A technique from Lovasz and Szegedy for showing that matrices related to set-functions are PSD

Chris Beck

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The goal in this note is to expose in detail a small but very interesting part of a paper of Lovasz & Szegedy titled "Limits of Dense Graph Sequences". In it, they employ a useful factorization of a class of combinatorial matrices which they can use to see that certain matrices are or are not PSD.

1 Möbius Inversion

It is helpful I think to give a linear-algebra oriented definition of Möbius Inversion to set the stage and fix notation. This part of the exposition is based on chapter 25 in Van Lint & Wilson's textbook.

Let P denote any finite partially ordered set, and let $\mathbb{F}$ denote any field.

Let $\mathcal{M}_{\mathbb{F}}(P)$ denote the algebra of matrices whose rows and columns are indexed by elements of P. (In other words it is the endomoprhism algebra of the vector space $\mathbb{F}^P$.)

The *incidence algebra* $\mathbb{A}_{\mathbb{F}}(P)$ is a subalgebra of $\mathcal{M}_{\mathbb{F}}(P)$, consisting of those matrices which have zeros at all positions (i, j) such that $i \not\leq j$.

(We will usually suppress $\mathbb{F}$.)

Alternatively, $\mathbb{A}(P)$ is the subalgebra generated by the elementary matrices $\{e_{i,j}\}_{i \leq j}$. It is easy to see that this set of matrices, together with the zero matrix, is closed as a monoid under multiplication, so the linear span of these elements is the whole subalgebra.

An element of $\mathbb{A}(P)$ that is important to our exposition is the *zeta function* of P, defined by

$$\zeta(x, y) = \begin{cases} 1 & \text{if } x \leq y \text{ in } P \\ 0 & \text{otherwise} \end{cases} .$$

ζ corresponds to the matrix Z in Lovasz & Szegedy's paper.

Because ζ has ones along the diagonal and is upper triangular otherwise (with respect to any total ordering extending P), ζ has an inverse in $\mathbb{A}(P)$, and the inverse matrix corresponds to the Möbius function of P.

Then (as is well known) the traditional statement of Möbius inversion can be stated linear algebraically: Suppose that f, g are two vectors in $\mathbb{F}^P$, such that $f = \zeta g$ as matrices. Then $\mu f = g$.

The more traditional formulation (which we will use below) is the following:

Theorem 1.1. Let $f : P \to A$ be any function from P to an abelian group A. Let g be the function defined by

$$g(x) := \sum_{x \leq y} f(y) \ ,$$

Then, it also holds that

$$f(x) = \sum_{x \leq y} \mu(x, y) g(y) \ .$$

Proof. If f, g are treated as column vectors, the assumption is equivalent to $g = \zeta f$, and the conclusion can be similarly seen to be equivalent to $f = \mu g$. To be completely formal and allow them to take values in an arbitrary abelian group (as the principle is traditionally stated), we should work over a $\mathbb{Z}$-module rather than a vector space over $\mathbb{F}$, which is sufficient to construct the incidence algebra, and build ζ and μ. Since any abelian group is a $\mathbb{Z}$-module trivially, this proves the traditional formulation. It is possible to prove by an explicit inductive construction that the inverse of ζ exists uniquely, so we can get μ without appealing to linear algebra. We'll omit this here. □

2 An application for PSD matrices

The following is implicit in Lovasz & Szegedy. They call this the "Lindstrom-Wilf formula", although they don't cite any particular source for this and I didn't find any reference for this formula online.

Lemma 2.1. (Lovasz & Szegedy) Let P be a finite lattice. Let f denote any function $f : P \to \mathbb{R}$, and let f' denote the Möbius inverse μf.

Let α denote the matrix defined by $\alpha(S, T) := f(S \cup T)$. Then α is PSD if and only if f' is everywhere nonnegative.

Proof. Let D denote the diagonal matrix defined by

$$D_{x,y} := \begin{cases} f'(x) & x = y \\ 0 & \text{otherwise} \end{cases} \ .$$

The lemma follows from the claim:

Claim 2.2. α can be factorized as

$$\alpha = \zeta D \zeta^T \ .$$

Note that, since ζ^T is not the inverse of ζ (that is μ), this is *not* a diagonalization of α. (As I erroneously claimed in Avi's office.) In particular, it does not imply that all matrices of the form α commute, so far as I know.

The lemma follows directly from the claim. On the one hand, if f' is nonnegative, then D is PSD, so we have, for any vector v,

$$v^T \alpha v = v^T \zeta D \zeta^T v = u^T D u \geq 0 \ ,$$

where $u = \zeta^T v$.

On the other hand, if f' is negative in some location, then clearly D is not PSD – we can take the vector u to be any e_i where $f(i) < 0$, and then we have u such that $u^T D u < 0$.

Then, since ζ is invertible, we can find a v such that $u = \zeta^T v$, and we have found a vector v such that $v^T \alpha v < 0$.

Now, let's prove the claim, which is an application of Möbius inversion.

Proof of Claim. Consider any entry of $\zeta D \zeta^T$, it is by definition

$$\begin{aligned}
\left(\zeta D \zeta^T\right)_{x,y} &:= \sum_{z \in P} \zeta_{x,z} \cdot D_{z,z} \cdot \zeta^T_{z,y} \\
&= \sum_{z \in P} f'(z) \cdot \zeta_{x,z} \cdot \zeta^T_{z,y} \\
&= \sum_{\substack{z \in P \\ x \leq z \\ y \leq z}} f'(z)
\end{aligned}$$

Now we use the fact that P is a lattice and not just a poset, so it has unique joins:

$$= \sum_{x \vee y \leq z} f'(z) \ .$$

This value is clearly equal to $(\zeta f')(x \vee y)$, but since f' is the Möbius inverse μf, by the principle of Möbius inversion this is just $f(x \vee y)$, or $\alpha_{x,y}$ as desired.

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