NOTES ON LOVASZ THETA

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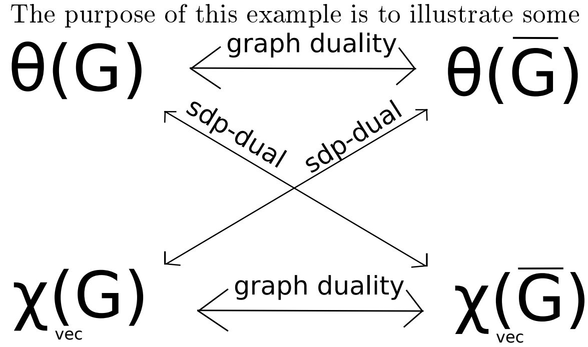
The purpose of this example is to illustrate some of the structure to $\vartheta(G)$.



Though the quantities above are scalars, they arise from arrangements of vectors. I will write down the vectors associated with each quantity above when G is the Petersen Graph.

Defining ϑ

First, we need a series of definitions to define ϑ[5]:

Definition 1. Given a graph G, an orthonormal representation of G is a mapping $r : V(G) \to \mathbb{S}^n \subset \mathbb{R}^{n+1}$ (for some $n \in \mathbb{N}$) such that if $i \neq j \in V(G)$, with $i \not\sim j$, then $r(i) \perp r(j)$. (Be careful: a vertex is not adjacent to itself).

Note that each graph has at least one representation, where v maps the verticies each to its own orthonormal vector.

Definition 2. A valuation of an orthonormal representation $val(r)$ is

$$\min_{\psi} \max_{v \in V(G)} \frac{1}{\left(\psi^T r(v)\right)^2}$$

where ψ ranges over all unit vectors (of the target space of r).

Given an orthonormal representation, its valuation is how tightly it can be embedded into a cone around some vector (ψ).

Definition 3. Define $\vartheta(G)$ to be the minimum valuation over all orthonormal representations of G.

We can show that this minimum is actually attained. We will use Bolzano-Weirstrass. To see this, fix n, and consider the orthonormal representations of the form: $v : V(G) \to \mathbb{S}^{n-1} \subset \mathbb{R}^n$. Observe that $\vartheta(G)$ remains unchanged if we require that $\psi = (1, 0, 0, 0 \dots)$: These valuations are defined by an inner product, which will not change if we apply a fixed unitary U to every vector. Choose U to send $\psi \mapsto (1, 0, 0, 0 \dots)$.

Fixing ψ, take a sequence of orthonormal representations whose values converge to $\vartheta(G)$. Observe that these orthonormal representations themselves can be considered as bounded vectors of dimension $n \cdot V(G)$, by concatenating all $V(G)$ vectors of dimension n. By the Bolzano-Weirstrass theorem, these have a convergent subsequence, so there is an accumulation point, r_∞, which we must show is an orthonormal representation.

Our convergent subsequence of orthonormal representations gives rise to $V(G)$ convergent sequences of vectors. We must show that each sequence of vectors goes to a unit vector, and that when $i \not\sim j$, with $i \neq j$, we have $r_\infty(i)^T r_\infty(j) = 0$. Both of these are consequences of the fact that dot products are continuous: $0 = \lim_{n\to\infty} r_n(i)^T r_n(j) = (\lim_{n\to\infty} r_n(i))^T (\lim_{n\to\infty} r_n(j))$.

There is no claim that such optimal representations are unique.

Graphs

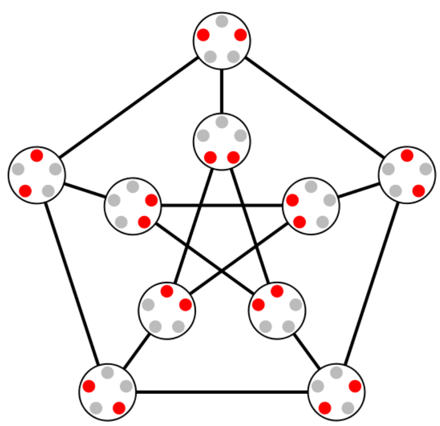
Definition 4. Define the Kneser Graph $k(n,r)$ to have $\binom{n}{r}$ verticies labeled by r-element subsets from a universe of size n. Two verticies are adjacent if their corresponding sets are disjoint. We assume that $n \geq 2r$

Kneser graphs are vertex and edge transitive. Given any two verticies (edges), there is an automorphism which sends one to the other.

Theorem 5. *If G is vertex and edge transitive, then $\vartheta(G)\vartheta(\overline{G}) = n$, and $\vartheta(G) = \frac{-n\lambda_n}{\lambda_1 - \lambda_n}$*

This powerful theorem was originally used to find $\vartheta(k(n,r))$. The proof of the theorem builds on the relations in the diagram.

Definition 6. The Petersen Graph, P, is the Kneser graph, $k(5,2)$.



We start with some graph properties.

Claim 7. The clique number of the kneser graph $\omega(k(n,r)) = \lfloor \frac{n}{r} \rfloor$, so $\omega(P) = 2$

A clique corresponds to a collection of disjoint sets.

Claim 8. [9]The coloring number $\chi(k(n,r)) = n - 2r + 2$, so $\chi(P) = 3$

This was a big open problem for many years. The optimal coloring is the following: Order the elements of the universe $u_1, \ldots, u_n$, and divide them into 3 pieces with sizes $n-2r$, r and r. Let x be an r-set. If it intersects the first piece, color x with the color i, where $i = \min\{i \mid u_i \in x\}$. Otherwise, x is contained entirely in the last two pieces. These remaining verticies form a subgraph, where each vertex has a unique neighbor, and these can be colored with two colors.

Claim 9. The independence number of the kneser graph is $\alpha(k(n,r)) = \binom{n-1}{r-1}$, so $\alpha(P) = 4$

The collection of r-subsets which each contain u_1 is a set of this size. It isn't hard to show this is optimal.

Claim 10. [9]The clique covering number is $q(k(n,r)) = \left\lceil \frac{\binom{n}{k}}{\lfloor \frac{n}{k} \rfloor} \right\rceil$, $q(P) = 5$

$\vartheta(k(n,r)) = \binom{n-1}{r-1}$, and $\vartheta(k(n,r)) = \frac{n}{r}$, so $\vartheta(P) = 4, \vartheta\left(\overline{P}\right) = \frac{5}{2}$

This is proven by Theorem 5 and some tricky algebra, but this avoids (or at least obscures) creating explicit orthonormal representations, which is the point of this example.

Relations between Graph Constants

Theorem 11. $\alpha(G)\chi(G) \geq \mid V(G) \mid$

Each color is an independent set, and a proper coloring colors every vertex.

Theorem 12. *For any graph G, $\alpha(G) \leq \vartheta(G) \leq \chi\left(\overline{G}\right) = q(G)$*

In an orthonormal representation, an independent set, α, of G must be sent to a collection of pairwise independent vectors. For such vectors, it is easy to see that $\max_{v_i \in \alpha} \frac{1}{(\psi^T r(v_i))^2}$ is minimized when $\psi = \frac{\sum_{v_i \in \alpha} r(v_i)}{\sqrt{|V(G)|}}$ (when ψ is between all the vectors.) In this case, $\frac{1}{(\psi^T r(v_i))^2} = \mid \alpha \mid$, and this lower bound holds for all orthonormal representations. This shows $\alpha(G) \leq \vartheta(G)$.

Suppose we have clique cover of size $q(G)$. Define an orthonormal representation by choosing $q(G)$ pairwise orthonormal vectors. Send each clique to one of these vectors. This provides an explicit orthonormal representation with valuation $q(G)$. The minimum over all orthonormal representations may be less.

Orthonormal Representations

We start with the graph $\overline{k(n,r)}$ and construct an optimal orthonormal representation in dimension n, with orthonormal basis $u_1, \ldots, u_n$ (overloading the names of the basis elements with the elements of the universe) The choice is obvious: disjoint sets need to go to orthonormal vectors. Set $u_i^T r(v_j) = \frac{1}{\sqrt{r}}$ if $u_i \in v_j$, and 0 otherwise. Set $\psi = \frac{1}{\sqrt{n}}(1, 1, \ldots, 1)$. It is immediate that this is an orthonormal representation with valuation $\frac{1}{(\psi^T r(v_i))^2} = \frac{r \cdot n}{r^2} = \frac{n}{r}$. This O.R. spans a space of dimension 5.

Definition 13. Given an orthonormal representation, we can define the cost of a vertex to be $c(v) = \left(\psi_1^T(r_1(v_i))\right)^2$. This corresponds to the quantum-mechanical probability of measuring $r_1(v_1)$ when measuring from state ψ.

Theorem 14. [4]*(Certification of Orthonormal Representations): if we have two orthonormal representations r_1, r_2 of G and $\overline{G}$ and for all $i \in V(G)$ we have $c_1(v_i) = \frac{1}{\vartheta}$, and we also have $\sum_i c_1(v_i) c_2(v_i) = 1$, then $\vartheta = \vartheta(G)$*

Proof. We have the explicit orthonormal representation r_1, so $\vartheta(G) \leq \vartheta$. For the other direction, we use an alternate definition ϑ, $\vartheta(G) = \max_{Rep(\overline{G})} \sum_i c(v_i)$.

$$\min_{r\in O.R.(G)} \max_i \frac{1}{c_r(v_i)} = \vartheta(G) \leq \sum_i \vartheta c_1(v_i) c_2(v_i) = \sum_i c_2 v_i \leq \max_{r\in O.R.(\overline{G})} \sum_i c_r(v_i) = \vartheta(G)$$

□

The argument above also shows that certificates always exist.

The next definition is crucial, and describes the relationship between $\vartheta(G)$ and $\vartheta(\overline{G})$. From the physical perspective, this will relate bell inequalities of completely different experiments. Can this relation be found using the Sheaf Theory?

Definition 15. [3]Given a non-empty closed convex set $P \subset \mathbb{R}^n_+$ with the property that $x \in P$ and $0 \leq x' \leq x$ then $x' \in P$, the antiblocker of P is

$$AB(P) = \left\{x \in \mathbb{R}^n_+ : y^T x \leq 1 \text{ for all } y \in P\right\}$$

The condition that $0 \leq x' \leq x \implies x' \in P$ implies that $AB(AB(P)) = P$.

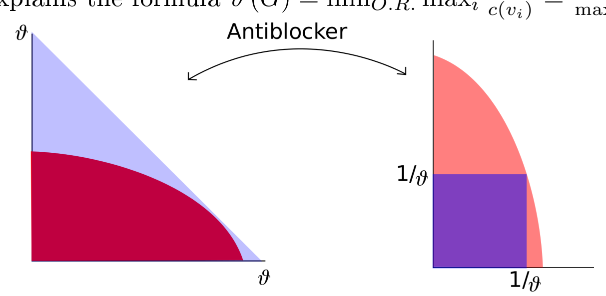
Example 16. Let $P_\vartheta = \left\{y \in \mathbb{R}^n_+ \mid \sum_{i=1}^n y_i \leq \vartheta\right\}$. Then $AB(P) = C_{\frac{1}{\vartheta}} = \left\{x \in \mathbb{R}^n_+ \mid \forall i, x_i \leq \frac{1}{\vartheta}\right\}$.

Proof. Let $y \in P_\vartheta, x \in C_{\frac{1}{\vartheta}}$. Then $y^T x = \sum_{i=1}^n y_i x_i \leq \frac{1}{\vartheta}\sum_{i=1}^n y_i \leq 1$. This shows $C_{\frac{1}{\vartheta}} \subset AB(P_\vartheta)$. Conversely, if $x \notin C_{\frac{1}{\vartheta}}$ for some $i \in V(G)$ $x_i > \frac{1}{\vartheta}$. Choose y such that $y_j = 0$ when $i \neq j$, and $y_i = \vartheta$. Then $y \in P_\vartheta$, and $x^T y > 1$, so $x \notin AB(P_\vartheta)$ □

Definition 17. $TH(G) = \left\{(c(v_i), v_i \in V(G)) \in \mathbb{R}^{V(G)}_+\right\}$. These are assignable probabilities, which (claim) satisfy the hypotheses of definition 6. (Note, these probablities do not need to sum to 1. We allow that some experiments have outcomes which are disregarded. The problem is intractable otherwise.)

Theorem 18. $AB(TH(G)) = TH(\overline{G})$

These concepts provide a geometric description of two definitions of ϑ. ϑ is the maximal of a linear functional over $TH(G)$: $\vartheta(G) = \max_{\overline{O.R.}} \sum_{i=1}^{|V(G)|} c(v_i)$. This linear functional has hyperplanes as its level sets, and the optimal value corresponds to a level set which lies tangent to $TH(G)$. Thus, $\vartheta(G)$ is the smallest simplex S_ϑ such that $TH(G) \subset S_\vartheta$. If we take the antiblocker of this picture, we seek the reciprocal of the largest cube $C_{\frac{1}{\vartheta}}$ such that $C_{\frac{1}{\vartheta}} \subset AB(TH(G)) = TH(\overline{G})$. This explains the formula $\vartheta(G) = \min_{O.R.} \max_i \frac{1}{c(v_i)} = \frac{1}{\max_{O.R.} \min_i c(v_i)}$.



Next, we give an orthonormal representation of $\vartheta(P)$, which will certify the optimality of the orthonormal representation given at the begining of this section.

Assume a basis of size 10, $\{e_{s_1}, e_{s_2}, \ldots, e_{s_{10}}\}$ labeled by the $\binom{5}{2}$ subsets of the graph. Let $\psi = \frac{1}{\sqrt{10}}(1, 1, \ldots, 1)$. Finally, assume that we will have $e^T_{s_i} r(v_j) =$

$x_{|s_i \cap v_j|}$. This is a plausible assumption, because it will result in vectors whose orthongonality relations are invariant with respect to the automorphism group of P.

The fact that intersecting sets must be sent to orthonormal vectors translates into the contstraint

$$x_0^2 + 3x_1^2 + 4x_0x_1 + 2x_1x_2 = 0$$

At the same time, we would like to minimize $\frac{10 \cdot \left(x_2^2 + 6x_1^2 + 3x_0^2\right)}{\left(x_2 + 6x_1 + 3x_0\right)^2}$. According to Wolfram Alpha the minimum is 4, when $(x_0, x_1, x_2) = \left(1, -4 - \sqrt{15}, 6 + \sqrt{15}\right)$, or when $(x_0, x_1, x_2) = (a, b, c) = \left(1, \sqrt{15} - 4, 6 - \sqrt{15}\right)$.

$$\begin{pmatrix} c & b & b & b & b & b & b & a & a & a \\ b & c & b & b & b & a & a & b & b & a \\ b & b & c & b & a & b & a & b & a & b \\ b & b & b & c & a & a & b & a & b & b \\ b & b & a & a & c & b & b & b & b & a \\ b & a & b & a & b & c & b & b & a & b \\ b & a & a & b & b & b & c & a & b & b \\ a & b & b & a & b & b & a & c & b & b \\ a & b & a & b & b & a & b & b & c & b \\ a & a & b & b & a & b & b & b & b & c \end{pmatrix}$$

These vectors span a space of dimension 6.

Remark 19. For any given graph G, it is not true that all optimal orthogonal representations have the same dimension. For example, there are two optimal orthonormal representations of C_4: $\{(0,1), (0,1), (1,0), (1,0)\}$ with handle $\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right)$, and $\{(a,a,0), (a,-a,0), (a,0,a), (a,0,-a)\}$ with handle $(1,0,0)$.

Finally, we apply the certification theorem. For the O.R. above, each cost is $\frac{1}{4}$, and $\sum_{i=1}^{10} \frac{1}{4} \cdot \frac{2}{5} = 1$. Hence, the O.R. above is optimal. Similarly, our *O.R.* of $\overline{K(n,r)}$ can be seen to be optimal.

Vector Colorings of Graphs

Definition 20. Given a graph G, we assign a unit vector to each vertex. This time, we would like adjacent verticies to be sent to vectors whose dot product is as negative as possible. If $\chi(G) = k$, then we can associate each color with a vector in the regular k-simplex in $\mathbb{R}^{k+1}$. Such vectors have inner product $\frac{-1}{k-1}$. In light of this, we define $\chi_{vec}(G) = \min\left\{k \mid v_i^T v_j = \frac{-1}{k-1}\right\}$

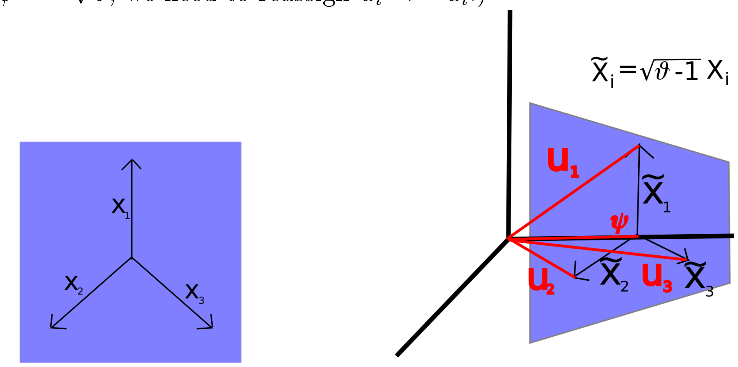
Theorem 21. $\chi_{vec}(G) = \vartheta\left(\overline{G}\right)$

This is proven by the fact that the two problems can be expressed as semidefinite-programming duals of one another. (The duality is between χ_{vec} and $\max_{\overline{O.R.}} \sum \left(\psi^T v_i\right)^2$.) Alternatively, there is a concrete way to move between optimal representations of the coloring problem and optimal representations for ϑ.

Proposition 22. *A vector coloring x_i is optimal (having value ϑ) iff $u_i = \frac{1}{\sqrt{\vartheta}}\left(\psi + \sqrt{\vartheta - 1}x_i\right)$ is an optimal Orthonormal representation (also having value ϑ).*

Proof. If x_i is an optimal vector-coloring for G with coloring number ϑ, and ψ is some unit vector orthogonal to each x_i, then we obtain an orthonormal representation $u_i = \frac{1}{\sqrt{\vartheta}}\left(\psi + \sqrt{\vartheta - 1}x_i\right)$. First, observe that these are all unit vectors. Secondly, let $u_i \neq u_j$ correspond to non-adjacent verticies in $\overline{G}$, so that $x_i^T x_j = \frac{-1}{\vartheta-1}$. Then $u_i^T u_j = \frac{1}{\vartheta}\left(1 + (\vartheta - 1)\frac{-1}{\vartheta-1}\right) = 0$, so u is an orthogonal representation of $\overline{G}$. Also, we have $\frac{1}{(\psi^T u_i)^2} = \vartheta$.

Conversely, if we start with the orthonormal representation with value ϑ (so $\vartheta = \frac{1}{\left(u_i^T\psi\right)^2}$ for all i. We have not yet shown that it's always possible to achieve equality, but it can be seen from the antiblocker picture.) we can recover the coloring by $x_i = \frac{\sqrt{\vartheta}u_i - \psi}{\sqrt{\vartheta-1}}$. Now, if $x_i \sim x_j$ in G, then $x_i^T x_j = \frac{-\sqrt{\vartheta}u_i^T\psi - \sqrt{\vartheta}u_j^T\psi + 1}{\vartheta-1} = \frac{-1}{\vartheta-1}$ so the coloring has value ϑ. Also, $x_i^2 = \frac{(\vartheta+1) - 2\sqrt{\vartheta}u_i\cdot\psi}{\vartheta-1} = 1$. (There is a slight issue: if $u_i \cdot \psi = -\sqrt{\vartheta}$, we need to reassign $u_i \mapsto -u_i$.)



vector coloring of C_3 representation of $\overline{C}_3$(not normalized) □

Next, we will provide an optimal vector coloring of P. Assume a basis of size 5, and that we will map $\star\star\circ\circ\circ \mapsto (a, a, b, b, b)$, and extend this map by permutations of S_5. If x, y are two vector representations of intersecting sets, we would like to minimize

$$min_{a,b}\frac{x^T y}{\|x\|\,\|y\|} = \frac{4ab + b^2}{2a^2 + 3b^2}$$

The minumum occurs at $a = -3, b = 2$, and gives

$$\frac{x^T y}{\|x\|\,\|y\|} = \frac{-24 + 4}{18 + 12} = -\frac{2}{3} = \frac{-1}{\frac{5}{2} - 1}$$

Using numpy.linalg, we can find that these vectors span a space of dimension 4.

Finally, an optimal vector coloring of $\overline{P}$ can be found by assuming a basis of size 10 (the same basis we used for $\vartheta(P)$) and three variables, x_0, x_1, x_2. This gives us the optimization problem:

$$min_{x_0,x_1,x_2}\frac{x^T y}{\|x\|\,\|y\|} = \frac{x_0^2 + 3x_1^2 + 4x_0x_1 + 2x_1x_2}{3x_0^2 + 6x_1^2 + x_2^2}$$

The minimum (according to Wolfram) is found at $\left(-\frac{1}{\sqrt{18}}, \frac{1}{\sqrt{18}}, -\frac{1}{\sqrt{2}}\right)$ and gives

$$\frac{x^T y}{\|x\|\,\|y\|} = \frac{\frac{1}{18} + \frac{3}{18} - 4\frac{1}{18} - 2\frac{1}{6}}{3\frac{1}{18} + 6\frac{1}{18} + \frac{1}{2}} = \frac{-6}{18} = \frac{-1}{4-1}$$

This spans a space of dimension 5.

Problem 23. Since we have established that vector colorings correspond to orthonormal representations, we actually have 2 orthonormal representations of the Petersen Graph and 2 for its complement. Are these the same?

Quantum Measurements

We fix a finite-dimensional vector space, known as the state space. Pure quantum states will be given by unit vectors in this space.

> A projective measurement is described by an observable, M, a Hermitian operator on the state space of the system being observed. The observable has a spectral decomposition
>
> $$M = \sum_m m P_m$$
>
> where P_m is the projector onto the eigenspace of M with eigenvalue m. The possible outcomes of the measurement correspond to the eigenvalues, m, of the observable. Upon measuring the state $|\psi\rangle$, the probability of getting result m is given by
>
> $$\langle\psi|\, P_m \,|\psi\rangle$$
>
> Given that the outcome m occured, the state of the quantum system immediately after the measurement is $\frac{P_m|\psi\rangle}{\sqrt{p(m)}}$[6]

(!) Naimark's Dilation Theorem states that all quantum measurements can be viewed as projective measurements on a larger system. The Spectral Theorem states that a Hermitian operator M always has a decomposition of the form

$$M = \sum_m m P_m$$

where m ranges over real numbers, and the ranges of the P_m's are pairwise orthogonal. Conversely, if we start with a collection of pairwise orthogonal vectors $\{|m\rangle\}_{m=1}^{n}$which span the state space, we can create a Hermitian operator which has those vectors as its eigenvectors: $M = \sum_{m=1}^{n} m\,|m\rangle\langle m|$. Thus, when specifying a PVM, we only need to supply an Orthonormal Basis.

Example 24. Polarizing sunglasses are an example of a PVM.

Light consists of an electric wave inducing a magnetic wave and vice versa. The direction of the electric wave determines the polarization of the light. A photon can be polarized in any 2-dimensional direction. Polarized lenses in sunglasses will let a photon through if it is polarized vertically, and will block it if it is polarized horizontally. The photon hitting the lens is a measurement. The state space is 2-dimensional, corresponding to the polarization directions. We are lucky in this case that polarization between horizontal and vertical directions has a direct physical meaning- that the light is polarized in a diagonal direction. Usually, this is not the case. Let $|v\rangle$ be the state of light which is polarized in the vertical direction and $|h\rangle$be the state of light polarized in the horizontal direction. When a vertically polarized photon hits a vertically polarized lens, it will surely pass through. We represent the observable for this lens by $L = 1 \cdot |v\rangle\langle v| + 0 \cdot |h\rangle\langle h|$. Suppose we have light that is polarized diagonally,

$$|\psi\rangle = \frac{1}{\sqrt{2}}|v\rangle + \frac{1}{\sqrt{2}}|h\rangle$$

The probability of the light passing through the lense is $(\langle v| + \langle h|)|v\rangle\langle v|(|v\rangle + |h\rangle) = \frac{1}{2}$, and if it does so, its state is $\frac{|v\rangle\langle v|\frac{1}{\sqrt{2}}(|v\rangle+|h\rangle)}{\sqrt{\frac{1}{2}}} = |v\rangle$. Observe that the probability that the light passes through the lens is the square of the inner product and the resultant state we're interested in. This is true in general.

Forward Example: The CHSH Inequality

There are two conceivable ways to use the machinery of ϑ to investigate contextuality. Usually we start with a collection of measurements and a linear functional on the outcomes of these measurements. By drawing the exclusion graph of the measurements, we can identify bounds (Bell Inequalities) on these linear functionals. We will see that these bounds are given by ϑ and α. Alternatively, we can go backwards and search for graphs which have a large gap between ϑ and α, then find orthonormal representations to realize these graphs as collections of quantum experiments. Ultimately, this is the direction that I would like to pursue, but we should start with the standard technique[2] first.

As an example of the forward method, we will investigate the CHSH inequality. Imagine Alice and Bob, separated in time and space and unable to communicate. However, they share qubits which make up a quantum state. That is, these particles may be entangled, so the total state space is 4-dimensional. Alice may choose between two measurements A and A', and Bob may also choose between two measurements B and B', so there are 4 total measurements which may occur: $\{AB, A'B, AB', A'B'\}$. Each of Alice and Bob's local measurements yield an outcome of 0 or 1, so each total measurement has 4 possible outcomes.

(One formulation of) the CHSH inequality begins with such a scenario and, if Alice and Bob both choose their experiments uniformly at random, and assigns a value of 1 whenever the their outcomes agree and A, B is not chosen, and a value of -1 whenever their outcomes disagree and A, B is not chosen. If A, B is chosen, then we reverse the valuations, so that 1 is assigned when their measurements disagree and -1 when the agree. The CHSH inequality concerns the expectation of such a valuation. To formalize this, let $E\left(A^{(\prime)}, B^{(\prime)}\right)$ be the probability that the outcomes agree, given that $A^{(\prime)}, B^{(\prime)}$ is measured. Then we have a value

$$S = -E(A, B) + E(A', B) + E(A, B') + E(A', B')$$

The CHSH inequality states that under classical assumptions

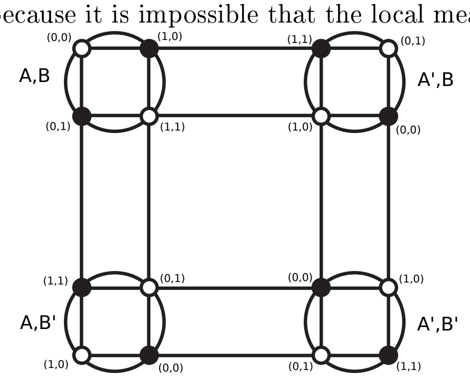
$$S \leq 2$$

We will see where this bound comes from. Yet using quantum mechanics, we may achive a value of

$$S = 2\sqrt{2}$$

Concretely, the measurements which realize this bound are: Alice may either measure in the standard basis (A), or in the basis $\left\{\frac{|0\rangle+|1\rangle}{\sqrt{2}}, \frac{|0\rangle-|1\rangle}{\sqrt{2}}\right\}$ (A'). Bob may either measure in the basis $\left\{\frac{\cos\left(\frac{\pi}{8}\right)|0\rangle-\sin\left(\frac{\pi}{8}\right)|1\rangle}{\sqrt{2}},\frac{\sin\left(\frac{\pi}{8}\right)|0\rangle+\cos\left(\frac{\pi}{8}\right)|1\rangle}{\sqrt{2}}\right\}(B)$ and in the basis $\left\{\frac{\cos\left(\frac{\pi}{8}\right)|0\rangle+\sin\left(\frac{\pi}{8}\right)|1\rangle}{\sqrt{2}},\frac{-\sin\left(\frac{\pi}{8}\right)|0\rangle+\cos\left(\frac{\pi}{8}\right)|1\rangle}{\sqrt{2}}\right\}$ (B'). (!) (TODO: check that this is accurate.)

To derive these bounds we first draw the exclusion graph for this scenario. The verticies of the graph are the 16 total outcomes which may occur (or, if you like, pairs of measurements and outcomes). Edges are drawn between vertices which cannot cooccur. For example, there is an edge between $(0,0 \mid AB)$ and $(1,0 \mid AB')$ because it is impossible that the local measurement A gives both 1 and 0.



Once the exclusion graph, H, is drawn, we obtain a weighting on the vertices which is determined by our valuation. For example, whenever the outcome $(1,1 \mid AB')$ occurs, we add 1 to our counter, and whenever $(0,0 \mid AB)$ occurs, we subtract 1 from our counter. Thus, each vertex gets a weight $w : V(G) \to \mathbb{R}$. We can insist that these weights be positive by adding 1 to all the experiments so that our final weighting corresponds to giving $w(v) = 2$ for the black vertices and $w(v) = 0$ for the white vertices. Typically, and in this case, all of the weights will be the same, except for those which are 0. Our weighting therefore identifies a subgraph, H'

To derive the classical bounds, observe that any classical state of the system must assign outcomes to all measurements, even those which have not occured. This means that a classical state will correspond to an independent set in the graph. It is intuitive (and easy to show, since S is a linear functional) S is maximized at a particular classical state rather than a mixture of them. The maximum value for S, classically, will correspond to an independent set and this independent set will restrict to an independent set of H'. Since $\alpha(H') = 3$, we can recover the classical bound on S by undoing our manipulations to the weighting.

$$S \leq_{classical} 2 \cdot 3 - 4 = 2$$

With respect to quantum mechanics, each of our outcomes corresponds to an eigenvector of an observable. Thus, each vertex in H' receives a vector. If the two outcomes associated with these vectors are exclusive, then the vectors must be orthogonal. Otherwise, it would be possible to measure the system, obtain one outcome, then measure the system again and obtain the other, exclusive outcome.

Therefore, the eigenvectors of the observables form an orthogonal representation of $\overline{H'}$. Recall our dual definition for $\vartheta(G) = \max_{\overline{OR}} \sum_i c(v_i)$ is exactly the maximum expected value in the quantum setting. Thus,

$$S \leq 2 \cdot \vartheta(G) - 4 = 2 \cdot \left(2 + \sqrt{2}\right) - 4 = 2\sqrt{2}$$

In this case, the bound is tight. This is not always the case, because the dimension of the optimal orthonormal representation may be too large.

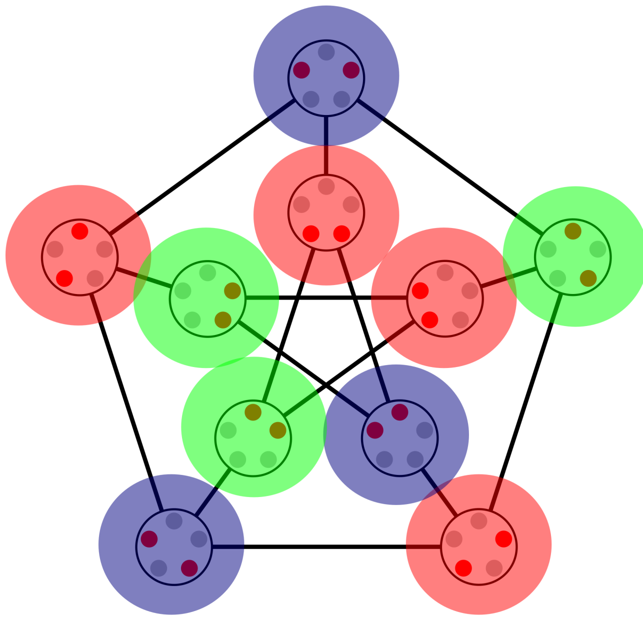
From Orthonormal Representations to Quantum Circuits

Next, we would like to sketch how we might find collections of quantum circuits which exhibit large amounts of contextuality. This procedure comes with many unanswered questions.

(1) Choose an optimal coloring of the graph.
(2) Produce an optimal orthonormal representation for this graph.
(3) Each color corresponds to a collection of pairwise orthonormal vectors. Extend each collection to an orthonormal basis.
(4) Find the unitary transformations from the given bases to the standard (computational) basis.
(5) All unitary transformations can be implemented by quantum gates.
(6) Our circuits consist of these unitary transformations, followed by measurement in the computational basis.

For a quantum circuit which takes some input state, ψ, applies a unitary transformation, U, then measures in the computational basis, the possible outcomes will be the elements of the computational basis. If x is one such basis element, the probability of measuring x is $\langle U\psi, x\rangle^2 = \langle \psi, U^\star x\rangle^2$. It is easier to think of the unitary transformations as moving the computational basis than moving the state. We will think of these quantum circuits as collections of bases under which to measure a particular state.

Since any two orthogonal vectors can be extended to a basis and we can perform a measurement (which will reveal one outcome) in that basis, two orthogonal vectors represent incompatible outcomes.



If we perform these steps, we will arive at $\chi(G)$ quantum circuits whose statistics on the input state ψ cannot be explained classically. Specifically, the results corresponding to vectors in our original Orthonormal Representation (prior to extending to a basis) will occur more often than is possible classically. The dimension of the orthonormal representation, d, is exactly the dimension of the hilbert space in which the quantum circuit lives, so we will need $\lceil \log_2 d \rceil$ qubits to implement such a circuit.

Some questions must be raised:

(1) Does the initial coloring matter?
(2) Can we effectively find the O.R. in step 2?
(3) How can we control the dimension of the optimal orthogonal representation? Can we use a non-optimal representation in a smaller dimension? (I have a specific construction, due to Lovasz in mind.)
(4) How can we control the circuit complexity of our resultant unitaries?
(5) Does it matter how extend our colored sets to bases?
(6) Can any of these circuits be achieved using only Clifford gates? Can we find a result linking the contextual resources (such as magic states) used to form the unitaries, and the final contextuality?

Graph Theory and Optimization

If we have an exclusivity graph G, we can consider the probabilities which may be assigned to vectors $\mathbb{R}_+^{V(G)}$. This identification also maps subgraphs of G to their incidence vectors. Recall that independent sets of our graph correspond to the classical, deterministic probablility distribution. The collection of classical distributions is therefore described by convex sums of our independent sets. The set of classical states is given by the "vertex polytope," VP

$$VP := CvxHull(\{vec_\alpha \mid \alpha \text{ is independent}\})$$

We may express α (we will omit the argument G in the notation) as an optimization problem over this set. Specifically, α may be defined by an integer linear program. We begin with variables $\{x_i \in \{0,1\}\}_{i=1}^{V(G)}$ which are intepreted as: $x_i = 1$ when v_i is in the indendent set in question. Our program is then:

$$\alpha = \max_x \left(\sum_{i=1}^{V(G)} x_i \right)$$

such that $x_i \in \{0,1\}$ and

$$x_i + x_j \leq 1, \text{ for } v_i \sim v_j$$

Equivalently, we could write our constraint as $x \in VP$.

This problem is intractible, so we might formulate a linear program by allowing $x_i \in [0,1]$ to take on a continum of values. The resulting problem is tractible, but is too relaxed. For example, $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$ is a solution to the triangle. Thus, we choose a different generalization of the constraints:

$$\alpha^\star = \max_x \left(\sum_{i=1}^{V(G)} x_i \right)$$

such that $x_i \in [0,1]$ and

$$\sum_{i \in K} x_i \leq 1 \text{ for all cliques } K$$

In this problem, our feasible set is the "fractional vertex packing polytope"

$$FVP = \left\{ x \mid \sum_{i \in K} x_i \leq 1, \forall \text{ cliques } K \right\}$$

This program is important enough to get a name: $\alpha^\star$, the fractional packing number. Moreover, the $\alpha^\star \neq \alpha$, since, for the 5-cycle we have the solution $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$.

The fractional packing number has a nice interpretation: If our variables x_i correspond to probabilities, then our constraint enforces that the sum of probabilities of pairwise exclusive events be bounded by 1, which is implied by one of Kolmogorov's Axioms for probability. General probabilistic models have their Bell Inequalities bounded by $\alpha^\star$ rather than ϑ.

This problem is NP-hard because there may be exponentially many cliques. For perfect graphs, however, $\alpha = \alpha^\star$ and both are polynomial-time computable.

Theorem 25. $FVP\left(\overline{G}\right) = AB\left(VP\left(G\right)\right)$.

Suppose $x \in FVP\left(\overline{G}\right)$. If we show that $x^T v_\alpha \leq 1$, for all indepdent sets α, we will have shown that $FVP\left(\overline{G}\right) \subset AB\left(VP\left(G\right)\right)$. Since α is an independent set of G, it is also a clique of $\overline{G}$, so $\sum_{a\in\alpha} x_a + \sum_{b \in G-\alpha} x_b \cdot 0 \leq 1 + 0 = 1$. The argument works conversely as well: If $x^T y \leq 1$ for all $y \in VP\left(G\right)$, then $x^T v_\alpha \leq 1$ for all independent α. Again, since these independent α in G become cliques ω in $\overline{G}$, our constraints precisely name FVP.

Linear Programming Duality

Every linear program comes with a dual program with the same optimum. The linear program

$$\text{Max}_x \left\{ c^T x \mid Ax \leq b, x \geq 0 \right\}$$

comes with the dual

$$\text{Min}_y \left\{ b^T y \mid A^T y \geq c, y \geq 0 \right\}$$

If the primal problem asks: “Given my ingredients and recipies for baking various cakes and the profits for each type of cake, how much of each cake should I make in order to maximize my profit? And what is my final profit?” Then the dual problem asks “What is the minimum amount of money I would accept to sell my ingredients, given that I could use them to make cakes and later sell these cakes? And how much money would I make from doing this.” In this formulation, it is intuitive that the primal and dual problems will have the same optimal.

Another way to think about the dual program that it provides upper bounds for the primal problem. In this perspective, the new variables y refer to different ways to linearly combine our constraint equation to achive(on the left side) a linear functionals $A^T y$ which is an upper bound on our primal functional, c. Meanwhile, on the right side of the inequality, we get $b^T y$, so this is an upper bound[1].

A third way to think about the dual problem is via Lagrange Multipliers. When optimizing a function over a feasible set, at the optimal solution, the direction in which the function increases the fastest increase must be parallel to the normal of the feasible set. The level sets of our objective function are hyperplanes, and our feasible set is a polytope. Clearly, maxima will occur at a vertex of the polytope. At this point, we will be able to combine the normals (which define the facets adjacent to the vertex) linearly, with non-negative coefficients to arrive at the normal of the objective function.

$$L(x, \lambda) = c^T x - \sum_i \lambda_i a_i^T x$$

In the dual formulation of $\alpha^\star$, we want to minimize the sum of cliques, such that the sum of cliques over any single vertex is at least one. Let $\{y_i \in [0,1]\}_N$, where N is the total number of cliques in the graph.

$$\alpha^\star = \min_y \left(\sum_{i=1}^N y_i \right)$$

under the constraints $y_i \in [0,1]$. For every vertex v,

$$\sum_{y_i \ni v} y_i \geq 1$$

Observe that if we form the associated integer linear program by restricting $y_i \in \{0,1\}$, then we will have the clique covering problem, so $\alpha^\star$ may also be also called $q^\star$. Thus, α and q are an example of dual integer linear programs which do not agree.

ϑ as a Semidefinite Program

Semidefinite programs are "vector relaxations." Instead of integers or real numbers, our variables range over vectors. In the case of ϑ, these are our Orthonormal Representations. These collections of vectors are in perfect correspondence with positive semidefinite matricies. A symmetric matrix $m \in \mathbb{R}^n \times \mathbb{R}^n$ is called positive semidefinite if $\langle x, mx \rangle \geq 0$ for all $x \in \mathbb{R}^n$. If this is the case, then we can define a new inner product as $(x, y) = \langle x, my \rangle$, sans positive-definiteness. To look at the entries of m, we can set x and y to be members of the basis. The ij^{th} element of m will be $m_{ij} = \langle e_i, me_j \rangle = (e_i, e_j)$. In other words, the matrix m tells us how our new inner product behaves on our basis elements. The argument also works conversely, so positive semidefinite matricies are in $1-1$ correspondence with gram matricies.

A semidefinite program is of the form

$$Min_X\,(C \cdot X) = Min_X\,(TR\,(CX))$$

such that X satisfies

$$X \succeq 0, \{D_i \cdot X = p_i\}_{i=1}^k$$

In such a problem, we will be supplied with the k $n \times n$ symmetric matricies C and $\{D_i\}$, along with real numbers $\{p_i\}_{i=1}^k$.

The notation $X \succeq 0$ states that X be positive semidefinite. As in the linear programming case, our objective function is some linear function of the variables. We are allowed linear equality constraints on the entries of X, which are in effect constraints of linear combinations of dot products of our vector assignments.

Rather than supplying the linear equality constraints $\{D_i \cdot X = p_i\}_{i=1}^k$, we could express the feasible set directly, in the form $X\,(y) = G_0 + \sum_{i=1}^m (y_i G_i)$ ard requiring that $X\,(y) \succeq 0$. Set $d_i = C \cdot G_i$. We obtain one equivalent formulation:

$$Min_y d^T y$$

such that

$$X\,(y) \succeq 0$$

Theorem 26. *We can express ϑ as a semidefinite program.*

Proof. Consider the following program, which computes the vector chromatic number:

$$\frac{-1}{\vartheta - 1} = \min_m\,(\alpha)$$

such that $m \succeq 0$ and

$$m_{ij} = \alpha \text{ if } v_i \sim v_j$$

$$m_{ii} = 1$$

It's clear that the program computes the vector chromatic number, but we have to justify that it is a semidefinite optimization problem, as defined above. In particular, the constraint $m_{ij} = \alpha$ is problematic, since α is our objective function. We can replace these constraints with a set of constraints which requires that all m_{ij}

where $v_i \sim v_j$ be equal. To do this, order the edges $e_1, e_2, \ldots, e_{E(G)}$ arbitrarily, and require that $m_{e_i} = m_{e_{i+1}}$. Rather than minimizing α, we can minimize m_{e_1}. Then we arrive at an equivalent problem, which is clearly semidefinite. Let $y \in \mathbb{R}^{k+1}$, and $d = (1, 0, 0, \ldots)$ Then

$$\frac{-1}{\vartheta - 1} = \min\left(d^T y\right)$$

subject to

$$I + y_1 A + \sum_{i=2}^{k} y_i D_i = M(y) \succeq 0$$

Here, J is the matrix of all 1's, $A \in \mathbb{R}^{n \times n}$ is the adjacency matrix of the graph, which which has the i, j^{th} entry 1 when $v_i \sim v_j$, and 0 otherwise. D_i's are the collection of matricies with 1 entry of 1 in the i, j^{th} entry where $v_i \not\sim v_j$.

Observe that if we scale the solution to the vector coloring problem so that each vector has length $\sqrt{\vartheta - 1}$, then this will imply that the dot products of adjacent vectors are -1. And conversely, if we have a solution to the scaled problem we can recover a solution to the original problem. Hence,

$$\vartheta - 1 = \frac{1}{n} I \cdot Z$$

subject to the constraints that

$$Z_{11} = Z_{22} = \cdots = Z_{n,n};\; Z_{ij} = -1 \text{ if } v_i \sim v_j; Z \succeq 0$$

□

Definition 27. Suppose we have semidefinite program in the second formulation. Its dual is defined[8] as

$$Max_Z\left(-G_0 \cdot Z\right)$$

such that

$$Z \succeq 0, \{G_i \cdot Z = d_i\}_{i=1}^{m}$$

Just as the linear programming duality arises from finding bounds on the optimal values for the primal program, the duality in semidefinite programming also arises in this way, since

$$d^T y + Z \cdot G_0 = \sum_{i=1}^{m} \left(Z \cdot G_i\right) y_i + Z \cdot G_0 = Z \cdot G(y) \geq 0$$

so

$$d^T y \geq -G_0 \cdot Z$$

In fact, we have equality, assuming that there is a positive definite feasible matrix in either the primal or dual problem. We can see that this occurs exactly when $Z \cdot G(y) = 0$. (!) This is the antiblocker theorem.

Theorem 28. *We can express ϑ as a semidefinite program*[5]*:*

$$\vartheta = \max (J \cdot B)$$

subject to

$$b_{ij} = 0 \text{ if } v_i \sim v_j; Tr(B) = 1$$

Where J is the 1's matrix (so $J \cdot B$) is the sum of entries in B.

Proof. We will take the dual of the semidefinite program is Theorem 27.

$$\frac{-1}{\vartheta - 1} = \max_Z (-I \cdot Z) = \max_Z -Tr(Z)$$

subject to the constraints

$$A \cdot Z = 1, \{D_i Z = 0\}_{i=1}^k$$

The second set of constraints implies that Z_{ij} is 0 whenever $v_i \sim v_j$. It follows that $J \cdot Z = (I + A) \cdot Z = Tr(Z) + A \cdot Z$. Thus, for the optimal $Z^\star$, $J \cdot Z = 1 + \frac{1}{\vartheta - 1} = \frac{\vartheta}{\vartheta - 1}$. Thus, if we scale up all the entries in Z by $\vartheta - 1$, we arrive at the desired semidefinite program. □

Remark 29. The feasible set B is related to the set of Orthonormal Representations in the *max* definition of ϑ. Given an O.R., one can compute its gram matrix and obtain a PSD matrix C such that $Tr(C) = n$. It is not obvious how to interpret the objective function, $J \cdot B$ as relating to $\sum_{i \in V(G)} \left(\psi^T v_i\right)^2$. Lovasz proves[5] our max definition from the SDP. In the course of his proof, he appears(!) to show that the optimal handle is always $\psi^\star = \frac{\sum v_i}{|\sum v_i|}$.

The Ellipsoid Method: Convex Optimization is Polynomial Time

There is a general technique to optimize any linear objective function over any convex feasible set. This technique is slow in practice, but runs in polynomial time. In particular, suggests that semidefinite optimization problems may be solved efficiently. A correct analysis of the technique is complicated because we need to take rounding errors into account. Since the optimal may not have a terminating decimal representation, we need to allow solutions which only approximate that optimal value up to ϵ, and we need to show that this approximation is polynomial in $\log\left(\frac{1}{\epsilon}\right)$. Furthermore, we need to take into account rounding errors in the representation convex set itself. The following description comes from [7]

In the following, a convex body will be modeled as an oracle which, given a point, will either assert that the point is in the convex body, or else it will return a separating hyperplane between the point and the body.

First, suppose that we have some convex body C and we wish to optimize $\max_{x \in C} \left(a^T x\right)$ with $\|a\| = 1$ Suppose we have a function *sample* (C) which takes a convex body and returns a point in that set or correctly asserts that C is empty. We must also assume that C contains a ball $b_{0,r}$ and is contained in a ball $B_{0,R}$. Then we can solve the optimization problem by means of a binary search. We know that $0 \leq \max_x \left\{a^T x \mid x \in C\right\} \leq R$. We can sample x_0 and calculate $a^T x_0$. Then, we consider $C_1 = C \cap \left\{x \mid a^T x \geq \frac{a^T x_0 + R}{2}\right\}$. We can sample again, and if we find a point, x_1, we known that $\max_{x \in C} \left(a^T x\right) \geq a^T x_1$. Otherwise, we know $\max_{x \in C} \left(a^T x\right) \leq a^T x_1$. In either case, we have halved the range of possible values for $\max_{x\in C}\left(a^T x\right)$, so it only takes one more iteration of the algorithm to calculate one more bit of the output. In other words, it is polynomial-time.

Thus, if we can find points inside a convex body, C, we can optimize over C in polynomial time. The ellipsoid method is a technique to find a point inside a convex body. If we know nothing about C, we are left guessing at points and the problem is hopeless. We must assume we are told our convex body is contained in a ball $S(0,B)$.

The ellipsoid method works via ellipsoids whose volumes shrink by constant factors. The first ellipsoid is the ball $S(0,B)$. Then, we guess a point at the center of the ellipsoid, 0. If this fails, the oracle will return a separating hyperplane to us. Call the halfspace containing C, H. We construct a new ellipsoid, which is the smallest ellipsoid containing $S(0,B)\cap H$. Generally, we guess at the center of the current ellipsoid, and if we're wrong, use the resulting hyperplane to construct an new ellipsoid with less volume by a constant (depending on the dimension) factor. These ellipsoids do not work in practice, but a simple (if you ignore precision) way to argue that optimization over a convex body can be achieved in polynomial time.

The ellipsoid method requires a separation oracle. For a semidefinite programming problem, we must be able to decide whether or not a point is in the feasible set, and if not, then we should be able to compute a separating hyperplane. Specifically, we need to be able to determine whether a symmetric matrix is positive semidefinite or not. First, we diagonalize the matrix is $O\left(n^3\right)$ time, thereby writing $M=UDU^T$ where U is orthonormal and D is diagonal. M is positive semidefinite exactly when D has non-negative entries. If D has a negative entry, then we can find a vector c such that U^Tc is the basis vector associated with that entry, and $c^TUDU^Tc=c^TMc<0$. Since $c^TMc=\sum c_ic_jm_{ij}$, this is a linear functional on M which separates M from the positive cone.

Interior Point Methods

Linear programming problems are usually solved by the simplex method, where the vertices of the feasible polytope are examined systematically. Our semidefinite programs do not have polytopes as feasible sets, so there would be infinitely many vertices to check. Instead, we use interior point methods, where we search the interior of the feasible set.

To do this, we assign a barrier function which is infinite at the boundary:

$$\phi(Z)=\begin{cases}\log\left(\det Z^{-1}\right) & \text{if } Z>0\\ \infty & else\end{cases}$$

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