on the equator (a *triangular bipyramid*), or the north pole together with a square at constant latitude in the southern hemisphere (a *square pyramid*). The square pyramid lies in a one-parameter family, where the latitude of the square depends on the choice of potential function. By contrast, the triangular bipyramid is in equilibrium for every potential function, but it becomes an unstable equilibrium for steep inverse power laws.

**Conjecture 3.1.** For each completely monotonic potential function, either the triangular bipyramid or a square pyramid minimizes energy for 5 points in $S^2$.

This conjecture really feels like it ought to be provable. Specifying five points on $S^2$ takes ten degrees of freedom, three of which are lost if we take the quotient by symmetries. Thus, we are faced with a calculus problem in just seven variables. However, despite a number of partial results \cite{30, 67, 10, 68}, no complete solution is known.

The known universal optima in spheres are listed in Table 1. Each of them is an exciting mathematical object that predates the study of universal optimality. For example, the 27 points in $\mathbb{R}^6$ correspond to the classical configuration of 27 lines on a cubic surface. One way of thinking about universal optimality is that it highlights similarities between various exceptional structure and helps characterize what’s so special about them. See \cite{17} for descriptions of these objects and how they are related. We’ll discuss the proof techniques in the fourth lecture, while \cite{17} contains detailed proofs.

One important source of universal optima is regular polytopes, the higher-dimensional generalizations of the Platonic solids. As in three dimensions, only some of them are universally optimal, specifically the ones with simplicial facets.$^2$

\footnote{Surprisingly, the minimal vectors of $D_4$ are not universally optimal \cite{14}, despite their beauty and symmetry. They are the vertices of a regular polytope with octahedral facets, called the regular 24-cell.}
Table 1. Known universal optima with \( N \) points on \( S^{n-1} \).

| \( n \) | \( N \) | Description |
|-------|-------|-------------|
| 2     | \( N \) | \( N \)-gon |
| \( n \) | \( N \leq n + 1 \) | simplex (generalized tetrahedron) |
| \( n \) | \( 2n \) | cross polytope (generalized octahedron) |
| 3     | 12    | icosahedron |
| 4     | 120   | regular 600-cell |
| 5     | 16    | hemicube |
| 6     | 27    | Schlӓfi graph |
| 7     | 56    | equiangular lines |
| 8     | 240   | \( E_8 \) root system |
| 21    | 112   | isotropic subspaces |
| 21    | 162   | strongly regular graph |
| 22    | 100   | Higman-Sims graph |
| 22    | 275   | McLaughlin graph |
| 23    | 891   | isotropic subspaces |
| 23    | 552   | equiangular lines |
| 23    | 4600  | kissing configuration of next line |
| 24    | 196560 | Leech lattice minimal vectors |

\[ q(q^3 + 1)/(q + 1)(q + 1)(q^3 + 1) \] isotropic subspaces (\( q \) is a prime power)

The shortest vectors in the \( E_8 \) lattice (called the \( E_8 \) root system) also form a universally optimal configuration, as do the shortest vectors in the Leech lattice.

It is difficult to depict high-dimensional objects on a two-dimensional page, but Figure 3 shows how the \( E_8 \) root system appears when viewed from random directions. It is so regular and symmetrical that even these random views display considerable structure. For comparison, Figure 4 shows similar projections of a random point configuration.

In up to 24 dimensions, all of the known universal optima are regular polytopes or cross sections of the \( E_8 \) or Leech configurations. However, the last line of Table 1 shows that there are more examples coming from finite geometry. It’s not plausible that Table 1 is the complete list of universal optima, and in fact \( q \) constructs two conjectural examples (40 points in \( \mathbb{R}^{10} \) and 64 points in \( \mathbb{R}^{14} \)), but it seems difficult to find or analyze further universal optima.

The gap between \( 8 \) and \( 21 \) dimensions in Table 1 is puzzling. Are the dimensions in between not favored by universal optimality, or do we just lack the imagination to construct new universal optima in these dimensions?

4. Optimality of simplices

It is not difficult to explore energy minimization via numerical optimization, but it is far from obvious how to prove anything about it. Developing proof techniques will occupy most of the remaining lectures, and we will start here by analyzing regular simplices, i.e., configurations of equidistant points.

In particular, we will study the spherical code problem: how can we maximize the closest distance between \( N \) points on the unit sphere \( S^{n-1} \)? This is an important
Figure 3. Four views of the $E_8$ root system, after orthogonal projection onto randomly chosen planes.

Figure 4. A random 240-point configuration in $S^7$, orthogonally projected onto randomly chosen planes.

It is a version of the sphere packing problem in spherical geometry, i.e., for spherical caps on the surface of a sphere. Furthermore, it is a degenerate case of energy minimization. If we look at the limit of increasingly steep potential functions, then asymptotically only the minimal distance matters and we obtain an optimal spherical code.

If we represent radio signals by vectors in $\mathbb{R}^n$ by measuring the amplitudes at different frequencies, then the squared vector length is proportional to the power of the radio signal. If we transmit a constant-power signal, then we need an error-correcting code on the surface of a sphere, i.e., a spherical code.
When $N \leq n + 1$, we will see shortly that the optimal solution is a regular simplex. In other words, the points are all equidistant from each other, forming an $n$-dimensional analogue of the equilateral triangle or regular tetrahedron. The cutoff at $n + 1$ simply reflects the fact that $\mathbb{R}^n$ cannot contain more than $n + 1$ equidistant points.

Let $\langle x, y \rangle$ denote the inner product of $x$ and $y$. Inner products can be used to measure distances on the unit sphere, since

$$|x - y|^2 = \langle x - y, x - y \rangle = |x|^2 + |y|^2 - 2\langle x, y \rangle = 2 - 2\langle x, y \rangle$$

when $|x| = |y| = 1$. Thus, maximizing the distance $|x - y|$ is equivalent to minimizing the inner product $\langle x, y \rangle$.

Note that if $x_1, \ldots, x_N$ are unit vectors forming the vertices of a regular simplex centered at the origin, then all the inner products between them must be $-1/(N-1)$.

To see why, observe that $x_1 + \cdots + x_N = 0$ and hence

$$0 = |x_1 + \cdots + x_N|^2 = N + \sum_{i \neq j} \langle x_i, x_j \rangle,$$

while all the $N(N-1)$ inner products in this sum are equal. This calculation already contains all the ingredients needed to prove that regular simplices are optimal spherical codes:

**Proposition 4.1.** If $N \leq n + 1$, then the unique optimal $N$-point spherical code in $S^{n-1}$ is the regular simplex centered at the origin.

Of course it is unique only up to rigid motions.

**Proof.** Suppose $x_1, \ldots, x_N$ are points on $S^{n-1}$. The fundamental inequality we'll use is

$$\left| \sum_{i=1}^N x_i \right|^2 \geq 0.$$

Using $|x_i|^2 = 1$, this inequality expands to

$$N + \sum_{i \neq j} \langle x_i, x_j \rangle \geq 0,$$

which amounts to

$$\frac{1}{N(N-1)} \sum_{i \neq j} \langle x_i, x_j \rangle \geq -\frac{1}{N-1}.$$

In other words, the average inner product is at least $-1/(N-1)$, and hence the maximal inner product (which corresponds to the minimal distance) must be at least that large. Equality holds iff all the inner products are the same and $\sum_i x_i = 0$. This condition is equivalent to all the points being equidistant with centroid at the origin, which can be achieved iff $N \leq n + 1$. \qed

**Exercise 4.2.** Prove that regular simplices are universally optimal, and more generally that they minimize $E_f$ for every decreasing, convex potential function $f$.

Our discussion here may give the impression that the existence of regular simplices is trivial, while their optimality is a little more subtle. This impression is reasonable for Euclidean space, but in projective spaces or Grassmannians the existence of regular simplices is far more mysterious. See, for example, [20].
The inequality
\[ \left| \sum_{i=1}^{N} x_i \right|^2 \geq 0 \]
is useful for analyzing simplices, but it is not obvious at a glance what its significance is or how it fits into a broader theory. It turns out to be a special case of Delsarte’s linear programming bounds, which are also equivalent to the nonnegativity of the structure factor in statistical physics. In the upcoming lectures, we’ll look at these connections. The fundamental theme will be geometrical constraints on correlation functions.
Lecture 3

Interlude: Spherical harmonics

Spherical harmonics are a spherical generalization of Fourier series and a fundamental tool for understanding particle configurations on the surface of a sphere. Despite their importance in mathematics, they are not nearly as well known as Fourier series are, so this lecture will be devoted to the basic theory. We’ll begin with a quick review of Fourier series, to establish notation and fundamental concepts, and then we’ll do the same things in higher dimensions. Our discussion will start off in a rather elementary fashion, but then gradually increase in sophistication. We won’t go through complete proofs of basic facts such as convergence of Fourier series under the $L^2$ norm, but we will at least see an outline of what is true and why, to a level of detail at which the proofs could be completed using standard facts from introductory graduate classes.

1. Fourier series

We will identify the circle $S^1$ with the quotient $\mathbb{R}/2\pi\mathbb{Z}$ via arc length (i.e., the quotient of the real line in which we wrap around after $2\pi$ units). In other words, a function on the circle is the same as a function on $\mathbb{R}$ with period $2\pi$.

We know from basic analysis that every sufficiently nice function $f$ from $\mathbb{R}/2\pi\mathbb{Z}$ to $\mathbb{C}$ can be expanded in a Fourier series

$$f(x) = \sum_{k \in \mathbb{Z}} a_k e^{ikx}.$$  \hspace{1cm} (1.1)

Of course we could replace the complex exponentials with trigonometric functions by writing $e^{ikx} = \cos kx + i \sin kx$, but the exponentials will be more pleasant.

The coefficients $a_\ell$ are determined by orthogonality via

$$a_\ell = \frac{1}{2\pi} \int_0^{2\pi} f(x)e^{-i\ell x} \, dx,$$

because we can interchange the sum (1.1) with the integral and apply

$$\frac{1}{2\pi} \int_0^{2\pi} e^{i(k-\ell)x} \, dx = \begin{cases} 1 & \text{if } k = \ell, \\ 0 & \text{otherwise}. \end{cases}$$  \hspace{1cm} (1.2)

The right setting for Fourier series is the space of square-integrable functions on $S^1$, i.e.,

$$L^2(S^1) = \left\{ f : \mathbb{R}/2\pi\mathbb{Z} \to \mathbb{C} \mid \int_0^{2\pi} |f(x)|^2 \, dx < \infty \right\}.$$  

This is a Hilbert space under the inner product $\langle \cdot, \cdot \rangle$ defined by

$$\langle f, g \rangle = \frac{1}{2\pi} \int_0^{2\pi} f(x)g(x) \, dx,$$  

27
which corresponds to the $L^2$ norm $\| \cdot \|_2$ defined by

$$\| f \|_2 = \sqrt{\langle f, f \rangle} = \sqrt{\frac{1}{2\pi} \int_0^{2\pi} |f(x)|^2 \, dx}.$$  

The exponential functions are orthonormal in $L^2(S^1)$: if $f_k$ is the function defined by $f_k(x) = e^{ikx}$, then (1.2) amounts to

$$\langle f_k, f_\ell \rangle = \begin{cases} 1 & \text{if } k = \ell, \\ 0 & \text{otherwise.} \end{cases}$$

Furthermore, these functions form an orthonormal basis of $L^2(S^1)$.

We can express this fact algebraically as follows. If $V_k$ consists of the complex multiples of the function $f_k$, then

$$L^2(S^1) = \bigoplus_{k \in \mathbb{Z}} V_k.$$  

(Here $\oplus$ is the orthogonal direct sum. The hat indicates a Hilbert space completion; without the hat, the direct sum would contain only sums of finitely many exponentials.) In other words, the partial sums of the Fourier series of an $L^2$ function converge to that function under the $L^2$ norm. However, it’s important to keep in mind that they needn’t converge pointwise.

The most important property of the decomposition

$$L^2(S^1) = \bigoplus_{k \in \mathbb{Z}} V_k.$$  

is that it is compatible with the symmetries of $S^1$ (i.e., the rigid motions that preserve $S^1$), as we will see shortly. Recall that the symmetry group $O(2)$ of $S^1$ consists of rotations and reflections that fix the center of the circle, with the subgroup $SO(2)$ consisting of just the rotations. The notation is based on the fact that these symmetries can be written in terms of orthogonal matrices, but we do not need that perspective here.

Each symmetry $g$ of $S^1$ acts on functions $f: S^1 \to \mathbb{C}$ by sending $f$ to the function $gf$ defined by $(gf)(x) = f(g^{-1}x)$. The inverse ensures that the associative law $(gh)f = g(hf)$ holds. For motivation, recall that moving the graph of a function $f(x)$ one unit to the right amounts to graphing $f(x-1)$, not $f(x+1)$. Similarly, the graph of $gf$ is simply the graph of $f$ transformed according to $g$.

Under this action, $L^2(S^1)$ is a representation of the group $O(2)$. In other words, the group $O(2)$ acts on $L^2(S^1)$ by linear transformations. In fact, it is a unitary representation, which means that symmetries of $S^1$ preserve the $L^2$ norm. We would like to decompose $L^2(S^1)$ into irreducible representations of $O(2)$ or $SO(2)$. In other words, we would like to break it apart into orthogonal subspaces preserved by these groups, with the subspaces being as small as possible.

For the rotation group $SO(2)$, we’re already done. In the $\mathbb{R}/2\pi\mathbb{Z}$ picture, rotations of $S^1$ correspond to translations of $\mathbb{R}$. The exponential functions are already invariant: if we translate $x \mapsto e^{ikx}$ by $t$, we get

$$e^{ik(x-t)} = e^{-ikt} e^{ikx}.$$
which is the original function \( x \mapsto e^{ikx} \) multiplied by the constant \( e^{-ikt} \). In other words, \( V_k \) is itself a representation of \( SO(2) \), and

\[
L^2(S^1) = \bigoplus_{k \in \mathbb{Z}} V_k
\]

is the complete decomposition of \( L^2(S^1) \) under this group action. Each summand must be irreducible, since it’s one-dimensional.

There are many ways to restate this decomposition, such as:

1. The Fourier basis simultaneously diagonalizes the translation operators on \( L^2(\mathbb{R}/2\pi\mathbb{Z}) \) (i.e., rotations of \( L^2(S^1) \)).
2. The exponential functions are simultaneous eigenfunctions for the translation operators.

It turns out that the reason why the Fourier decomposition is particularly simple, with one-dimensional summands, is that the rotation group \( SO(2) \) is abelian.

But what about the full symmetry group \( O(2) \)? It is generated by \( SO(2) \) and any one reflection, because all the reflections are conjugate by rotations. In the \( \mathbb{R}/2\pi\mathbb{Z} \) picture, we can use the reflection \( x \mapsto -x \). The nonconstant exponential functions are not preserved by this reflection, because it takes \( x \mapsto e^{ikx} \) to \( x \mapsto e^{-ikx} \). In other words, it interchanges \( k \) with \( -k \).

However, this is no big deal. Instead of keeping the representations \( V_k \) and \( V_{-k} \) separate, we combine them to form \( W_k = V_k \oplus V_{-k} \) when \( k > 0 \) (while we take \( W_0 = V_0 \)). Now \( W_k \) is the span of \( x \mapsto e^{ikx} \) and \( x \mapsto e^{-ikx} \), or equivalently \( x \mapsto \cos kx \) and \( x \mapsto \sin kx \) if we expand \( e^{\pm ikx} = \cos kx \pm i\sin kx \). These spaces \( W_k \) are preserved by \( O(2) \), because this group is generated by \( SO(2) \) and \( x \mapsto -x \). Thus, the decomposition of \( L^2(S^1) \) into irreducible representations of \( O(2) \) is

\[
L^2(S^1) = \bigoplus_{k \geq 0} W_k.
\]

This decomposition is just slightly more complicated than the one for \( SO(2) \), because \( \dim W_k = 2 \) when \( k > 0 \).

Another way to think of this equation is as the spectral decomposition of the Laplacian operator \( d^2/dx^2 \). Specifically,

\[
\frac{d^2}{dx^2}e^{ikx} = -k^2 e^{ikx}.
\]

Thus, \( W_k \) is the eigenspace with eigenvalue \(-k^2\). The Laplacian plays a fundamental role, since it is invariant under the action of \( O(2) \). (In other words, translating or reflecting a function commutes with taking its Laplacian.) In fact, the Laplacian generates the algebra of isometry-invariant differential operators on \( S^1 \), but that’s going somewhat far afield from anything we will need.

### 2. Fourier series on a torus

The \( S^1 \) theory generalizes pretty straightforwardly if we think of \( S^1 \) as a one-dimensional torus. We can view a higher-dimensional flat torus as \( \mathbb{R}^n/\Lambda \), where \( \Lambda \) is a lattice in \( \mathbb{R}^n \). In other words, we simply take a fundamental cell for \( \Lambda \) and wrap around whenever we cross the boundary. When we looked at \( S^1 \), we wrote it as \( \mathbb{R}^1/\Lambda \) with \( \Lambda = 2\pi\mathbb{Z} \), and it’s worth keeping this example in mind.
We can decompose $L^2(\mathbb{R}^n/\Lambda)$ into exponential functions in exactly the same way as we did for $S^1$. It works out particularly simply since $\mathbb{R}^n/\Lambda$ is an abelian group. To write this decomposition down, we need to figure out which exponential functions are periodic modulo $\Lambda$. Suppose $y \in \mathbb{R}^n$, and consider the exponential function $x \mapsto e^{2\pi i \langle x, y \rangle}$ from $\mathbb{R}^n$ to $\mathbb{C}$. Here $\langle \cdot, \cdot \rangle$ denotes the usual inner product on $\mathbb{R}^n$ (not the inner product on functions used in the previous section). This formula defines a function on $\mathbb{R}^n/\Lambda$ if and only if it is invariant under translation by vectors in $\Lambda$.

What happens if we translate the function $x \mapsto e^{2\pi i \langle x, y \rangle}$ by a vector $z$? It gets multiplied by $e^{-2\pi i \langle z, y \rangle}$, and so it is always an eigenfunction of the translation operator. Furthermore, it is invariant under translation by vectors in $\Lambda$ if and only if $y$ satisfies

$$e^{2\pi i \langle z, y \rangle} = 1$$

for all $z \in \Lambda$, which is equivalent to $\langle z, y \rangle \in \mathbb{Z}$ for all $z \in \Lambda$.

Let $\Lambda^\ast = \{ y \in \mathbb{R}^n \mid \langle z, y \rangle \in \mathbb{Z} \text{ for all } z \in \Lambda \}$ be the dual lattice to $\Lambda$. Thus, the exponential functions that are periodic modulo $\Lambda$ are parameterized by $\Lambda^\ast$.

**Exercise 2.1.** Prove that $\Lambda^\ast$ is a lattice. Specifically, prove that if $v_1, \ldots, v_n$ is any basis of $\Lambda$, then $\Lambda^\ast$ has $v_1^\ast, \ldots, v_n^\ast$ as a basis, where these vectors are the dual basis vectors satisfying

$$\langle v_i, v_j^\ast \rangle = \begin{cases} 1 & \text{if } i = j, \text{ and} \\ 0 & \text{otherwise}. \end{cases}$$

Deduce also that $(\Lambda^\ast)^\ast = \Lambda$.

Let $V_y$ be the complex multiples of $x \mapsto e^{2\pi i \langle x, y \rangle}$. Then

$$L^2(\mathbb{R}^n/\Lambda) = \bigoplus_{y \in \Lambda^\ast} V_y,$$

which is the decomposition into irreducible representations under the translation action.

When $n = 1$, the lattice $\Lambda$ is determined up to scaling. In the previous section we took $\Lambda = 2\pi \mathbb{Z}$, in which case $\Lambda^\ast = (2\pi)^{-1}\mathbb{Z}$. The elements of $\Lambda^\ast$ are $(2\pi)^{-1}k$, where $k$ is an integer, and $V_{(2\pi)^{-1}k}$ is spanned by $x \mapsto e^{ikx}$. Thus, we recover exactly the same theory as in the previous section, except that we now write $V_{(2\pi)^{-1}k}$ instead of $V_k$. It’s arguably prettier to take $\Lambda = \mathbb{Z}$ and use the functions $x \mapsto e^{2\pi i k x}$, but this is a matter of taste.

The higher-dimensional analogue of the $O(2)$ theory is a little more subtle. The map $x \mapsto -x$ is always a symmetry of $\mathbb{R}^n/\Lambda$, and taking it into account means combining $V_y$ with $V_{-y}$ as before. Generically, all the symmetries of $\mathbb{R}^n/\Lambda$ are generated by translations and $x \mapsto -x$. However, particularly nice lattices may have further symmetries. If $G$ is the automorphism group of the lattice itself, then the full group of isometries of $\mathbb{R}^n/\Lambda$ is the semidirect product of $G$ with the additive group $\mathbb{R}^n/\Lambda$. What effect this has on the decomposition of $L^2(\mathbb{R}^n/\Lambda)$ depends on the representation theory of $G$. However, for many purposes this is not important, and the decomposition under translations alone will suffice.
3. Spherical harmonics

If we think of $S^1$ as a one-dimensional sphere, rather than a one-dimensional torus, then it is less clear how to generalize Fourier series. Instead of exponential functions, we’ll have to use spherical harmonics.

The symmetry group of the unit sphere

$$ S^{n-1} = \{ x \in \mathbb{R}^n \mid |x|^2 = 1 \} $$

is the orthogonal group $O(n)$, which consists of $n \times n$ orthogonal matrices. As before, $L^2(S^{n-1})$ is a Hilbert space under the inner product

$$ \langle f, g \rangle = \int_{S^{n-1}} f(x) g(x) \, dx, $$

where the integral is taken with respect to the surface measure on $S^{n-1}$, and $L^2(S^{n-1})$ is a unitary representation of $O(n)$. We would like to decompose it into irreducible representations of $O(n)$.

To get a handle on $L^2(S^{n-1})$, we will study the polynomials on $S^{n-1}$. Let $\mathcal{P}_k$ be the subset of $L^2(S^{n-1})$ consisting of polynomials on $\mathbb{R}^n$ of total degree at most $k$. (Strictly speaking, it consists of the restrictions of these polynomials to $S^{n-1}$, since two different polynomials can define the same function on the unit sphere.) Then

$$ \mathcal{P}_0 \subseteq \mathcal{P}_1 \subseteq \mathcal{P}_2 \subseteq \ldots, $$

and each $\mathcal{P}_k$ is a representation of $O(n)$. To see why, note that rotating or reflecting a polynomial gives another polynomial of the same degree; in fact, this is true for any invertible linear transformation.

Let $W_0 = \mathcal{P}_0$, and for $k > 0$ let $W_k$ be the orthogonal complement of $\mathcal{P}_{k-1}$ in $\mathcal{P}_k$. Then $W_k$ is a representation of $O(n)$, because $\mathcal{P}_{k-1}$ and $\mathcal{P}_k$ are representations and the inner product in $L^2(S^{n-1})$ is $O(n)$-invariant. Iterating this decomposition shows that

$$ \mathcal{P}_k = W_0 \oplus W_1 \oplus \cdots \oplus W_k. $$

Furthermore, $\bigcup_k \mathcal{P}_k$ is dense in $L^2(S^{n-1})$, and hence

$$ L^2(S^{n-1}) = \bigoplus_{k \geq 0} W_k. $$

We have thus decomposed $L^2(S^{n-1})$ into finite-dimensional representations of $O(n)$. In fact they are irreducible, as we will see in the next lecture, but that fact is by no means obvious.

This decomposition may sound abstract, but it’s actually quite elementary, since it is simply given by polynomials. Let’s check that it agrees with what we did for $S^1$. Polynomials on $\mathbb{R}^2$ can be written in terms of the coordinate variables $x$ and $y$, and in the $\mathbb{R}/2\pi \mathbb{Z}$ picture we have $x = \cos \theta$ and $y = \sin \theta$ with $\theta \in \mathbb{R}/2\pi \mathbb{Z}$. Thus, $\mathcal{P}_k$ consists of polynomials of degree at most $k$ in the functions $\theta \mapsto \cos \theta$ and $\theta \mapsto \sin \theta$. If we write $\cos \theta = (e^{i\theta} + e^{-i\theta})/2$ and $\sin \theta = (e^{i\theta} - e^{-i\theta})/(2i)$, then we find that the elements of $\mathcal{P}_k$ involve powers of $e^{i\theta}$ ranging from $-k$ to $k$, and every such power is in $\mathcal{P}_k$. In other words,

$$ \mathcal{P}_k = V_{-k} \oplus V_{-(k-1)} \oplus \cdots \oplus V_{k-1} \oplus V_k $$

1Continuous functions are dense in $L^2(S^{n-1})$, and the Stone-Weierstrass theorem tells us that polynomials are dense in the space of continuous functions.
in the notation from [11]. In particular, the orthogonal complement $W_k$ of $P_{k-1}$ in $P_k$ is indeed $V_{-k} \oplus V_k$ when $k > 0$, which agrees with our previous construction.

Returning to $L^2(S^{n-1})$, we call the elements of $W_k$ spherical harmonics of degree $k$. Note that the word "harmonic" generalizes the term from music theory for a note whose frequency is an integer multiple of the base frequency; this term literally describes $W_k$ when $n = 2$, and it is applied by analogy in higher dimensions.

Writing $W_k$ down explicitly is a little subtle, because two different polynomials on $\mathbb{R}^n$ can restrict to the same function on $S^{n-1}$. For example, $x_1^2 + \cdots + x_n^2$ and $1$ are indistinguishable on the unit sphere. To resolve this ambiguity, we will choose a canonical representative for each equivalence class.

**Lemma 3.1.** For each polynomial on $\mathbb{R}^n$, there is a unique harmonic polynomial on $\mathbb{R}^n$ with the same restriction to $S^{n-1}$.

Recall that harmonic means $\Delta g = 0$, where

$$\Delta = \frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_n^2}$$

is the Laplacian on $\mathbb{R}^n$. If $f$ is a harmonic polynomial with $f|_{S^{n-1}} = g|_{S^{n-1}}$, then $f$ is called a harmonic representative for $g$.

The main fact we’ll need about harmonic functions is the maximum principle [4, p. 7]: the maximum of a harmonic function on a domain $D$ cannot occur in the interior of $D$ (instead, it must occur on the boundary). Of course, multiplying the function by $-1$ shows that the same is true for the minimum.

**Proof.** Uniqueness follows immediately from the maximum principle: if $g_1|_{S^{n-1}} = g_2|_{S^{n-1}}$ with both $g_1$ and $g_2$ harmonic, then $g_1 - g_2$ is a harmonic function that vanishes on $S^{n-1}$. It must therefore vanish inside the sphere as well (since its minimum and maximum over the ball must be attained on the sphere), which implies that $g_1 = g_2$ because they are polynomials.

Proving existence of a harmonic representative is only slightly trickier. Let $Q_k$ denote the space of polynomials of degree at most $k$ on $\mathbb{R}^n$. Note that the difference between $P_k$ and $Q_k$ is that $P_k$ consists of the restrictions to $S^{n-1}$, and thus $P_k$ is the quotient of $Q_k$ by the polynomials whose restrictions vanish. Multiplication by $x_1^2 + \cdots + x_n^2 - 1$ maps $Q_{k-2}$ injectively to $Q_k$, and its image vanishes on $S^{n-1}$, so

$$\dim P_k \leq \dim Q_k - \dim Q_{k-2}.$$ 

On the other hand, $\Delta$ maps $Q_k$ to $Q_{k-2}$, and hence

$$\dim \ker \Delta|_{Q_k} \geq \dim Q_k - \dim Q_{k-2} \geq \dim P_k.$$ 

By uniqueness, the restriction map from $\ker \Delta|_{Q_k}$ to $P_k$ is injective, and thus the inequality $\dim \ker \Delta|_{Q_k} \geq \dim P_k$ implies that each polynomial in $P_k$ must have a harmonic representative (and $\dim \ker \Delta|_{Q_k} = \dim P_k$).

Another way to understand spherical harmonics is as eigenfunctions of the spherical Laplacian $\Delta_{S^{n-1}}$, which acts on $C^2$ functions on the sphere (i.e., twice continuously differentiable functions). The right setting for this operator is the theory of Laplace-Beltrami operators in Riemannian geometry, but we can give a
quick, ad hoc definition as follows. Given a function \( f \) on \( S^{n-1} \), extend it to a radially constant function \( f_{\text{radial}} \) on \( \mathbb{R}^n \setminus \{0\} \). Then we define \( \Delta_{S^{n-1}} \) by

\[
\Delta_{S^{n-1}} f = \left( \Delta f_{\text{radial}} \right) \big|_{S^{n-1}}.
\]

In other words, \( \Delta_{S^{n-1}} f \) measures the Laplacian of \( f \) when there is no radial change.

It is often notationally convenient to extend the operator \( \Delta_{S^{n-1}} \) to apply to functions \( f: \mathbb{R}^n \setminus \{0\} \to \mathbb{R} \), rather than just functions defined on the unit sphere. We can do so by rescaling everything to the unit sphere. More precisely, to define \( \Delta_{S^{n-1}} f \) at the point \( x \), we consider the function \( g: S^{n-1} \to \mathbb{R} \) defined by \( g(y) = f(|x|y) \), and we let

\[
\Delta_{S^{n-1}} f(x) = \Delta_{S^{n-1}} g(x/|x|).
\]

The advantage of being able to apply \( \Delta_{S^{n-1}} \) to functions on \( \mathbb{R}^n \setminus \{0\} \) is that it becomes the angular part of the Euclidean Laplacian in spherical coordinates:

**Exercise 3.2.** Prove that if \( r \) denotes the distance to the origin and \( \partial/\partial r \) is the radial derivative, then for every \( C^2 \) function \( f: \mathbb{R}^n \to \mathbb{R} \),

\[
\Delta f = \frac{\partial^2 f}{\partial r^2} + \frac{n - 1}{r} \frac{\partial f}{\partial r} + \frac{1}{r^2} \Delta_{S^{n-1}} f
\]

when \( r \neq 0 \).

If \( f \) is homogeneous of degree \( k \), then (3.1) becomes

\[
\Delta f = \frac{k(k - 1)f}{r^2} + \frac{(n - 1)k}{r^2} + \frac{1}{r^2} \Delta_{S^{n-1}} f.
\]

Then \( \Delta f = 0 \) is equivalent to \( \Delta_{S^{n-1}} f = -k(k + n - 2)f \). In other words, harmonic functions that are homogeneous of degree \( k \) are eigenfunctions of the spherical Laplacian with eigenvalue \( -k(k + n - 2) \). We will see shortly that the spherical harmonics in \( W_k \) are all homogeneous of degree \( k \), and thus that the spaces \( W_k \) are the eigenspaces of \( \Delta_{S^{n-1}} \).

First note, that the Euclidean Laplacian maps homogeneous polynomials of degree \( k \) to homogeneous polynomials of degree \( k - 2 \). Thus, every harmonic polynomial is the sum of homogeneous harmonics.

In terms of spherical harmonics, \( P_k \) is the sum of the eigenspaces of \( \Delta_{S^{n-1}} \) with eigenvalues \( -\ell(\ell + n - 2) \) for \( \ell = 0, 1, \ldots, k \). These eigenspaces are orthogonal, because the spherical Laplacian is symmetric:

**Lemma 3.3.** For \( C^2 \) functions \( f \) and \( g \) on \( S^{n-1} \),

\[
\langle f, \Delta_{S^{n-1}} g \rangle = \langle \Delta_{S^{n-1}} f, g \rangle.
\]

**Proof.** This identity is well-known for the Laplace-Beltrami operator, but verifying it using our ad hoc definition takes a short calculation. Replace \( f \) and \( g \) with their radial extensions to \( \mathbb{R}^n \setminus \{0\} \), and let

\[
\Omega = \{ x \in \mathbb{R}^n \mid 1/2 \leq |x| \leq 2 \}.
\]

Equation (3.1) implies that

\[
(\langle f, \Delta_{S^{n-1}} g \rangle - \langle \Delta_{S^{n-1}} f, g \rangle) \int_{1/2}^2 \omega_{n-1} r^{n-3} \, dr = \int_{\Omega} f \Delta g - g \Delta f,
\]

where the integral over \( \Omega \) is with respect to Lebesgue measure and \( \omega_{n-1} \) is the surface area of \( S^{n-1} \). In this equation, \( \omega_{n-1} r^{n-3} \) combines the volume factor from spherical coordinates with the \( 1/r^2 \) factor multiplying \( \Delta_{S^{n-1}} f \) in (3.1).
Now Green’s identity tells us that
\[
\int_\Omega f \Delta g - g \Delta f = \int_{\partial \Omega} f \frac{\partial g}{\partial n} - g \frac{\partial f}{\partial n},
\]
where \( \frac{\partial}{\partial n} \) denotes the normal derivative and the integral over \( \partial \Omega \) is with respect to surface measure. It vanishes because \( \frac{\partial f}{\partial n} = \frac{\partial g}{\partial n} = 0 \) by construction.

Because \( P_k \) is the sum of the eigenspaces of \( \Delta_{S^{n-1}} \) with eigenvalues \( -\ell(\ell + n - 2) \) for \( \ell = 0, 1, \ldots, k \) and these eigenspaces are orthogonal, the orthogonal complement of \( P_{k-1} \) in \( P_k \) must be the \( -k(k + n - 2) \) eigenspace. Thus, \( W_k \) consists of the harmonic polynomials that are homogeneous of degree \( k \). This gives a rather concrete, if cumbersome, description of the space of spherical harmonics. By contrast, people sometimes make spherical harmonics look unnecessarily exotic by writing them in spherical coordinates as eigenfunctions of the Laplacian.

**Exercise 3.4.** Compute the homogeneous harmonic polynomials explicitly when \( n = 2 \), and check that this computation agrees with our earlier analysis of \( S^1 \).

We will see in the next lecture that \( W_k \) is an irreducible representation of \( O(n) \). Thus, we have found the complete decomposition of \( L^2(S^{n-1}) \) into irreducible representations, as well as the spectral decomposition of the Laplacian. The biggest conceptual difference from \( S^1 \) is that the space \( W_k \) of degree \( k \) spherical harmonics has much higher dimension than 2 in general, but that’s not an obstacle to using this theory.
LECTURE 4

Energy and packing bounds on spheres

1. Introduction

In this lecture, we will use spherical harmonics to prove bounds for packing and energy minimization on spheres. Our technique will be essentially the same as in the proof of Proposition 4.1 from the second lecture, but the bounds will be more sophisticated algebraically and much more powerful. By the end of the lecture we will be able to solve the kissing problem in $\mathbb{R}^8$ and $\mathbb{R}^{24}$, as well as analyze almost all of the known cases of universal optimality. In the next lecture we will tackle Euclidean space using much the same approach, but the analytic technicalities will be greater and it will be useful to have looked at the spherical case first.

Everything we do will be based on studying the distances that occur between pairs of points. Motivated by error-correcting codes, we call a finite subset $C$ of $S^{n-1}$ a code. The distance distribution of a code measures how often each pairwise distance occurs. For $-1 \leq t \leq 1$, define the distance distribution $A_t$ of $C$ by

$$A_t = \# \{(x, y) \in C^2 \mid \langle x, y \rangle = t\},$$

where $\langle \cdot, \cdot \rangle$ denotes the usual inner product on $\mathbb{R}^n$. Recall that $|x - y|^2 = 2 - \langle x, y \rangle$ when $x$ and $y$ are unit vectors; thus, $A_t$ counts the number of pairs at distance $\sqrt{2 - 2t}$, but inner products are a more convenient way to index these distances. In physics terms [75, p. 63], the distance distribution is equivalent to the pair correlation function, although it is formulated a little differently.

We can express the energy for a pair potential function $f$ in terms of the distance distribution via

$$\sum_{x, y \in C \atop x \neq y} f(|x - y|^2) = \sum_{-1 \leq t < 1} f(2 - 2t) A_t. \tag{1.1}$$

(In the sum on the right, there are uncountably many values of $t$, but only finitely many of the summands are nonzero. Note that the restriction to $t < 1$ is to avoid self-interactions; it corresponds to $x \neq y$ on the left.) Thus, figuring out which energies can be attained amounts to understanding what the possible pair correlation functions are. Which constraints must they satisfy?

We have made an important trade-off here. The dependence of energy on the distance distribution is as simple as possible, because the right side of (1.1) is a linear function of the variables $A_t$. However, the nonlinearity in this problem cannot simply disappear. Instead, it reappears in the question of which distance distributions occur for actual point configurations.

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1 Analogous techniques work in various other settings, such as projective spaces or Grassmannians.
There are some obvious constraints for an \(N\)-point code: \(A_t \geq 0\) for all \(t\), \(A_1 = N\), and \(\sum_t A_t = N^2\). They follow trivially from the definition
\[
A_t = \# \{(x, y) \in C^2 \mid \langle x, y \rangle = t\}.
\]

Another obvious constraint is that \(A_t\) must be an integer for each \(t\), but we will generally ignore this constraint, because optimization theory does not handle integrality constraints as seamlessly as it handles inequalities.

There are also less obvious constraints, such as
\[
\sum_t A_t t \geq 0.
\]
To see why this inequality holds, note that
\[
\sum_t A_t t = \sum_{x, y \in C} \langle x, y \rangle,
\]
because \(A_t\) counts how often \(t\) occurs as an inner product between points in \(C\). Thus,
\[
\sum_t A_t t = \sum_{x, y \in C} \langle x, y \rangle = \left(\sum_{x \in C} x, \sum_{y \in C} y\right) = \sum_{x \in C} x^2 \geq 0.
\]

Recall that this is the inequality we used to analyze simplices at the end of the second lecture.

Delsarte discovered an infinite sequence of linear inequalities generalizing this one\(^2\). The factor of \(t\) above is replaced with certain special functions, namely Gegenbauer or ultraspherical polynomials, which are a family \(P^\mu_n\) of polynomials in one variable with \(\deg(P^\mu_n) = k\). The Delsarte inequalities then say that whenever \(A\) is the distance distribution of a configuration in \(S^{n-1}\),
\[
\sum_t A_t P^\mu_k(t) \geq 0
\]
for all \(k\). In particular, \(P^0_n(t) = t\), from which we recover the previous inequality, and \(P^1_n(t) = 1\), while the higher-degree polynomials depend on \(n\).

The Delsarte inequalities are far from a complete characterization of the distance distributions of codes. However, they are particularly beautiful and important constraints on these distance distributions.

An equivalent reformulation of (1.2) is that for every finite set \(C \subset S^{n-1}\),
\[
\sum_{x, y \in C} P^\mu_k(\langle x, y \rangle) \geq 0.
\]
We will return in \(\S\) to what ultraspherical polynomials are and why they have this property. In the meantime, we will treat them as a black box while we explore how the Delsarte inequalities are used to prove bounds.

\(^2\)Delsarte’s initial discovery was in a discrete setting [28], but analogous techniques apply to spheres [29] [41].
2. Linear programming bounds

The energy of a code is given by the linear function

\[ \frac{1}{2} \sum_{-1 \leq t < 1} f(2 - 2t) A_t \]

of its distance distribution, and the Delsarte inequalities

\[ \sum_t A_t P^n_k(t) \geq 0 \]

are linear in \( A \) as well. The linear programming bounds minimize the energy subject to these linear constraints. Because of the linearity, these bounds are particularly well behaved and useful. The only computational difficulty is that there are infinitely many variables \( A_t \).

Let’s write down the linear programming bounds more precisely. To begin with, we are given the dimension \( n \), number \( N \) of points, and potential function \( f \). Then linear programming bounds attempt to choose \( A_t \) for \(-1 \leq t \leq 1\) so as to minimize

\[ \frac{1}{2} \sum_{-1 \leq t < 1} A_t f(2 - 2t) \]

subject to

\[ A_1 = N, \]
\[ A_t \geq 0 \text{ for } -1 \leq t \leq 1, \]
\[ \sum_t A_t = N^2, \text{ and} \]
\[ \sum_t A_t P^n_k(t) \geq 0 \text{ for all } k \geq 1. \]

This optimization problem gives us a lower bound for the energy of codes in \( S^{n-1} \), because every code has a corresponding distance distribution. However, there is no reason to expect the bound to be sharp in general: the optimal choice of \( A_t \) will usually not even be integral, let alone come from an actual code. Of course one could improve the bound by imposing integrality, but then the optimization problem would become far less tractable. In particular, it would no longer be a convex optimization problem.

Linear programming bounds are well suited to computer calculations, but they have not yet been fully optimized. Any given case can be solved numerically, but the general pattern is unclear. In particular, for most \( n \), \( N \), and \( f \) we do not know the optimal solution.

In practice, it is useful to apply linear programming duality, in which we try to prove bounds on energy by taking linear combinations of the constraints. If we multiply the Delsarte inequalities

\[ \sum_t A_t P^n_k(t) \geq 0 \]

by constants \( h_k \) and then sum over \( k \), we obtain the following theorem.

---

3Recall that “linear programming” means optimizing a linear function subject to linear constraints. There are efficient algorithms to solve finite linear programs.
Theorem 2.1 (Yudin [81]). Suppose $h = \sum_k h_k P_k^n$ with $h_k \geq 0$ for $k \geq 1$, and suppose $h(t) \leq f(2 - 2t)$ for $t \in [-1, 1)$. Then every $N$-point configuration $\mathcal{C}$ on $S^{n-1}$ satisfies
\[
\sum_{x, y \in \mathcal{C}} f(|x - y|^2) \geq N^2 h_0 - N h(1).
\]

The auxiliary function $h$ is generally a polynomial, in which case $h_k = 0$ for all sufficiently large $k$, but convergence of $\sum_k h_k P_k^n$ on $[-1, 1]$ suffices. (It turns out that $|P_k^n| \leq P_k^n(1)$ on $[-1, 1]$, and hence the convergence is automatically absolute and uniform.)

Proof. We have
\[
\sum_{x, y \in \mathcal{C}} f(|x - y|^2) \geq \sum_{x, y \in \mathcal{C}} h(\langle x, y \rangle) \quad \text{(because $f(2 - 2t) \geq h(t)$ pointwise)}
\]
\[
= \sum_{x, y \in \mathcal{C}} h(\langle x, y \rangle) - N h(1)
\]
\[
= N^2 h_0 - N h(1) + \sum_{k \geq 1} h_k \sum_{x, y \in \mathcal{C}} P_k^n(\langle x, y \rangle)
\]
\[
\geq N^2 h_0 - N h(1),
\]
as desired. \qed

Note that the proof rests on the fundamental inequality
\[
\sum_{x, y \in \mathcal{C}} P_k^n(\langle x, y \rangle) \geq 0.
\]
The proof technique might seem extraordinarily wasteful, since it involves throwing away many terms in our sum. However, $P_k^n(\langle x, y \rangle)$ averages to zero over the whole sphere when $k \geq 1$, which suggests that the double sums
\[
\sum_{x, y \in \mathcal{C}} P_k^n(\langle x, y \rangle)
\]
may not be so large after all when $\mathcal{C}$ is well distributed over the sphere.

Theorem 2.1 tells us that to prove a lower bound for $f$-energy, all we need is a lower bound $h$ for the potential function $f$ such that $h$ has non-negative ultraspherical coefficients. Such an auxiliary function is a convenient certificate for a lower bound.

Outside of a few special cases, nobody knows the optimal $h$ for a given $f$. However, numerical optimization is an effective way to compute approximations to it. One can use more sophisticated techniques such as sums of squares and semidefinite programming, but even the most straightforward approach works well in practice: let $h$ be a polynomial of degree $d$, and instead of imposing the inequality $h(t) \leq f(2 - 2t)$ for all $t$, impose it just at finitely many locations (chosen fairly densely in $[-1, 1)$, of course). Then we are left with a finite linear program, i.e., a linear optimization problem with only finitely many variables and constraints, which is easily solved numerically using standard software. The resulting auxiliary function $h$ might not satisfy $h(t) \leq f(2 - 2t)$ everywhere, but any violations will be small, and we can eliminate them by adjusting the constant term $h_0$ without substantially changing the energy bound.
3. Applying linear programming bounds

Linear programming bounds are behind almost every case in which universal optimality, or indeed any sharp bound on energy, is known. As mentioned above, they are generally far from sharp, but for certain codes they miraculously give sharp bounds. This is the case for all the universal optima listed in Table 1 from the second lecture.

When could the bound be sharp for a configuration $C$? Equality holds in Theorem 2.1 iff every term we throw away in the proof is actually already zero. Inspecting the proof leads to the following criteria:

**Lemma 3.1.** The energy lower bound in Theorem 2.1 is attained by a code $C$ if and only if

$$ f(|x - y|^2) = h(\langle x, y \rangle) $$

for all $x, y \in C$ with $x \neq y$, and

$$ \sum_{x, y \in C} P^k(\langle x, y \rangle) = 0 $$

for all $k \geq 1$ for which $h_k > 0$.

The first condition says that $h(t) = f(2 - 2t)$ whenever $t = \langle x, y \rangle$ with $x, y \in C$ and $x \neq y$. Because $h(t) \leq f(2 - 2t)$ for all $t$, the functions $h$ and $f$ cannot cross. Instead, they must agree to order at least 2 whenever they touch.

In practice, sharp bounds are usually obtained in the simplest possible way based on this tangency constraint. We choose $h$ to be a polynomial of as low a degree as possible subject to agreeing with $f$ to order 2 at each inner product that occurs between distinct points in $C$. This specifies a choice of $h$, but it is not obvious that it has any of the desired properties. For example, the inequality $h(t) \leq f(2 - 2t)$ might be violated in between the points at which we force equality, and there is no obvious reason to expect the ultraspherical coefficients $h_k$ to be nonnegative.

This construction of $h$ is generally far from optimal when it works at all, but for particularly beautiful codes it does remarkably well at proving sharp bounds. For example, let’s show that regular simplices are universally optimal, which was Exercise 4.2 from the second lecture. Recall that for $N \leq n + 1$, the $N$-point regular simplex $C$ in $S^{n-1}$ has all inner products equal to $-1/(N - 1)$.

**Proposition 3.2.** For $N \leq n + 1$, the $N$-point regular simplex is universally optimal in $S^{n-1}$.

We’ll describe the proof in terms of linear programming bounds, but one could reword it to use just the inequality

$$ \left| \sum_{x \in C} x \right|^2 \geq 0 $$

(as was intended in Exercise 4.2 from the second lecture).

**Proof.** We will show that the simplex in fact minimizes energy for every decreasing, convex potential function $f$, which is an even stronger property than universal optimality. Let $h(t)$ be the tangent line to $f(2 - 2t)$ at $t = -1/(N - 1)$; in other words,

$$ h(t) = f(2 + 2/(N - 1)) - 2f'(2 + 2/(N - 1))(t + 1/(N - 1)). $$
This function is the lowest-degree polynomial that agrees with $f(2 - 2t)$ to order 2 at all the inner products occurring in the regular simplex, which makes it a special case of the construction outlined above.

Because $f$ is convex, $h(t) \leq f(2 - 2t)$ for all $t$. Thus, the first inequality we need for $h$ does in fact hold. To check the nonnegativity of the ultraspherical coefficients (aside from the constant term), note that the first two ultraspherical polynomials are 1 and $t$. If we express $h(t)$ in terms of this basis, then the coefficient of $t$ is $-2f'(2 + 2/(N - 1))$, which is nonnegative since $f$ is decreasing. Thus, $h$ satisfies the hypotheses of Theorem 2.1. Furthermore, $h(t) = f(2 - 2t)$ when $t = -1/(N - 1)$ by construction, and

$$\sum_{x, y \in C} \langle x, y \rangle = \left| \sum_{x \in C} x \right|^2 = 0.$$  

These are the conditions for a sharp bound in Lemma 3.1, and so we conclude that our energy bound is equal to the energy of the regular simplex. Hence regular simplices minimize energy for all decreasing, convex potential functions, and in particular they are universally optimal.

Codes with more inner products are more complicated to handle, but in any given case one can figure out whether this approach works. If one analyzes the technique in sufficient generality, it proves the following theorem, which extends a theorem of Levenshtein [51].

**Theorem 3.3** (Cohn and Kumar [17]). Every $m$-distance set that is a spherical $(2m - 1)$-design is universally optimal.

Here an $m$-distance set is a set in which $m$ distances occur between distinct points, and a spherical $k$-design is a finite subset $\mathcal{D}$ of the sphere $S^{n-1}$ such that for every polynomial $p: \mathbb{R}^n \to \mathbb{R}$ of total degree at most $k$, the average of $p$ over $\mathcal{D}$ is equal to its average over the entire sphere $S^{n-1}$. In other words, averaging at the points of $\mathcal{D}$ is an exact numerical integration formula for polynomials up to degree $k$, which means these points are exceedingly well distributed over the sphere.

This theorem suffices to handle every known universal optimum on the surface of a sphere (see Table 1 in the second lecture) except the regular 600-cell, which is dealt with in §7 of [17]. Surely that’s not the only exception, but it is unclear where to find other universal optima that go beyond Theorem 3.3.

### 4. Spherical codes and the kissing problem

Recall that the spherical code problem asks whether $N$ points can be arranged on $S^{n-1}$ so that no two are closer than angle $\theta$ to each other along the great circle connecting them. In other words, the minimal angle between the points is at least $\theta$. This is a packing problem: how many spherical caps of angular radius $\theta/2$ can we pack on the surface of a sphere?

The most famous special case is the kissing problem discussed in the first lecture. Given a central unit ball, the kissing problem asks how many non-overlapping unit balls can be arranged tangent to it. Equivalently, the points of tangency should form a spherical code with minimal angle at least $60^\circ$ (see Figure 1).

Linear programming bounds apply to this problem. In fact, packing problems were the original application for these bounds [28], before Yudin applied them to energy minimization [81].
Theorem 4.1. Suppose \( h = \sum h_k P^n_k \) with \( h_k \geq 0 \) for \( k \geq 0 \) and \( h_0 > 0 \), and suppose \( h(t) \leq 0 \) for \( t \in [-1, \cos \theta] \). Then every code \( C \) in \( S^{n-1} \) with minimal angle at least \( \theta \) satisfies
\[
|C| \leq h(1)/h_0.
\]

Proof. We have
\[
|C| h(1) \geq \sum_{x,y \in C} h(x,y) = \sum_k h_k \sum_{x,y \in C} P^n_k (\langle x, y \rangle) \geq |C|^2 h_0. \quad \square
\]

As in the case of energy minimization, this bound is generally not sharp, but on rare occasions we are lucky enough to get a sharp bound. The most famous case is the kissing problem in \( \mathbb{R}^8 \) and \( \mathbb{R}^{24} \), which was solved independent by Levenshtein [50] and Odlyzko and Sloane [59]. In particular, the kissing number is 240 in \( \mathbb{R}^8 \) and 196560 in \( \mathbb{R}^{24} \), as achieved by the \( E_8 \) lattice and the Leech lattice. It is not so difficult to prove these upper bounds using Theorem 4.1. In particular, we take
\[
h(t) = (t+1)(t+1/2)^2 t^2(t-1/2)
\]
in the \( \mathbb{R}^8 \) case, and
\[
h(t) = (t+1)(t+1/2)^2(t+1/4)^2 t^2(t-1/4)^2(t-1/2)
\]
in the \( \mathbb{R}^{24} \) case. (The roots correspond to the inner products that occur in the kissing configurations.) Checking that these polynomials satisfy the hypotheses of Theorem 4.1 and prove sharp bounds is a finite calculation. Of course presenting it this way makes the proof look like a miracle, and explaining it conceptually requires a deeper analysis [51].

5. Ultraspherical polynomials

So far, we have treated ultraspherical polynomials as a black box and taken the Delsarte inequalities on faith. In this section, we will finally examine where these polynomials come from and why the inequalities hold.
One simple (albeit unmotivated) description is that ultraspherical polynomials for $S^{n-1}$ are \textit{orthogonal polynomials} with respect to the measure $(1-t^2)^{(n-3)/2} \, dt$ on $[-1,1]$. In other words,

$$\int_{-1}^{1} P^n_k(t)P^n_\ell(t)(1-t^2)^{(n-3)/2} \, dt = 0$$

for $k \neq \ell$. Equivalently, $P^n_k$ is orthogonal to all polynomials of degree less than $k$ with respect to this measure, because all such polynomials are linear combinations of $P^n_0, \ldots, P^n_{k-1}$. We’ll see shortly where the measure comes from and why this orthogonality characterizes the ultraspherical polynomials, but first let’s explore its consequences.

Orthogonality uniquely determines the ultraspherical polynomials up to scaling (and the scaling is irrelevant for our purposes, as long as we take $P^n_k(1) > 0$ so as not to flip the Delsarte inequality). Specifically, we just apply Gram-Schmidt orthogonalization to $1,t,t^2,\ldots$, which gives an algorithm to compute these polynomials explicitly. It’s not the most efficient method, but it works.

Although orthogonality may sound like an arcane property of a sequence of polynomials, it has many wonderful and surprising consequences. For example, it implies that $P^n_k$ has $k$ distinct roots in $[-1,1]$. To see why, suppose $P^n_k$ changed sign at only $m$ points $r_1, \ldots, r_m$ in $[-1,1]$, with $m < k$. Then the polynomial $P^n_k(t)(t-r_1)\ldots(t-r_m)$ would never change sign on $[-1,1]$, which would contradict

$$\int_{-1}^{1} P^n_k(t)(t-r_1)\ldots(t-r_m)(1-t^2)^{(n-3)/2} \, dt = 0$$

(which holds because $(t-r_1)\ldots(t-r_m)$ has degree less than $k$). Thus, $m = k$ and $P^n_k$ has $k$ distinct roots in $[-1,1]$, which means it’s a highly oscillatory function.

Although ultraspherical polynomials can be characterized via orthogonality, it’s not really a satisfactory explanation of where they come from. To explain that, we will use spherical harmonics. Recall that as a representation of $O(n)$, we can decompose $L^2(S^{n-1})$ as

$$L^2(S^{n-1}) = \bigoplus_{k \geq 0} W_k,$$

where $W_k$ consists of degree $k$ spherical harmonics.

We can obtain ultraspherical polynomials by studying the \textit{evaluation map}: let $x \in S^{n-1}$, and consider the linear map that takes $f \in W_k$ to $f(x)$. By duality for finite-dimensional vector spaces, this map must be the inner product with some unique element $w_{k,x}$ of $W_k$, called a \textit{reproducing kernel}. That is,

$$f(x) = \langle w_{k,x}, f \rangle$$

for all $f \in W_k$. Note that here $\langle \cdot, \cdot \rangle$ denotes the inner product on $L^2(S^{n-1})$. We will use the same notation for both this inner product and the standard inner product on $\mathbb{R}^n$; to distinguish between them, pay attention to which vector spaces their arguments lie in.

The function $w_{k,x}$ on $S^{n-1}$ has considerable structure. For example, it is invariant under all symmetries of $S^{n-1}$ that fix $x$:

\textbf{Lemma 5.1.} If $T$ is an element of $O(n)$ such that $Tx = x$, then $Tw_{k,x} = w_{k,x}$. 

Proof. This lemma follows easily from the invariance of the inner product on $W_k$ under $O(n)$. We have $\langle w_{k,x}, f \rangle = \langle Tw_{k,x}, f \rangle$ for all $f \in W_k$, because $\langle w_{k,x}, f \rangle = f(x) = (T^{-1}f)(x) = \langle w_{k,x}, T^{-1}f \rangle = \langle Tw_{k,x}, f \rangle$, and hence $w_{k,x} = Tw_{k,x}$. □

Equivalently, $w_{k,x}(y)$ can depend only on the distance between $x$ and $y$, and therefore it must be a function of $\langle x, y \rangle$ alone. We define $P^n_k$ by $w_{k,x}(y) = P^n_k(\langle x, y \rangle)$.

The reproducing kernel $w_{k,x}$ is a polynomial of degree $k$ in several variables, because it is a spherical harmonic in $W_k$, and thus $P^n_k$ must be a polynomial of degree $k$ in one variable. (Technically this definition is off by a constant factor from the special case $P^n_1(t) = t$ mentioned earlier, but we could easily rectify that by rescaling so that $P^n_k(1) = 1$.)

We have finally explained where ultraspherical polynomials come from. They describe reproducing kernels for the spaces $W_k$, and the importance of reproducing kernels is that they tell how to evaluate spherical harmonics at points.

The drawback of the reproducing kernel definition is that it does not make it clear how to compute these polynomials in any reasonable way. In principle one could choose a basis for the homogeneous harmonic polynomials of degree $k$, integrate over the sphere to obtain the inner products of the basis vectors in $W_k$, write down the evaluation map explicitly relative to this basis, and solve simultaneous linear equations to obtain the reproducing kernel. However, that would be unpleasantly cumbersome. The beauty of the orthogonal polynomial characterization of ultraspherical polynomials is that it is much more tractable, but we must still see why it is true.

First, observe that $w_{k,x}$ and $w_{\ell,x}$ are orthogonal in $L^2(S^{n-1})$ for $k \neq \ell$, since they are spherical harmonics of different degrees. Thus,

\[(5.1) \quad \int_{S^{n-1}} P^n_k(\langle x, y \rangle) P^n_\ell(\langle x, y \rangle) d\mu(y) = 0,\]

where $\mu$ is surface measure. We can now obtain the orthogonality of the ultraspherical polynomials from the following multivariate calculus exercise:

Exercise 5.2. Prove that under orthogonal projection from the surface of the sphere onto a coordinate axis, the measure $\mu$ projects to a constant times the measure $(1 - t^2)^{(n-3)/2} dt$ on $[-1, 1]$. (See [13] p. 2434 for a simple solution.)

If we apply this orthogonal projection onto the axis between the antipodal points $\pm x$, then (5.1) becomes

\[\int_{-1}^{1} P^n_k(t) P^n_\ell(t) (1 - t^2)^{(n-3)/2} dt = 0,\]

as desired.

As a side comment, we can now see that $W_k$ is an irreducible representation of $O(n)$. If it broke up further, then each summand would have its own reproducing kernel, which would yield two different polynomials of degree $k$ that would be orthogonal to each other as well as to lower degree polynomials. That’s impossible, since the space of polynomials of degree at most $k$ has dimension too low to contain so many orthogonal polynomials.
All that remains to prove is the Delsarte inequalities. The key observation is that $P_n^k(\langle x, y \rangle)$ can be written as the inner product of two vectors in $W_k$ depending only on $x$ and $y$, namely the reproducing kernels:

**Lemma 5.3.** For all $x, y \in S^{n-1}$ and $k \geq 0$,

$$P_n^k(\langle x, y \rangle) = \langle w_{k,x}, w_{k,y} \rangle.$$

**Proof.** Recall that the reproducing kernel property means $\langle w_{k,x}, f \rangle = f(x)$ for all $f \in W_k$. In particular, taking $f = w_{k,y}$ yields $\langle w_{k,x}, w_{k,y} \rangle = w_{k,y}(x)$. Now $w_{k,y}(x) = P_n^k(\langle x, y \rangle)$ implies that $P_n^k(\langle x, y \rangle) = \langle w_{k,x}, w_{k,y} \rangle$, as desired. □

**Corollary 5.4.** For every finite subset $C \subseteq S^{n-1}$ and $k \geq 0$,

$$\sum_{x,y \in C} P_n^k(\langle x, y \rangle) \geq 0.$$

**Proof.** We have

$$\sum_{x,y \in C} P_n^k(\langle x, y \rangle) = \sum_{x,y \in C} \langle w_{k,x}, w_{k,y} \rangle = \left| \sum_{x \in C} w_{k,x} \right|^2 \geq 0,$$

as desired. □

This argument is a perfect generalization of $\left| \sum_{x \in C} x \right|^2 \geq 0$, except instead of summing the vectors $x$, we are summing vectors $w_{k,x}$ in the Hilbert space $W_k$. One interpretation is that $x \mapsto w_{k,x}$ maps $S^{n-1}$ into a sphere in the higher-dimensional space $W_k$, and we're combining the trivial inequality

$$\left| \sum_{x \in C} w_{k,x} \right|^2 \geq 0$$

with that nontrivial mapping. When $n = 2$, the space $W_k$ has dimension $2$ for $k \geq 1$, and so up to scaling we are mapping $S^1$ to itself. This map wraps $S^1$ around itself $k$ times, while the analogues for $n \geq 3$ are more subtle.

It’s natural to wonder whether ultraspherical polynomials span all the functions $P$ satisfying

$$\sum_{x,y \in C} P(\langle x, y \rangle) \geq 0$$

for all $C$. In fact, they do not. Pfender has constructed further such functions and used them to obtain improvements on linear programming bounds [62]. However, the numerical improvements so far have been relatively modest.

Instead, Schoenberg proved that the ultraspherical polynomials span the space of positive-definite kernels [64], i.e., functions $P$ such that for all $x_1, \ldots, x_N \in S^{n-1}$, the $N \times N$ matrix with entries $P(\langle x_i, x_j \rangle)$ is positive semidefinite. The reason why ultraspherical polynomials are positive-definite is Lemma 5.3: the matrix with
entries \( \langle w_{k,x_i}, w_{k,x_j} \rangle \) is a Gram matrix and is thus positive semidefinite. Positive-definite kernels play an important role in representation theory, which contributes to the importance of ultraspherical polynomials.

As a final comment, everything we have done in this lecture has been restricted to analyzing pairwise distance distributions. It’s natural to ask what happens if one looks at triples of points instead of pairs, or even larger subconfigurations. The Delsarte inequalities can be generalized to semidefinite constraints on these higher-order correlation functions, and thus we can obtain semidefinite programming bounds \[65, 5, 47\], which are a powerful and important extension of linear programming bounds. For reasons that have not yet been understood, these higher-order bounds seem less fruitful for obtaining sharp bounds, but several sharp cases are known \[6, 22\] and others presumably remain to be discovered.
PACKING BOUNDS IN EUCLIDEAN SPACE

1. Introduction

In this lecture we will study linear programming bounds for the sphere packing problem in Euclidean space. The basic principles are closely analogous to those we saw for spherical codes in the fourth lecture. However, the way the bounds behave in Euclidean space is far more mysterious. They almost certainly solve the sphere packing problem in $\mathbb{R}^8$ and $\mathbb{R}^{24}$, by matching the densities of the $E_8$ and Leech lattices, but nobody has been able to prove it.

We will focus on the sphere packing problem, rather than energy minimization. Everything we will do works just as well in the latter case (see §9 of [17]), but sphere packing already illustrates the essential features of these bounds.

To begin, let’s review the statement and proof of linear programming bounds for spherical codes, i.e., Theorem 4.1 from the last lecture:

**Theorem 1.1.** Suppose $h = \sum_k h_k P_n^k$ with $h_k \geq 0$ for $k \geq 0$ and $h_0 > 0$, and suppose $h(t) \leq 0$ for $t \in [-1, \cos \theta]$. Then every code $C$ in $S^{n-1}$ with minimal angle at least $\theta$ satisfies

$$|C| \leq h(1)/h_0.$$  

**Proof.** We have

$$|C|h(1) \geq \sum_{x,y \in C} h(\langle x, y \rangle) = \sum_k h_k \sum_{x,y \in C} P_n^k(\langle x, y \rangle) \geq |C|^2 h_0. \tag*{□}$$

How could we generalize this argument? First, we need functions on Euclidean space that can play the same role as ultraspherical polynomials. In particular, we need an analogue of the positivity property

$$\sum_{x,y \in C} P_n^k(\langle x, y \rangle) \geq 0.$$

As it turns out, the Euclidean functions are considerably more familiar, namely exponentials $x \mapsto e^{2\pi i \langle t, x \rangle}$. If we apply them to two points via $(x, y) \mapsto e^{2\pi i \langle t, x-y \rangle}$, then for every finite subset $C$ of $\mathbb{R}^n$,

$$\sum_{x, y \in C} e^{2\pi i \langle t, x-y \rangle} = \left| \sum_{x \in C} e^{2\pi i \langle t, x \rangle} \right|^2 \geq 0. \tag{1.1}$$

As in the third lecture, these functions have representation-theoretic origins, but we will not take up that subject here.

In the same way we previously made use of nonnegative linear combinations of ultraspherical polynomials, we will now need to use nonnegative linear combinations of exponentials. The natural setting for linear combinations of exponentials is
the Fourier transform. Define the Fourier transform \( \hat{f} \) of an integrable function \( f: \mathbb{R}^n \rightarrow \mathbb{R} \) by

\[
\hat{f}(t) = \int_{\mathbb{R}^n} f(x) e^{-2\pi i \langle t, x \rangle} \, dx.
\]

If \( f \) is continuous and \( \hat{f} \) is integrable as well, then Fourier inversion tells us that

\[
f(x) = \int_{\mathbb{R}^n} \hat{f}(t) e^{2\pi i \langle t, x \rangle} \, dt.
\]

In other words, the Fourier transform \( \hat{f} \) gives the coefficients needed to express \( f \) as a continuous linear combination of exponentials. Thus, we will be particularly interested in functions \( f \) for which \( \hat{f} \geq 0 \).

If \( \hat{f}(t) \geq 0 \) for all \( t \), then Fourier inversion implies that

\[
\sum_{x, y \in C} f(x - y) \geq 0
\]

whenever \( C \) is a finite subset of \( \mathbb{R}^n \), because

\[
\sum_{x, y \in C} f(x - y) = \int_{\mathbb{R}^n} \hat{f}(t) \left| \sum_{x \in C} e^{2\pi i \langle t, x \rangle} \right|^2 \, dt
\]

by \([11]\). Thus, functions with nonnegative Fourier transforms have exactly the property we need to generalize the Delsarte inequalities to Euclidean space.

However, using these functions to prove sphere packing bounds requires some finesse. In the spherical case, we looked at the double sum

\[
\sum_{x, y \in C} h(\langle x, y \rangle)
\]

and bounded it on both sides to get

\[
|C|h(1) \geq \sum_{x, y \in C} h(\langle x, y \rangle) = \sum_k h_k \sum_{x, y \in C} P^n_k(\langle x, y \rangle) \geq |C|^2 h_0.
\]

In Euclidean space, the corresponding double sum would be

\[
\sum_{x, y \in C} f(x - y),
\]

where \( C \) is a dense sphere packing, or rather the set of sphere centers in such a packing. Unfortunately, there’s an obvious problem with this approach: \( C \) will be infinite and the double sum will diverge. For example, if \( C \) is a lattice, then every term in the sum occurs infinitely often, because there are infinitely many ways to write each lattice vector as a difference of lattice vectors.

Can we somehow renormalize the double sum and use it to complete the proof? The answer is yes if we’re careful; see the proof of Theorem 3.3 in \([23]\), which controls the sum over a packing by subtracting a uniform background distribution of equal density. However, in this lecture we’ll take an arguably more fundamental approach using the Poisson summation formula.
2. Poisson summation

Poisson summation is a remarkable duality between summing a function over a lattice and summing its Fourier transform over the dual lattice.

We’ll take a somewhat cavalier attitude towards analytic technicalities: we will manipulate sums and integrals however we like, and include enough hypotheses to justify these manipulations. Specifically, we will deal with what we’ll call admissible functions $f : \mathbb{R}^n \to \mathbb{R}$, those for which $|f(x)| = O((1 + |x|)^{-n-\varepsilon})$ and $|\hat{f}(t)| = O((1 + |t|)^{-n-\varepsilon})$ for some $\varepsilon > 0$. This decay rate is fast enough for sums over lattices to converge with room to spare. In practice, we can simply read “admissible” as “sufficiently rapidly decreasing and smooth for everything to work.”

**Theorem 2.1** (Poisson summation). If $f : \mathbb{R}^n \to \mathbb{R}$ is an admissible function and $\Lambda$ is a lattice in $\mathbb{R}^n$, then

$$\sum_{x \in \Lambda} f(x) = \frac{1}{\text{vol}(\mathbb{R}^n / \Lambda)} \sum_{t \in \Lambda^*} \hat{f}(t).$$

Here $\text{vol}(\mathbb{R}^n / \Lambda)$ is the volume of a fundamental cell of $\Lambda$, i.e., the determinant of $\Lambda$, and $\Lambda^* = \{ t \in \mathbb{R}^n \mid \langle x, t \rangle \in \mathbb{Z} \text{ for all } x \in \Lambda \}$ is the dual lattice (see Exercise 2.1 in the third lecture).

**Proof.** The key idea is to prove an even more general formula, by looking at the Fourier expansion of the periodization of $f$ under $\Lambda$. Let

$$F(y) = \sum_{x \in \Lambda} f(x + y),$$

so that $F$ is periodic modulo $\Lambda$. We can expand $F$ as a Fourier series

$$F(y) = \sum_{t \in \Lambda^*} c_t e^{2\pi i \langle t, y \rangle}$$

for some coefficients $c_t$, where $\Lambda^*$ occurs because it specifies the exponentials that are periodic modulo $\Lambda$ (see Exercise 2.2 in the third lecture).

Let $D$ be a fundamental domain for $\Lambda$. By orthogonality,

$$c_t = \frac{1}{\text{vol}(D)} \int_D F(y)e^{-2\pi i \langle t, y \rangle} \, dy$$

$$= \frac{1}{\text{vol}(\mathbb{R}^n / \Lambda)} \int_D F(y)e^{-2\pi i \langle t, y \rangle} \, dy$$

$$= \frac{1}{\text{vol}(\mathbb{R}^n / \Lambda)} \sum_{x \in \Lambda} \int_D f(x + y)e^{-2\pi i \langle t, y \rangle} \, dy$$

$$= \frac{1}{\text{vol}(\mathbb{R}^n / \Lambda)} \sum_{x \in \Lambda} \int_D f(x + y)e^{-2\pi i \langle t, x + y \rangle} \, dy \quad (x \in \Lambda \text{ and } t \in \Lambda^*)$$

$$= \frac{1}{\text{vol}(\mathbb{R}^n / \Lambda)} \int_{\mathbb{R}^n} f(y)e^{-2\pi i \langle t, y \rangle} \, dy \quad (\text{translates of } D \text{ tile } \mathbb{R}^n)$$

$$= \frac{1}{\text{vol}(\mathbb{R}^n / \Lambda)} \hat{f}(t).$$

In other words, the Fourier coefficients $c_t$ of the periodization of $f$ are simply proportional to $\hat{f}(t)$, with constant of proportionality $1/\text{vol}(\mathbb{R}^n / \Lambda)$.
Thus,
\[
\sum_{x \in \Lambda} f(x + y) = \frac{1}{\text{vol}(\mathbb{R}^n / \Lambda)} \sum_{t \in \Lambda^*} \hat{f}(t) e^{2\pi i (t, y)},
\]
and setting \(y = 0\) yields Poisson summation. \(\square\)

The more general formula
\[
\sum_{x \in \Lambda} f(x + y) = \frac{1}{\text{vol}(\mathbb{R}^n / \Lambda)} \sum_{t \in \Lambda^*} \hat{f}(t) e^{2\pi i (t, y)}
\]
is important in its own right, not just as tool for proving Poisson summation. At first it looks considerably more general than Poisson summation, but it is simply Poisson summation applied to the function \(x \mapsto f(x + y)\) in place of \(f\).

3. Linear programming bounds

We can now state and prove the linear programming bounds for Euclidean sphere packings.

**Theorem 3.1** (Cohn and Elkies [15]). Let \(f : \mathbb{R}^n \to \mathbb{R}\) be an admissible function with \(f(x) \leq 0\) for \(|x| \geq 2\), \(\hat{f}(t) \geq 0\) for all \(t\), and \(\hat{f}(0) > 0\). Then the sphere packing density in \(\mathbb{R}^n\) is at most
\[
\frac{\pi^{n/2}}{(n/2)!} \cdot \frac{f(0)}{\hat{f}(0)}.
\]

As before, \((n/2)!\) means \(\Gamma(n/2 + 1)\) when \(n\) is odd. The factor of \(\pi^{n/2}/(n/2)!\) is the volume of a unit ball. It occurs because we are looking at packing density, rather than just the number of balls per unit volume in space.

We will prove Theorem 3.1 using Poisson summation [15]. Several other proofs are known, but they are longer [12] or more delicate [23]. One advantage of the proof in [23] is that it weakens the admissibility hypothesis, so that we can use a more robust space of functions; however, it obscures when a sharp bound can be obtained.

Before we turn to the proof, let's compare Theorem 3.1 with Theorem 1.1, its spherical analogue. One difference is that the Euclidean case involves a function of \(n\) variables, as opposed to one variable in the spherical case. However, this difference is illusory: we might as well radially symmetrize \(f\) in the Euclidean case (since both the hypotheses and the bound are radially symmetric), after which it becomes a function of one variable.

Table 1 gives a dictionary with which these theorems can be compared. They really are fully analogous, with the biggest discrepancy being that we use inner products to measure distances in the spherical case but Euclidean distance in the Euclidean case.

**Proof.** As a warm-up, let’s prove the linear programming bounds for lattice packings. Suppose \(\Lambda\) is a lattice packing with unit balls (since we can specify the packing radius without loss of generality). In other words, the minimal vector length of the lattice \(\Lambda\) is at least 2.

By Poisson summation,
\[
\sum_{x \in \Lambda} f(x) = \frac{1}{\text{vol}(\mathbb{R}^n / \Lambda)} \sum_{t \in \Lambda^*} \hat{f}(t).
\]
Table 1. A dictionary for comparing linear programming bounds on spheres and in Euclidean space.

| space    | $S^{n-1}$ | $\mathbb{R}^n$ |
|-----------|-----------|----------------|
| function  | $h$       | $f$            |
| transform | $h_k$     | $\hat{f}(t)$  |
| balls don’t overlap | $t \in [-1, \cos \theta]$ | $|x| \geq 2$ |
| value at distance zero | $h(1)$ | $f(0)$ |
| bound     | $h(1)/h_0$ | $f(0)/\hat{f}(0)$ |

We will apply the contrasting inequalities $f(x) \leq 0$ (for $|x| \geq 2$) and $\hat{f}(t) \geq 0$ to this identity. We have

$$f(0) \geq \sum_{x \in \Lambda} f(x)$$

because $f(x) \leq 0$ for $|x| \geq 2$, while

$$\sum_{t \in \Lambda^*} \hat{f}(t) \geq \hat{f}(0)$$

because $\hat{f}(t) \geq 0$ for all $t$. Thus,

$$f(0) \geq \frac{\hat{f}(0)}{\text{vol}(\mathbb{R}^n/\Lambda)}.$$

The number of balls per unit volume in the packing is $1/\text{vol}(\mathbb{R}^n/\Lambda)$, and its density is therefore $1/\text{vol}(\mathbb{R}^n/\Lambda)$ times the volume of a unit ball. Thus, the density is at most

$$\frac{\pi^{n/2}}{(n/2)!} \cdot \frac{f(0)}{\hat{f}(0)}$$

as desired.

So far, we have done nothing but apply the given inequalities to both sides of Poisson summation. Handling general packings will require a little more work, but nothing too strenuous.

Without loss of generality, we can restrict our attention to periodic packings, since they come arbitrarily close to the optimal packing density. In other words, we can suppose our packing consists of $N$ translates of a lattice $\Lambda$, namely

$$\Lambda + y_1, \ldots, \Lambda + y_N.$$

Now the number of balls per unit volume in the packing is $N/\text{vol}(\mathbb{R}^n/\Lambda)$, and the condition that they should not overlap says that $|x + y_j - y_k| \geq 2$ for $x \in \Lambda$ as long as $x \neq 0$ or $j \neq k$.

A little manipulation based on the translated Poisson summation formula

$$\sum_{x \in \Lambda} f(x + y) = \frac{1}{\text{vol}(\mathbb{R}^n/\Lambda)} \sum_{t \in \Lambda^*} \hat{f}(t)e^{2\pi i \langle t, y \rangle}$$

shows that

$$\sum_{x \in \Lambda} \sum_{j,k=1}^N f(x + y_j - y_k) = \frac{1}{\text{vol}(\mathbb{R}^n/\Lambda)} \sum_{t \in \Lambda^*} \hat{f}(t) \left| \sum_{j=1}^N e^{2\pi i \langle y_j, t \rangle} \right|^2.$$
The inequalities on $f$ and $\hat{f}$ show that the left side is at most $N f(0)$ and the right side is at least $\frac{N^2 \hat{f}(0)}{\text{vol}(\mathbb{R}^n/\Lambda)}$. It follows that $\frac{\pi^{n/2}}{(n/2)!} \cdot \frac{N}{\text{vol}(\mathbb{R}^n/\Lambda)} \leq \frac{\pi^{n/2}}{(n/2)!} \cdot \frac{f(0)}{\hat{f}(0)}$, which completes the proof.

In this proof, the inequality $\sum_{x \in \Lambda} \sum_{j,k=1}^N f(x + y_j - y_k) \geq \frac{N^2 \hat{f}(0)}{\text{vol}(\mathbb{R}^n/\Lambda)}$ plays the role of the Delsarte inequalities. Note that the left side is essentially summing $f$ over the distance distribution of the packing, but renormalized so that the distances do not occur infinitely often.

In physics terms [75, p. 72], this inequality says that the structure factor (the Fourier transform of $g_2 - 1$, where $g_2$ is the pair correlation function) is nonnegative. The structure factor plays an important role in the theory of scattering, and its nonnegativity is a fundamental constraint on the pair correlations that can occur in any material.

The Poisson summation approach to linear programming bounds generalizes naturally to the Selberg trace formula [69, 33]. Specifically, one can use a pretrace formula to prove density bounds in hyperbolic space [23]. However, several things that are known in the Euclidean case remain mysterious in hyperbolic geometry. In particular, the bounds based on the pretrace formula have been proved only for periodic packings, which are not known to come arbitrarily close to the optimal density in hyperbolic space, and it is not known how to decrease the hypotheses on the auxiliary function $f$ along the lines of the proof for Euclidean space in [23].

4. Optimization and conjectures

As in the spherical case, nobody knows how to choose the optimal auxiliary function in the linear programming bounds. It is not difficult to obtain a trivial bound as follows:

**Exercise 4.1.** Let $\chi_B$ be the characteristic function of the unit ball centered at the origin in $\mathbb{R}^n$. Show that the convolution $f = \chi_B * \chi_B$ satisfies the hypotheses of Theorem 3.1 and yields an upper bound of 1 for the sphere packing density.

Despite the triviality of the bound, this function is of some interest [71], but better constructions are needed if we are to prove nontrivial bounds. See, for example, §6 of [15] for constructions based on Bessel functions.

The behavior of the optimized linear programming bound in $\mathbb{R}^n$ as $n \to \infty$ is unclear. Cohn and Zhao [23] showed that it is at least as good as the Kabatiansky-Levenshtein bound of $2^{-0.5990 \cdots + o(1)n}$, while Torquato and Stillinger [76] showed that it can be no better than $2^{-0.7786 \cdots + o(1)n}$. In particular, it comes nowhere near the density of $2^{-1 + o(1)n}$ attained by the best sphere packings currently known, although it might come much closer than the Kabatiansky-Levenshtein bound does. Aside from these constraints, the asymptotics are a mystery.

We will focus instead on how the bounds behave in low dimensions, by which I mean “not tending to infinity” rather than low in the everyday sense. Linear
programming bounds are nearly the best bounds known in four or more dimensions (there is a small improvement based on incorporating one more term from Poisson summation \[46\]). As shown in Figure 1, they are not so far from the truth in eight or fewer dimensions, but they gradually drift away from the current record densities in high dimensions. Note that the jaggedness of the record densities reflects their subtle dependence on the dimension.

The most remarkable feature of Figure 1 is that the curves appear to touch in eight and twenty-four dimensions. If true, this would settle the sphere packing problem in those dimensions, without the difficulties that plague three dimensions.

**Conjecture 4.2** (Cohn and Elkies \[15\]). *The linear programming bounds for sphere packing density in \(\mathbb{R}^n\) are sharp when \(n = 2, 8,\) or \(24\).*

Equality holds to at least fifty decimal places \[21\], but no proof is known. It is furthermore conjectured that the linear programming bounds for energy are sharp, which would lead to universal optimality in Euclidean space \[17\], \(\S 9\).

Examining the proof of Theorem 3.1 shows that the auxiliary function \(f\) proves a sharp bound for a lattice \(\Lambda\) iff \(f(x) = 0\) for all \(x \in \Lambda \setminus \{0\}\) and \(\hat{f}(t) = 0\) for all \(t \in \Lambda^* \setminus \{0\}\). In other words, all we have to do is to ensure that \(f\) and \(\hat{f}\) have certain roots without developing any unwanted sign changes. That sounds like a manageable problem, but unfortunately it seems difficult to control the roots of a function and its Fourier transform simultaneously.

\[1\] Viazovska \[80\] has recently proved the conjecture for \(n = 8\).
Linear programming bounds seem not to be sharp in $\mathbb{R}^n$ except when $n = 1, 2, 8,$ or $24$. We can’t rule out the possibility of sharp bounds in other dimensions, but nobody has been able to identify any plausible candidates. The $n = 1$ case follows from Exercise [1.1] but sharpness is not known even for $n = 2$, let alone 8 or 24. That makes it seem all the more mysterious: eight or twenty-four dimensions could be truly deep, but two dimensions cannot transcend human understanding.

The strongest evidence for the sharpness of these bounds is the numerics, but there are also analogies with related bounds that are known to be sharp in these dimensions, such as those for the kissing problem [50, 59]. It is worth noting that the kissing bounds are not just sharp, but sharp to an unnecessary degree. Because the kissing number is an integer, any bound with error less than 1 could be truncated to the exact answer, but that turns out not to be necessary. In particular, the bound in Theorem [1.1] is generally not an integer, but for the kissing problem it miraculously turns out to be integral in $\mathbb{R}^8$ and $\mathbb{R}^{24}$: it is exactly 240 in $\mathbb{R}^8$ and exactly 196560 in $\mathbb{R}^{24}$. This unexpected exactness raises the question of whether sharp bounds hold also for quantities such as packing density, where integrality does not apply, and indeed they do seem to.

The computations behind Figure 1 are based on numerical optimization within a restricted class of auxiliary functions. Specifically, they use functions of the form $f(x) = p(|x|^2)e^{-\pi|x|^2}$, where $p$ is a polynomial of one variable. Such functions are relatively tractable, while being dense among all reasonable radial functions.

To carry out explicit computations, it is convenient to write $p$ in terms of an eigenbasis of the Fourier transform:

**Exercise 4.3.** Let

$$\mathcal{P}_k = \left\{ \text{functions } x \mapsto p(|x|^2)e^{-\pi|x|^2} \text{ on } \mathbb{R}^n \mid p \text{ is a polynomial and } \deg(p) \leq k \right\}.$$  

Prove that $\mathcal{P}_k$ is closed under the Fourier transform. What are the eigenvalues of the Fourier transform on $\mathcal{P}_k$? Show that the polynomials $p$ corresponding to an eigenbasis are orthogonal with respect to a certain measure on $[0, \infty)$, and compute that measure.

The most general approach to optimizing the linear programming bounds over $\mathcal{P}_k$ is to impose the sign conditions on $f$ and $\hat{f}$ via sums of squares and then optimize using semidefinite programming [60]. This technique will produce the best possible polynomial $p$ of any given degree. (Another approach is to force roots for $f$ and $\hat{f}$ and then optimize the root locations [15].) However, we cannot obtain a sharp bound by using polynomials, because they have only finitely many roots. The best we can do is to approximate the optimal bound.

By contrast, in the spherical case we can prove sharp bounds using polynomials. That is one reason why linear programming bounds are so much more tractable for spheres than they are in Euclidean space.

Numerical computations have thus far shed little light on the high-dimensional asymptotics of linear programming bounds. These bounds are difficult to compute precisely in high dimensions, because such computations seem to require using high-degree polynomials. Computing the linear programming bound in $\mathbb{R}^{1000}$ to fifteen decimal places would be an impressive benchmark, which might be possible but would not be easy. Even just a few decimal places would be interesting, as would an order of magnitude estimate in $\mathbb{R}^{10000}$. 
Table 2. Numerically computed Taylor series coefficients of the hypothetical sphere packing functions in $\mathbb{R}^n$, normalized so $f(0) = \hat{f}(0) = 1$.

| $n$ | function | order | coefficient | conjecture |
|-----|-----------|-------|-------------|------------|
| 8   | $f$       | 2     | $-2.700000000000000000000000000\ldots$ | $-27/10$   |
| 8   | $\hat{f}$ | 2     | $-1.500000000000000000000000000\ldots$ | $-3/2$     |
| 24  | $f$       | 2     | $-2.6276567765567765677656776\ldots$ | $-14347/5460$ |
| 24  | $\hat{f}$ | 2     | $-1.314102564102564102564102564\ldots$ | $-205/156$ |
| 8   | $f$       | 4     | $4.216751240968298210998965628\ldots$ | ?           |
| 8   | $\hat{f}$ | 4     | $-1.23976907029598026220596589\ldots$ | ?           |
| 24  | $f$       | 4     | $3.8619903167183007758184168473\ldots$ | ?           |
| 24  | $\hat{f}$ | 4     | $-0.7376727789015323203799539712\ldots$ | ?           |

Even without being able to prove that the linear programming bounds are sharp in $\mathbb{R}^8$ and $\mathbb{R}^{24}$, they can be combined with further arguments to prove optimality among lattices:

**Theorem 4.4** (Cohn and Kumar [18]). The Leech lattice is the unique densest lattice in $\mathbb{R}^{24}$.

See also the exposition in [16]. Aside from $\mathbb{R}^{24}$, the optimal lattices are known only in up to eight dimensions [9, 79].

Cohn and Miller observed that the hypothetical auxiliary functions proving sharp bounds in $\mathbb{R}^8$ and $\mathbb{R}^{24}$ have additional structure, which has not yet been explained. The patterns are prettiest if we rescale the function $f$ and its input so that $f(0) = \hat{f}(0) = 1$, in which case the linear programming bounds amount to minimizing the radius $r$ such that $f(x) \leq 0$ for $|x| \geq r$ (see Theorem 3.2 in [15]). Then the quadratic Taylor coefficients appear to be rational numbers:

**Conjecture 4.5** (Cohn and Miller [21]). The quadratic Taylor coefficients of the optimal radial functions $f$ and $\hat{f}$, normalized as above with $f(0) = \hat{f}(0) = 1$, are rational numbers when $n = 8$ or $n = 24$, as shown in Table 2.

Because $f$ and $\hat{f}$ are even functions, the odd-degree Taylor coefficients vanish. The fourth-degree coefficients shown in Table 2 remain unidentified. If all the coefficients could be determined, it would open the door to solving the sphere packing problem in $\mathbb{R}^8$ and $\mathbb{R}^{24}$. 
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