Flag Algebras on Limits of Graph Sequences

Today, we finally define some algebras $\mathcal{A}$ and $\mathcal{A}^\sigma$. We try to develop an analogue for $P(.,G)$ in the limit. We start by defining $\mathcal{A}$. We denote the set all graphs up to isomorphism by $\mathcal{F}$ and the set of all graphs on exactly ℓ vertices by $\mathcal{F}_\ell$. Let $\mathbb{R}\mathcal{F}$ be the set of all formal linear combinations of graphs in $\mathcal{F}$. This $\mathbb{R}\mathcal{F}$ will be used to derive $\mathcal{A}$. In order to do that, we need to somehow define addition and multiplication on $\mathbb{R}\mathcal{F}$.

1: How to *obviously* define the addition of elements in $\mathbb{R}\mathcal{F}$ and the multiplication by a real number?

Solution: For addition of $a, b \in \mathbb{R}\mathcal{F}$, just add the coefficients together.

Recall we used linear combinations of graphs last time, but they had some extra interpretation using $P(.,G)$. Our goal is to eventually have a similar interpretation for $\mathbb{R}\mathcal{F}$ and $\mathcal{A}$.

2: Let $F_1, F_2 \in \mathcal{F}$. Can you write $F_1 \cdot F_2$ as an element in $\mathbb{R}\mathcal{F}$ inspired by our efforts last time?

Solution:

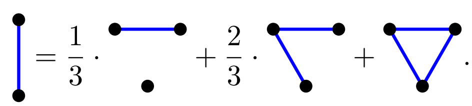
$$F_1 \cdot F_2 = \sum_{F \in F_\ell} P(F_1, F_2; F) F,$$

where $v(F_1) + v(F_2) = \ell$. Notice, there is NO $+o(1)$.

3: How to "define" a multiplication of $a, b \in \mathbb{R}\mathcal{F}$?

Solution: One could say that having $a, b \in \mathbb{R}\mathcal{F}$ it would be possible to do entry wise product from the previous exercise. A small trouble is that $F_1 \cdot F_2$ can be written in many ways as a linear combination so this is not a great multiplication.

In addition to the "uniqueness trouble" in multiplication for $\mathbb{R}\mathcal{F}$, we would also like to enforce identities such as


(1)

We do this by factorizing $\mathbb{R}\mathcal{F}$ by a suitable subspace $\mathcal{K}$. Let $\mathcal{K}$ be a linear subspace of $\mathbb{R}\mathcal{F}$ generated by all elements of the form

$$F - \sum_{F' \in \mathcal{F}_\ell} P(F, F') F', \tag{2}$$

where $F \in \mathcal{F}$ and $v(F) \leq \ell$.

4: What is the value of (2) in our previous interpretation using $P(.,G)$?

Solution: 0

Finally, the algebra $\mathcal{A}$ is $\mathbb{R}\mathcal{F}$ factorized by $\mathcal{K}$. Notice that $a, b \in \mathbb{R}\mathcal{F}$ belong to the same equivalence class iff $a = b + c$ for some $c \in \mathcal{K}$.

This also fixes the uniqueness in multiplication (which we are not proving here). Personal note: I just think of it all as $\mathbb{R}\mathcal{F}$, where some additional equations hold. Not as the formal $\mathcal{A}$. An analogue is $\mathbb{Q}$ for $\mathcal{A}$ and $\mathbb{Z} \times \mathbb{Z}$ for $\mathbb{R}\mathcal{F}$. We get $\frac{1}{2} = \frac{2}{4} = \frac{4}{8} = \frac{3}{6} = \cdots$.

Now we try to make $\mathcal{A}$ somehow useful by providing a similar interpretation as $P(?, G)$ from last time. Notice we do not have $+o(1)$ in multiplication, so we cannot really use $P(?, G)$ but we will use limits of $P(?, G)$.

Definition: A sequence of graphs $(G_n)_{n\in\mathbb{N}}$ is *convergent* if for every finite graph H, $\lim_{n\to\infty} P(H, G_n)$ exists.

Notice that the *limit of convergent sequence* can be viewed as vector of numbers in $[0, 1]$ indexed by all finite graphs, i.e., a function $\mathcal{F} \to [0, 1]$.

5: Show that $(K_n)_{n\in\mathbb{N}}$ is convergent, where K_n is the complete graph on n vertices. What is the limit?

Solution: The limit is quite simple. If H is a complete graph, then the limit of $p(H, K_n)$ is 1, otherwise it is 0.

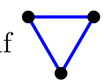
6: Show that $(P_n)_{n\in\mathbb{N}}$ is convergent, where P_n is a path on n vertices. What is the limit?

Solution: The limit is not difficult. For any H that contains an edge, $p(H, P_n)$ is 0 and if H has no edges, then $p(H, P_n) = 1$.

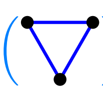
Now we get to the promised replacement of $P(., G)$. Let $Hom(\mathcal{A}, \mathbb{R})$ be the set of all homomorphisms from $\mathcal{A}$ to $\mathbb{R}$. So for any $\phi \in Hom(\mathcal{A}, \mathbb{R})$ and $a, b \in \mathcal{A}$, we have that $\phi(a + b) = \phi(a) + \phi(b)$ and $\phi(a \cdot b) = \phi(a) \cdot \phi(b)$. Since $p(H, G) \in [0, 1]$, we consider only $Hom^+(\mathcal{A}, \mathbb{R})$, which are homomorphism ϕ such that $\phi(H) \geq 0$ for all $H \in \mathcal{F}$. Notice $\phi(\emptyset) = 1$.

It can be proved, that $Hom^+(\mathcal{A}, \mathbb{R})$ corresponds exactly to the convergent sequences of graphs.

Theorem (special for graphs) Let $a \in \mathbb{R}\mathcal{F}$. $\phi(a) = 0$ for all $\phi \in Hom^+(\mathcal{A}, \mathbb{R})$ iff $a \in \mathcal{K}$.

7: Recall that previously we stated Mantel's theorem as  $\leq \frac{1}{2}$ if  $= 0$. What does it formally translate in our new interpretation using $Hom^+(\mathcal{A}, \mathbb{R})$?

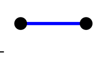
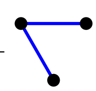
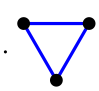
Solution: It is saying that for every $\phi \in Hom^+(\mathcal{A}, \mathbb{R})$ holds that

if $\phi\Big($  $\Big) = 0$ then $\phi\Big($  $\Big) \leq \frac{1}{2}$.

We could also develop the whole flag algebras with $\mathcal{F}$ being *triangle-free* graphs instead of all graphs. Let's call such algebras $\mathcal{A}_{\nabla}$. Then the statement would be that for all $\phi \in Hom^+(\mathcal{A}_{\nabla}, \mathbb{R})$ holds $\phi\Big($  $\Big) \leq \frac{1}{2}$.

We are interested in finding $a \in \mathcal{A}$ such that for EVERY $\phi \in Hom^+(\mathcal{A}, \mathbb{R})$ we have $\phi(a) \geq 0$. If this happens, we just write $a \geq 0$. Note that Hatami and Norin showed that determining if $a \geq 0$ is not algorithmically decidable.

Example of such a was given last time

$0 \leq 3 \cdot$ $-$  $-$  $+ 3 \cdot$  . (3)

Now we explore a way how to obtain various $a \in \mathcal{A}$ such that $a \geq 0$. Last time we also considered labeled graphs with some fixed embedding of a graph σ. By following the same path as for the unlabeled case, we can define $\mathcal{A}^\sigma$. Let $\sigma \in F$ be graph with vertices labeled by $1, \ldots, v(\sigma)$.

- $\mathcal{F}^\sigma$ is the set of all graphs each containing a fixed induced labeled copy of σ.
- $\mathcal{F}^\sigma_\ell$ is the set of elements in $\mathcal{F}^\sigma$ on ℓ vertices.

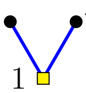
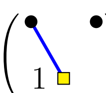
- $\mathbb{R}\mathcal{F}^\sigma$ are all formal linear combinations of elements in $\mathcal{F}^\sigma$.
- $\mathcal{K}^\sigma$ is a linear subspace generated by $F - \sum_{F' \in \mathcal{F}^\sigma_\ell} P(F, F')F'$, where $F \in \mathcal{F}^\sigma$ and $v(F) \le \ell$.
- $\mathcal{A}^\sigma$ is $\mathbb{R}\mathcal{F}^\sigma$ factorized by $\mathcal{K}^\sigma$.
- addition in $\mathcal{A}^\sigma$ comes from $\mathbb{R}\mathcal{F}^\sigma$
- multiplication in $\mathcal{A}^\sigma$ defined as an extension of $F_1 \cdot F_2 = \sum_{F \in F^\sigma_\ell} P(F_1, F_2; F)F$, where $F_1, F_2 \in \mathcal{F}$ and $v(F_1) + v(F_2) - v(\sigma) = \ell$.
- $Hom^+(\mathcal{A}^\sigma, \mathbb{R})$ is the set of homomorphism ϕ^σ, where $\phi^\sigma(F) \ge 0$ for all $F \in \mathcal{F}^\sigma$.
- $F \in \mathcal{F}^\sigma$ is called a *σ-flag*.

8: What is 1 for multiplication in $\mathcal{A}^\sigma$? Let $a, b \in \mathcal{A}^\sigma$ and $ab = a$. What is b?

Solution: $b = \sigma$, it also means the equivalence class of σ in $\mathcal{A}$.

Let σ be fixed. We will describe an interaction between $Hom^+(\mathcal{A}, \mathbb{R})$ and $Hom^+(\mathcal{A}^\sigma, \mathbb{R})$. First, we fix some $\phi \in Hom^+(\mathcal{A}, \mathbb{R})$. This ϕ corresponds to some converging graph sequence $(G_n)_{n \in \mathbb{N}}$. In order to make some connection with $\mathcal{A}^\sigma$, we would need a sequence of labeled graphs in $\mathcal{F}^\sigma$. However, instead of creating a sequence of labeled graphs, we create a sequence of probability distributions generated by picking different copies of σ. For each n separately, we do the following. Pick uniformly at random a labeled copy of σ in G_n, denote result by G_n^σ. This allows us to evaluate $P(F, G_n^\sigma)$ for all $F \in \mathcal{A}^\sigma$. By the random choice of σ in G_n, we get some probability distribution $\mathbf{P}^\sigma_{G_n}$ on the functions $P(., G_n^\sigma)$. These $\mathbf{P}^\sigma_{G_n}$ then weakly converge to a (unique) probability distribution $\mathbf{P}^\sigma_\phi$ on $\phi^\sigma \in Hom^+(\mathcal{A}^\sigma, \mathbb{R})$. We will get back to $\mathbf{P}^\sigma_\phi$ in a bit.

Let σ be fixed. Our next goal is to define an *averaging* operator that can translate expressions from $\mathcal{A}^\sigma$ to $\mathcal{A}$. Let $F \in \mathcal{F}^\sigma$. Since F has a labeled copy of σ, we can view F and (G, θ), where $G \in \mathcal{F}$ is an unlabeled copy of F and θ is a function from $1, \ldots, v(\sigma)$ to $V(G)$ that identifies the labeled copy of σ. Let θ' be an injective function from $1, \ldots, v(\sigma)$ to $V(G)$ chosen uniformly at random. Define $q_\theta(F)$ to be the probability that (G, θ') is isomorphic to F.

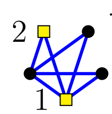
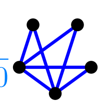
9: Calculate $q_\theta\Bigg($  $\Bigg) = \frac{1}{3}$ $\qquad$ $q_\theta\Bigg($  $\Bigg) = \frac{2}{3}$

Finally, for any type σ and $F \in \mathcal{F}^\sigma$, we define $[\![\cdot]\!]_\sigma : \mathcal{F}^\sigma \to \mathbb{R}\mathcal{F}$ as

$$[\![F]\!]_\sigma = q_\theta(F) \cdot G,$$

where G is an unlabeled F. Its linear extension is then the *averaging operator* $[\![\cdot]\!]_\sigma : \mathbb{R}\mathcal{F}^\sigma \to \mathbb{R}\mathcal{F}$. It is linear mapping, *not* a homomorphism.

10: Calculate

$\Bigg[\!\!\Bigg[$  $\Bigg]\!\!\Bigg]_\sigma = \frac{6}{20}$ 

A *crucial feature* is that if $a \in \mathcal{A}^\sigma$ and $\phi \in Hom^+(\mathcal{A}, \mathbb{R})$, then $\phi([\![a]\!]_\sigma)$ is closely related to the expected value of $\phi^\sigma(a)$, where ϕ^σ is chosen according to $\mathbf{P}^\sigma_\phi$. Specifically,

$$\phi([\![\sigma]\!]_\sigma) \cdot \mathbb{E}_{\mathbf{P}^\sigma_\phi}[\phi^\sigma(a)] = \phi([\![a]\!]_\sigma). \tag{4}$$

This can be viewed as an analogue of $P(B) \cdot P(A|B) = P(A \wedge B)$. Bonus: For a given $\phi \in Hom^+(\mathcal{A}, \mathbb{R})$, it can be directly shown there exists a unique probability distribution $\mathbf{P}^\sigma_\phi$ satisfying (4). This distribution is indeed the weak limit of $(\mathbf{P}^\sigma_{G_n})_{n \in \mathbb{N}}$ obtained from any sequence $(G_n)_{n \in \mathbb{N}}$ that converges to ϕ. Equation (4) is especially useful when $\phi^\sigma(a) \geq 0$ with probability one. In this case, (4) yelds $\phi([\![a]\!]_\sigma) \geq 0$. In particular, we will use that for any $\phi \in Hom^+(\mathcal{A}, \mathbb{R})$ and any $a \in \mathcal{A}^\sigma$

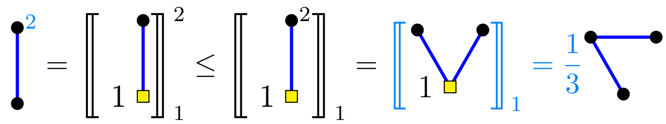
$$\phi([\![a \cdot a]\!]_\sigma) \geq 0.$$

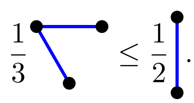
In the simplified notation, we could just write $[\![a \cdot a]\!]_\sigma \geq 0$. Note, the inequality $[\![a^2]\!]_\sigma \geq 0$ can be also obtained from the following flag version of Cauchy-Schwarz inequality

$$[\![a^2]\!]_\sigma \cdot [\![b^2]\!]_\sigma \geq [\![ab]\!]_\sigma^2. \tag{5}$$

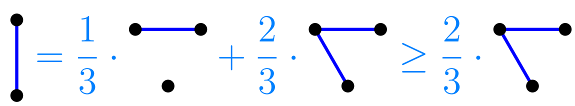
We try another proof of Mantel's theorem. Recall, we consider only triangle-free graphs. We denote the type of one labeled vertex simply by 1.

11: Complete the following inequality into an inequality between unlabeled triangle-free graphs (do not multiply unlabeled graphs)



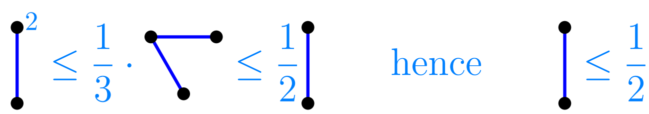
12: Use (1) to show 

Solution:



13: Combine the previous two questions to show Mantel's theorem.

Solution:



Generating $a \geq 0$ using $\mathcal{A}^\sigma$ and $[\![.]\!]_\sigma$

Recall that a symmetric real matrix $M \in \mathbb{R}^{n \times n}$ is *positive semidefinite* if $x^T M x \geq 0$ for all $x \in \mathbb{R}^n$. Denoted by $M \succcurlyeq 0$.

14: How to check if $M \in \mathbb{R}^{n \times n}$ is positive semidefinite?

Solution: All eigenvalues of M are non-negative. $M = U^T U$ for some matrix U. All principal minors are non-negative.

Main observation Let σ be fixed. If $M \succcurlyeq 0$ and X is a vector $(\mathcal{F}_\ell^\sigma)^n$, then for any ϕ^σ holds

$$0 \leq \phi^\sigma\left(X^T M X\right) \qquad \text{hence} \qquad [\![X^T M X]\!]_\sigma \geq 0.$$

Next we show, that using a semidefinite matrices is analogous to using sum of squares.

Let $a \in \mathcal{A}^\sigma$ be a linear combination of σ-flags. Let X be vector of flags in a and let v be a vector of coefficients.

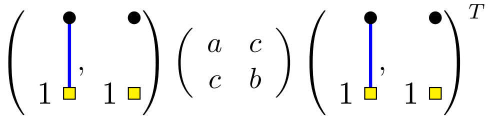
15: Show that $a^2 = X^T M X$ for some matrix $M \succeq 0$. Hint: $M = vv^T$.

Solution: Just expand it: $X^T M X = X^T v v^T X = X^T v \cdot (X^T v) = a \cdot a = a^2$.

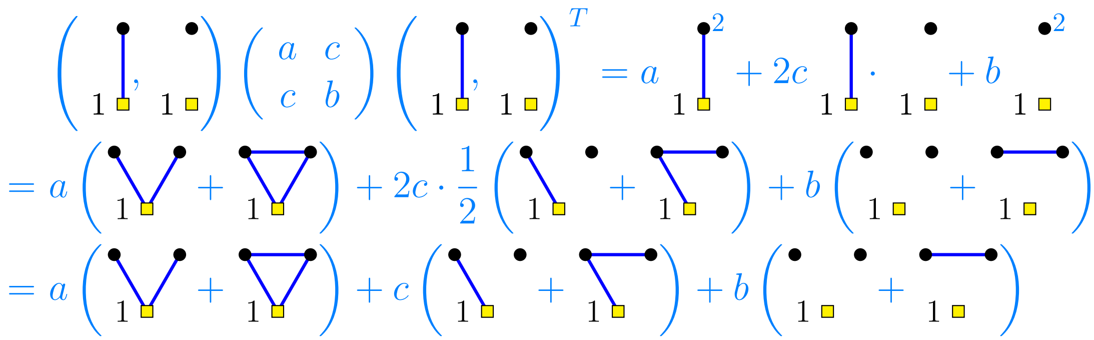
16: In light of the previous exercise, what is X^TMX for general $M \succeq 0$.

Solution: Since we can decompose every $M \in \mathbb{R}^{m\times m}$ into U^TU, we can decompose X^TMX into sum of (at most) m squares.

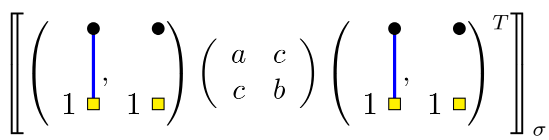
17: Let $M \in \mathbb{R}^{2\times 2}$, σ be one labeled vertex and X be a vector containing all labeled graphs in $\mathcal{F}_2^\sigma$. Evaluate X^TMX, which is can be also written as: (now we are NOT triangle-free)



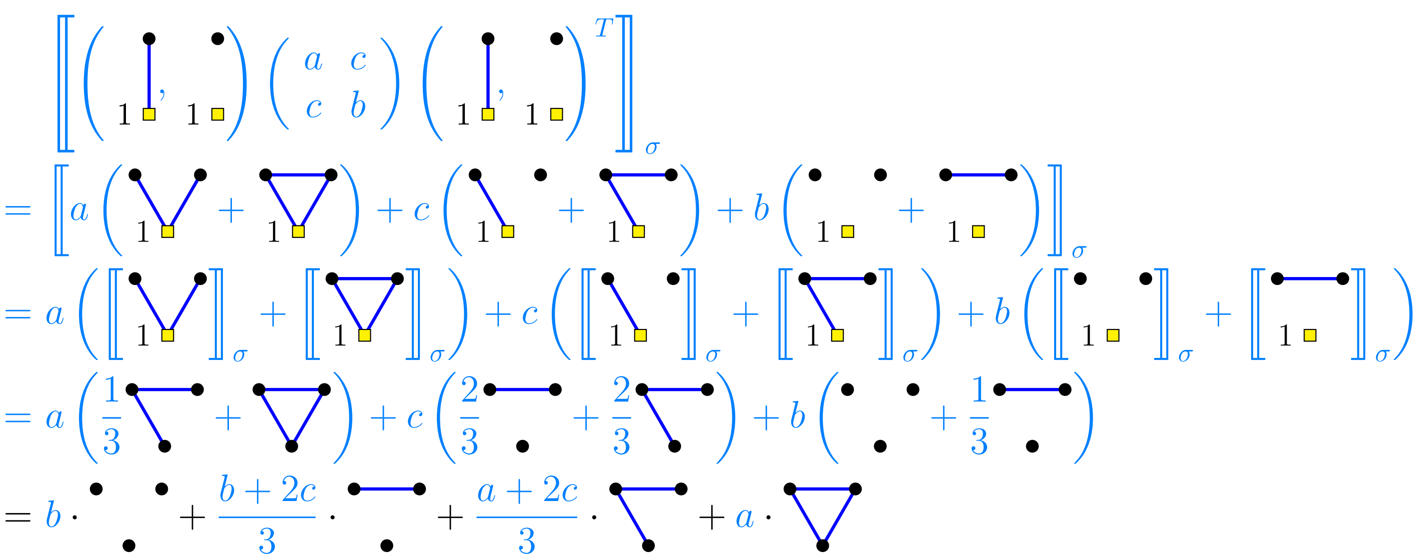
Solution:



18: Use the solution of the previous exercise to evaluate



Solution:



19: Recall that $[\![X^TMX]\!]_\sigma \geq 0$ is true for ANY $M \succcurlyeq 0$. Prove that inequality (3) is valid by finding a suitable M. Hint: Use the last solution.

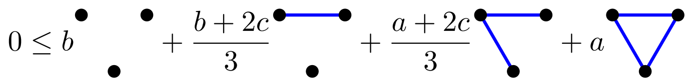
Solution: Take

$$M = \begin{pmatrix} a & c \\ c & b \end{pmatrix} = \begin{pmatrix} 3 & -3 \\ -3 & 3 \end{pmatrix}$$

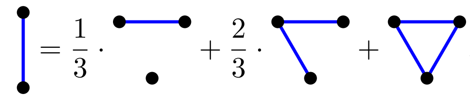
This matrix has eigenvalues 0 and 6 with eigenvectors $(1,1)$ and $(1,-1)$. Plugging it into the last line of previous question gives exactly (3).
It is also possible to see that M is positive semidefinite since all principal minors are non-negative.

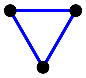
Bonus: A sufficient condition for M being positive semidefinite is that leading principal minors are positive except the last one, which is non-negative. Our matrix satisfies this too. It is easier to verify.

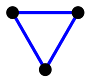
20: We try to prove Mantel's theorem again. Start by summing

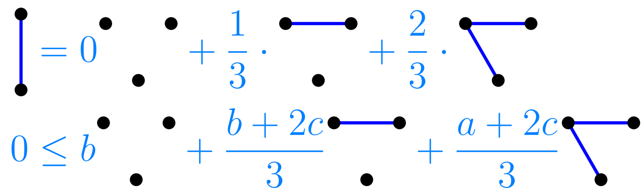


and

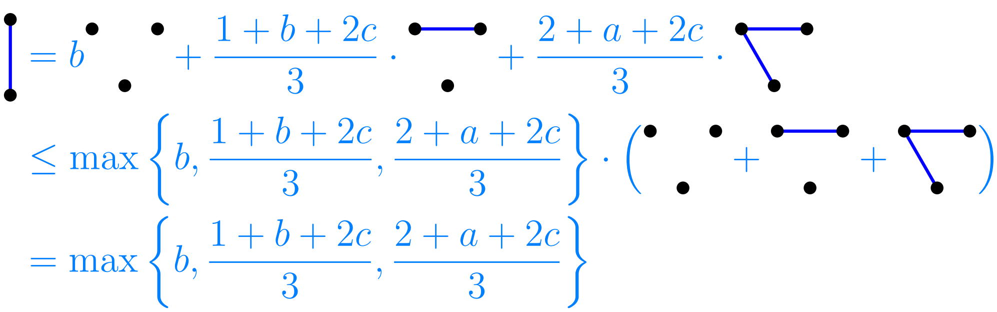


Use  $= 0$ and try to get  $\leq$ *function*(a, b, c). *Hint: function containing* max. Can you guess a, b, c?

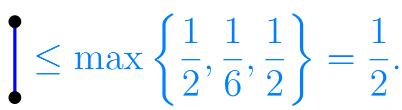
Solution: Since  $= 0$, we just ignore it in the calculation.



Summing together we get



Since we want the upper bound to be $\leq 1/2$, we can go with $b = 1/2$. To make the whole thing fit, we pul also $a = 1/2$ and $c = -1/2$. Then we get



Notice that a part of the last solution for Mantel's theorem can be stated as

$$\le \max\left\{b, \frac{1+b+2c}{3}, \frac{2+a+2c}{3}\right\}$$

while a, b, c had to form a positive semidefinite matrix. It is not completely obvious how to guess a, b, c. This can be written as a semidefinite program. One could think of it as a linear program with a bonus constraint that the variables together form a positive semidefinite matrix. A writeup of the program follows.

$$(SDP)\begin{cases}\text{Minimize} & t\\ \text{subject to} & a \le t\\ & \frac{1+a+2c}{3} \le t\\ & \frac{2+b+2c}{3} \le t\\ & \begin{pmatrix} a & c\\ c & b\end{pmatrix} \succcurlyeq 0\\ & t \ge 0\end{cases}$$

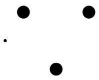
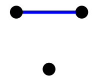
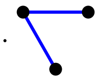
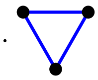
(SDP) can be solved on computers using freely available software CSDP or SDPA. What many flag algebra applications do is set up a semidefinite program and try to solve it. We will explore semidefinite programming next time.

21: What constraints must be satisfied by a, b, c to guarantee that

$$\begin{pmatrix} a & c\\ c & b\end{pmatrix} \succcurlyeq 0$$

Solution: Positive semidefinite matrix must have entries in the diagonal ≥ 0. Hence $a, b \ge 0$. Then also the determinant must be non-negative. So $ab - c^2 \ge 0$. Notice that this is giving some kind of a quadratic constraint on c.

22: Calculate the following product as a linear combination of graphs on 3 vertices.

$K_1 \cdot$  $= 0 \cdot$  $+ \frac{1}{3} \cdot$  $+ \frac{2}{3} \cdot$  $+ 1 \cdot$ 

Solution: Notice that that the right-hand side is *identical* to (1).

23: Let H be a fixed graph on ℓ vertices. Calculate the following product as a linear combination of graphs on $\ell + 1$ vertices.

$$K_1 \cdot H = \sum_{F \in \mathcal{F}_{\ell+1}} P(H, F) \cdot F$$

Solution: Recall that

$$H = \sum_{F \in \mathcal{F}_{\ell+1}} P(H, F) \cdot F$$

24: Let H be a fixed graph and $\mathcal{F}$ be a class of graphs closed under taking subrgaphs. For example, triangle-free graphs. Show that

$$\lim_{n \to \infty} \max\{P(H, G) : G \in \mathcal{F}_\ell\}$$

exists.

Solution: We show that $\max\{P(H, G) : G \in \mathcal{F}_\ell\}$ is monotone non-increasing. Suppose that $\max\{P(H, G) : G \in \mathcal{F}_\ell\} = a \in [0, 1]$. Suppose for contradiction that there exists $G' \in \mathcal{F}_{\ell'}$, where $\ell' > \ell$ and $P(H, G') > a$. Then

$$a < P(H, G') = \sum_{F \in \mathcal{F}_\ell} P(H, F) \cdot P(F, G') \leq \sum_{F \in \mathcal{F}_\ell} a \cdot P(F, G') = a,$$

which is a contradiction.

25: Use (5), i.e., $[\![a^2]\!]_\sigma \cdot [\![b^2]\!]_\sigma \geq [\![ab]\!]_\sigma^2$, to show

$$[\![a^2]\!]_\sigma \geq \frac{[\![a]\!]_\sigma^2}{[\![\sigma]\!]_\sigma}.$$

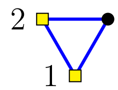
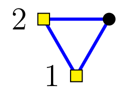
Solution: We use $b = \sigma$ and get

$$[\![a^2]\!]_\sigma \cdot [\![\sigma]\!]_\sigma = [\![a^2]\!]_\sigma \cdot [\![\sigma^2]\!]_\sigma \geq [\![a\sigma]\!]_\sigma^2 = [\![a]\!]_\sigma^2.$$

26: Let $(G_n)_{n \in \mathbb{N}}$ be a convergent sequence, where G_n is disjoint union of a clique on n vertices and n isolated vertices ($v(G_n) = 2n$). Denote the corresponding homomorphism by ϕ.

- Show that $(G_n)_{n \in \mathbb{N}}$ is indeed convergent.
- Let σ be 

. Determine $\mathbf{P}_\phi^\sigma$.

- Compute $\mathbb{E}_{\mathbf{P}^\sigma_\phi}\left[\phi^\sigma\left(\right.\right.$  $\left.\left.\right)\right]$, $\phi\left(\left[\!\left[\right.\right.\right.$  $\left.\left.\left.\right]\!\right]_\sigma\right)$, and $\phi([\![\sigma]\!]_\sigma)$. Compare with (4), which states

$$\phi([\![\sigma]\!]_\sigma) \cdot \mathbb{E}_{\mathbf{P}^\sigma_\phi}\left[\phi^\sigma(a)\right] = \phi([\![a]\!]_\sigma).$$

27: The proof of Mantel's theorem can be written as just one square instead of the whole positive semidefinite matrix. Can you find how?