Bakry-Émery curvature on graphs as an eigenvalue problem

David Cushing[1], Supanat Kamtue[1], Shiping Liu[2], and Norbert Peyerimhoff[1]

[1]Department of Mathematical Sciences, Durham University, Durham
[2]School of Mathematical Sciences and CAS Wu Wen-Tsun Key Laboratory of Mathematics, University of Science and Technology of China, Hefei

Abstract

In this paper, we reformulate the Bakry-Émery curvature on a weighted graph in terms of the smallest eigenvalue of a rank one perturbation of the so-called curvature matrix using Schur complement. This new viewpoint allows us to show various curvature function properties in a very conceptual way. We show that the curvature, as a function of the dimension parameter, is analytic, strictly monotone increasing and strictly concave until a certain threshold after which the function is constant. Furthermore, we derive the curvature of the Cartesian product using the crucial observation that the curvature matrix of the product is the direct sum of each component. Our approach of the curvature functions of graphs can be employed to establish analogous results for the curvature functions of weighted Riemannian manifolds. Moreover, as an application, we confirm a conjecture (in a general weighted case) of the fact that the curvature does not decrease under certain graph modifications.

1 Introduction and statements of result

The Ricci curvature is a fundamental notion in Riemannian geometry. It is also an essential ingredient in Einstein's formulation of general relativity. Lower Ricci curvature bounds on a Riemannian manifold allow one to extract various global geometric and topological information [25, 46]. The notion of Ricci curvature or its lower bound has been extended in various ways to general metric measure spaces. One of such extensions is Bakry-Émery's curvature dimension inequalities $CD(\mathcal{K}, N)$ [1, 2]. Bakry and Émery demonstrated that lower Ricci curvature bounds can be understood entirely in terms of the Laplace-Beltrami operator: On an n-dimensional Riemannain manifold (M^n, g), for any $N \in [n, \infty]$, the Ricci curvature is lower bounded by $\mathcal{K}$ at a point $x \in M$ if and only if the inequality $CD(\mathcal{K}, N)$, which can be formulated purely in terms of the Laplace-Beltrami operator, holds at x [1, pp.93-94].

Bakry-Émery theory has been a source of spectacular mathematical results [3]. In recent years, the discrete Bakry-Émery theory on graphs has become an active emerging research field. There are a growing number of articles investigating this theory, see e.g., [7, 8, 9, 10, 11, 12, 14, 15, 17, 20, 21, 22, 23, 24, 26, 27, 28, 29, 31, 32, 33, 34, 35, 37, 38, 39, 41, 42, 44, 45, 47, 48, 49, 52]. Let us mention here important related works on non-linear discrete curvature dimension inequalities, see e.g., [4, 13, 18, 19, 43].

A basic fact about the *optimal* lower Ricci curvature bound at a point x of a Riemannian manifold (M^n, g) is that it is equal to the smallest eigenvalue of the Ricci curvature tensor at x (when treated as a symmetric $(1,1)$-tensor) [46, Section 3.14].

In this paper, we provide an analogue of this basic fact in discrete Bakry-Émery theory. That is, we reformulate the *optimal* lower curvature bound $\mathcal{K}$ in Bakry-Émery's curvature dimension inequality $CD(\mathcal{K}, N)$ at a vertex x of a weighted graph as the smallest eigenvalue of a rank-one perturbation of the so-called *curvature matrix* (see Theorem 1.2). The curvature matrix at x is of size $m \times m$, where m is the number of neighbours of x in the graph. This might be surprising at first glance: Graphs are discrete and there are no way to define any curvature tensor directly. For instance, there are even no chain rule and the Laplacian is not diffusion [33, 4]. We achieve our result and conceive the concept of curvature matrix by combing an idea of Schmuckenschläger [49] with the trick of Schur complements [5, 6, 16], see also [12, Proposition 5.13]. This new viewpoint leads to a confirmation of [12, Conjecture 6.13] concerning the monotonicity of the Bakry-Émery curvature under certain graph modifications.

We further study the Bakry-Émery curvature as a function of the dimension parameter. Building upon the new viewpoint, we study the shape of the Bakry-Émery curvature functions systematically, especially the relation between the shape of the function and the spectrum of the curvature matrix. Very interestingly, the curvature matrix of a Cartesian product of two graphs is simply the direct sum of the curvature matrix of each graph. We use this to prove that the curvature function of Cartesian product is the star product (see Definition 1.11) of the curvature function of each factor.

The method we developed is also applicable to the setting of weighted Riemannian manifolds. Our results about the curvature functions of graphs can be transferred to the weighted manifold setting straightforwardly. In particular, we derive an analogous result about the curvature functions of Cartesian products of weighted Riemannian manifolds.

In the sequel, we will survey our results in more detail.

Let $G = (V, w, \mu)$ be a weighted graph consisting of a vertex set V, a vertex measure $\mu : V \to \mathbb{R}^+$, and an edge-weight function $w : V \times V \to \mathbb{R}^+ \cup \{0\}$ which is a symmetric function with $w_{xx} = 0$ for all $x \in V$. Two vertices $x, y \in V$ are adjacent if and only if $w_{xy} > 0$. The graph G is assumed to be *locally finite*, that is, each vertex has only finitely many neighbours. For $r \in \mathbb{N}$, the *combinatorial sphere* (resp. *ball*) of radius r centered at $x \in V$, denoted by $S_r(x)$ (resp. $B_r(x)$), is the set of all vertices whose minimum number of edges from x is equal to (resp. less than or equal to) r. In particular, $S_1(x)$ contains all neighbours of x.

Furthermore, let $d_x := \sum_{y \in V} w_{xy}$ be the *vertex degree* of x, and $p_{xy} := \frac{w_{xy}}{\mu_x}$ be the *transition rate* from x to y. In the special case of $d_x = \mu_x$ (that is, $\sum_{y \in V} p_{xy} = 1$) for all $x \in V$, the terms p_{xy} can be understood as transition probabilities of a reversible Markov chain. Another special situation is a *non-weighted* (or combinatorial) graph $G = (V, E)$ where E is the set of edges (without loops and multiple edges), that is, $\mu \equiv 1$ and $w_{xy} = 1$ iff x is adjacent to y, and $w_{xy} = 0$ otherwise.

The Laplacian $\Delta : C(V) \to C(V)$ (where $C(V)$ is the vector space of all functions $f : V \to$

$\mathbb{R}$) is given by

$$\Delta f(x) := \frac{1}{\mu_x} \sum_{y \in V} w_{xy}(f(y) - f(x)) = \sum_{y \in V} p_{xy}(f(y) - f(x)).$$

The Laplacian associated to non-weighted graphs is also known as the *non-normalised Laplacian.*

The Laplacian Δ gives rise to the symmetric bilinear forms Γ and Γ_2, namely,

$$\begin{aligned} 2\Gamma(f,g) &:= \Delta(fg) - f\Delta g - g\Delta f, \\ 2\Gamma_2(f,g) &:= \Delta(\Gamma(f,g)) - \Gamma(f,\Delta g) - \Gamma(g,\Delta f), \end{aligned}$$

with additional notations $\Gamma(f) := \Gamma(f,f)$ and $\Gamma_2(f) := \Gamma_2(f,f)$.

These bilinear forms are important for the following Ricci curvature notion due to Bakry-Émery [2], which is motivated by a fundamental identity in Riemannian Geometry called Bochner's formula.

Definition 1.1 (Bakry-Émery curvature)**.** Let $G = (V, w, \mu)$ be a locally finite weighted graph. Let $\mathcal{K} \in \mathbb{R}$ and $N \in (0, \infty]$. We say that a vertex $x \in V$ satisfies the Bakry-Émery's *curvature-dimension inequality* $CD(\mathcal{K}, N)$, if for any $f : V \to \mathbb{R}$, we have

$$\Gamma_2(f)(x) \geq \frac{1}{N}(\Delta f(x))^2 + \mathcal{K}\Gamma(f)(x), \tag{1.1}$$

where N is a dimension parameter and $\mathcal{K}$ is regarded as a lower Ricci curvature bound at x. The Bakry-Émery curvature, denoted by $\mathcal{K}(G, x; N)$, is then defined to be the largest $\mathcal{K}$ such that x satisfies $CD(\mathcal{K}, N)$.

The *Bakry-Émery curvature function* of x, namely $\mathcal{K}_{G,x}(N) := \mathcal{K}(G, x; N)$ can be reformulated as the solution to the following semidefinite programming:

$$\begin{aligned} &\text{maximize } K \qquad\qquad\qquad\qquad (P) \\ &\text{subject to } \Gamma_2(x) - \frac{1}{N}\Delta(x)^\top \Delta(x) - K\Gamma(x) \succeq 0, \end{aligned}$$

where the symmetric matrices $\Gamma(x)$ and $\Gamma_2(x)$ correspond to the symmetric bilinear forms Γ and Γ_2 at x. The explicit expression of these matrices is given in Appendix A. Here, $M \succeq 0$ (resp. $M \succ 0$) means M is positive semidefinite (resp. positive definite). The above computing method has been studied by Schmuckenschläger [49], and later on in [38], [36] and [12].

In this paper, we reformulate the above semidefinite programming problem as a smallest eigenvalue problem by employing the Schur complement of a square block matrix M_{22} in $M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}$, namely $M/M_{22} := M_{11} - M_{12}M_{22}^{-1}M_{21}$, applied to the matrix

$$\Gamma_2(x)_{\hat{1}} = \begin{pmatrix} \Gamma_2(x)_{S_1,S_1} & \Gamma_2(x)_{S_1,S_2} \\ \Gamma_2(x)_{S_2,S_1} & \Gamma_2(x)_{S_2,S_2} \end{pmatrix}.$$

Here the matrix $\Gamma_2(x)_{\hat{1}}$ refers to the principle submatrix of $\Gamma_2(x)$ obtained by removing its first row and column corresponding to the central vertex x. The matrix $\Gamma_2(x)_{S_i,S_j}$

refers to the submatrix of $\Gamma_2(x)$ whose rows and columns are indexed by the vertices of the combinatorial spheres $S_i(x)$ and $S_j(x)$.

We use the notation $Q(x) := \Gamma_2(x)_{\hat{1}}/\Gamma_2(x)_{S_2,S_2}$ for simplicity, and define

$$\begin{aligned} A_\infty(x) &:= 2\,\mathrm{diag}(\mathbf{v}_0(x))^{-1}Q(x)\,\mathrm{diag}(\mathbf{v}_0(x))^{-1}, \\ A_N(x) &:= A_\infty(x) - \frac{2}{N}\mathbf{v}_0(x)\mathbf{v}_0(x)^\top, \end{aligned} \tag{1.2}$$

where $\mathbf{v}_0(x) := (\sqrt{p_{xy_1}}\ \sqrt{p_{xy_2}}\ ...\ \sqrt{p_{xy_m}})^\top$ with $S_1(x) = \{y_1, y_2, ..., y_m\}$ labelling the neighbours of x. Note that the matrices $Q(x), A_\infty(x), A_N(x)$ are all symmetric matrices, and that $A_N(x)$ is a rank one perturbation of $A_\infty(x)$. All our subsequent results are based on the following theorem.

Theorem 1.2. *Let $G = (V, w, \mu)$ be a weighted graph. For $x \in V$ and $N \in (0, \infty]$, the Bakry-Émery curvature $\mathcal{K}_{G,x}(N)$ is the smallest eigenvalue of the symmetric matrix $A_N(x)$, that is,*

$$\mathcal{K}_{G,x}(N) = \lambda_{\min}(A_N(x)).$$

Theorem 1.2 is proved in Section 2. This concept of the curvature expression as eigenvalues was discussed in [12, Section 5] in the special case that a vertex x is S_1-out regular. Henceforth we will use the simplified notations $\mathbf{v}_0$, Q, A_∞ and A_N for the vector $\mathbf{v}_0(x)$ and the matrices $Q(x)$, $A_\infty(x)$ and $A_N(x)$, where x is a fixed vertex of G. We may refer to the matrix $A_\infty = A_\infty(x)$ as ***the curvature matrix*** of x.

The relation $\mathcal{K}_{G,x}(N) = \lambda_{\min}(A_N)$ allows us to investigate various properties of the curvature function $\mathcal{K}_{G,x} : (0, \infty] \to \mathbb{R}$. Some of the results here were already introduced in [12] in the case of non-weighted graphs, but this paper presents a unified and simplified approach to these results by employing the variational description of minimal eigenvalues via the Rayleigh quotient

$$\lambda_{\min}(A_N) = \inf_{v \neq 0} \frac{v^\top A_N v}{v^\top v}.$$

We first describe the shape of the curvature functions (see proofs in Section 3).

Theorem 1.3. *Let $G = (V, w, \mu)$ be a weighted graph, and fix $x \in V$. Then the curvature function $\mathcal{K}_{G,x} : (0, \infty] \to \mathbb{R}$ is continuous and there exists a unique threshold $N_1 \in (0, \infty]$ (possibly, $N_1 = \infty$) with the following properties:*

- *(i) $\mathcal{K}_{G,x}$ is analytic, strictly monotone increasing and strictly concave on $(0, N_1]$ with $\lim_{N\to 0} \mathcal{K}_{G,x}(N) = -\infty$ and $\lim_{N\to N_1} \mathcal{K}_{G,x}(N) =: K_1 < \infty$.*
- *(ii) $\mathcal{K}_{G,x}$ is constant on $[N_1, \infty]$ and equal to K_1.*

In fact, the threshold N_1 is the minimal $N \in (0, \infty]$ for which $\lambda_{\min}(A_N)$ is not simple. Another interesting threshold is given when the curvature function vanishes. Here we have the following result.

Proposition 1.4. *Assume that $A_\infty \succ 0$ (that is $\mathcal{K}_{G,x}(\infty) > 0$). Then there exists a unique $N_0 \in (0, \infty)$ such that $\mathcal{K}_{G,x}(N_0) = 0$, and it is given by*

$$N_0 = 2\mathbf{v}_0^\top A_\infty^{-1}\mathbf{v}_0 = 2\sum_{i,j} \sqrt{p_{xy_i}p_{xy_i}}(A_\infty^{-1})_{ij}.$$

Next we prove in Section 4 the following curvature bounds. The upper bound, in particular, plays an important role in our curvature analysis, where we study the situation when this upper bound is attained (called curvature sharpness; see the definition below). The notion of curvature sharpness was introduced [12] and studied in, e.g., [10].

Theorem 1.5 (Upper and lower curvature bounds)**.** *Let $G = (V, w, \mu)$ be a weighted graph. Then we have for $x \in V$ and $N \in (0, \infty]$,*

$$\mathcal{K}_{G,x}(\infty) - \frac{2}{N}\frac{d_x}{\mu_x} \leq \mathcal{K}_{G,x}(N) \overset{(*)}{\leq} \mathcal{K}^0_\infty(x) - \frac{2}{N}\frac{d_x}{\mu_x} \tag{1.3}$$

with

$$\mathcal{K}^0_\infty(x) := \frac{\mathbf{v}_0^\top A_\infty \mathbf{v}_0}{\mathbf{v}_0^\top \mathbf{v}_0} = \frac{1}{2}\left(\frac{d_x}{\mu_x} + 3\frac{\mu_x}{d_x}p^{(2)}_{xx} - \frac{\mu_x}{d_x}\sum_{z\in S_2(x)} p^{(2)}_{xz}\right).$$

Here we use the notation $p^{(2)}_{uv} := \sum_{w\in V} p_{uw}p_{wv}$. Moreover, a vertex $x \in V$ is called N- **curvature sharp** *iff (*) in (1.3) holds with equality.*

The next proposition clarifies the relation between curvature sharpness and the appearance of the following shapes of the curvature function $\mathcal{K}_{G,x}$:

- $\mathcal{K}_{G,x}(N) = c - \frac{2}{N}\frac{d_x}{\mu_x}$ (with a constant $c \in \mathbb{R}$) for all N near 0, and
- $\mathcal{K}_{G,x}(N)$ is constant for N near ∞.

Proposition 1.6. *If x is N_1-curvature sharp for some $N_1 \in (0, \infty]$, it is also N-curvature sharp for all $N \in (0, N_1]$. If x is N_1-curvature sharp for a maximally chosen N_1, then this N_1 is the threshold mentioned in Theorem 1.3, and hence $\mathcal{K}_{G,x}(N) = \mathcal{K}^0_\infty(x) - \frac{2}{N}\frac{d_x}{\mu_x}$ for all $N \in (0, N_1]$ and $\mathcal{K}_{G,x}$ is constant on $[N_1, \infty]$. Conversely, if $\mathcal{K}_{G,x}(N) = c - \frac{2}{N}\frac{d_x}{\mu_x}$ for some constant $c \in \mathbb{R}$ on some nontrivial interval (N', N''), then x is N''-curvature sharp.*

The following proposition provides insights into relations between curvature sharpness and the spectrum of the curvature matrix A_∞.

Proposition 1.7. *Let $G = (V, w, \mu)$ be a weighted graph and fix a vertex $x \in V$. Denote $E_{\min}(A_\infty)$ to be the minimal eigenspace of A_∞.*

(i) $\mathbf{v}_0$ *is an eigenvector of A_∞ if and only if x is N_1-curvature sharp for some $N_1 \in (0, \infty]$.*

(ii) $\mathbf{v}_0 \in E_{\min}(A_\infty)$ *if and only if x is ∞-curvature sharp.*

(iii) $\mathbf{v}_0$ *is perpendicular to $E_{\min}(A_\infty)$ if and only if $\mathcal{K}_{G,x}$ is constant on $[N_1, \infty]$ for some $N_1 < \infty$.*

The proofs of Propositions 1.6 and 1.7 are provided in Section 5.

Remark 1.8. If $\mathbf{v}_0$ is an eigenvector of A_∞ corresponding to a non-smallest eigenvalue of A_∞, then $\mathbf{v}_0$ is perpendicular to $E_{\min}(A_\infty)$. The converse is not true; a counterexample is the non-weighted Cartesian product $P_3 \times P_2$, discussed in Example 5.2. In this example, $\mathbf{v}_0$ is perpendicular to $E_{\min}(A_\infty)$ but it is not an eigenvector of A_∞, and its curvature function $\mathcal{K}_{G,x}$ is strictly increasing and strictly concave (but not curvature sharp) on $(0, N_1]$ and constant on $[N_1, \infty]$.

In Section 6, we discuss an important property of the curvature matrix A_∞, that is, the curvature matrix of the the Cartesian product of two graphs is simply the direct sum of the curvature matrices of each graph.

Definition 1.9 (weighted Cartesian product)**.** Given two weighted graphs G, G' and two fixed positive numbers $\alpha, \beta \in \mathbb{R}^+$, the weighted Cartesian product $G \times_{\alpha,\beta} G'$ is defined with the following weight function and vertex measure: for $x, y \in G$ and $x', y' \in G'$,

$$\begin{aligned} w_{(x,x')(y,x')} &:= \alpha w_{xy}\mu_{x'}, \\ w_{(x,x')(x,y')} &:= \beta w_{x'y'}\mu_x, \\ \mu_{(x,x')} &:= \mu_x\mu_{x'}. \end{aligned}$$

The parameters α and β serve two purposes.

1. In the case of non-weighted graphs G and G' (i.e., $\mu \equiv 1$ and $w \in \{0,1\}$), the choice of $\alpha = \beta = 1$ gives the usual Cartesian product graph $G \times G'$.
2. In the case of G and G' representing Markov chains (i.e., when $\sum_y w_{xy} = \mu_x$ and $\sum_{y'} w_{x'y'} = \mu_{x'}$), the choice of $\alpha + \beta = 1$ gives the weighted product $G \times_{\alpha,\beta} G$ which represents the random walk with probability α and β following horizontal and vertical edges, respectively.

Theorem 1.10. *The curvature matrix of the product $G \times_{\alpha,\beta} G'$ is the weighted direct sum of the curvature matrices G and G':*

$$A_\infty^{G\times_{\alpha,\beta}G'}((x,x')) = \alpha A_\infty^G(x) \oplus \beta A_\infty^{G'}(x').$$

As a consequence, we give a new proof (in a more general case of weighted graphs) of the fact that the curvature function of a Cartesian product is the star product of the curvature function in each factor (see Theorem 1.12 below).

Definition 1.11 (star product [12, Definition 7.1])**.** Let $f_1, f_2 : (0,\infty] \to \mathbb{R}$ be continuous and monotone increasing functions with $\lim_{t\to 0} f_1(t) = \lim_{t\to 0} f_2(t) = -\infty$. Then the function $f_1 * f_2 : (0,\infty] \to \mathbb{R}$ is defined by

$$f_1 * f_2(t) := f_1(t_1) = f_2(t_2),$$

where $t_1 + t_2 = t$ such that $f_1(t_1) = f_2(t_2)$.

Let us remark also that the star product is commutative and associative [12, Propositions 7.5 and 7.6].

Theorem 1.12. *The curvature function of the product $G \times_{\alpha,\beta} G'$ satisfies the following inequalities:*

$$\min\{\alpha\mathcal{K}_{G,x}, \beta\mathcal{K}_{G',x'}\} \le \mathcal{K}_{G\times_{\alpha,\beta}G',(x,x')} \le \max\{\alpha\mathcal{K}_{G,x}, \beta\mathcal{K}_{G',x'}\}.$$

Consequently, we have $\mathcal{K}_{G\times_{\alpha,\beta}G',(x,x')} = (\alpha\mathcal{K}_{G,x}) * (\beta\mathcal{K}_{G',x'})$.

In Section 7, we discuss analogous results in the smooth setting of weighted manifolds. Consider a weighted Riemannian manifold $(M^n, g, e^{-V} d\mathrm{vol}_g)$ of dimension n, with a metric g, the volume element $d\mathrm{vol}_g$, and a smooth real function $V : M \to \mathbb{R}$. The Bakry-Émery curvature function $\mathcal{K}_{M,V,x} : (0,\infty] \to \mathbb{R}$ at $x \in M$ is defined as

$$\mathcal{K}_{M,V,x}(N) := \inf_{v \in S_x(M)} \mathrm{Ric}_{N+n,V}(v,v), \qquad \forall N \in (0,\infty],$$

where $S_x(M)$ is the space of unit tangent vectors at x, and

$$\mathrm{Ric}_{N,V} := \mathrm{Ric} + \mathrm{Hess}\, V - \frac{\mathrm{grad}\, V \otimes \mathrm{grad}\, V}{N-n}, \ \forall N \in (n,\infty],$$

where we follow the notation in [54, Equation (14.36)]. We define $\mathcal{K}_{M,V,x}$ as a function on the interval $(0,\infty]$ instead of on $(n,\infty]$ to make it compatible with the curvature functions of graphs. All the results (Theorems 1.3, 1.5 and 1.12, Propositions 1.4, 1.6 and 1.7) have analogous counterparts in the manifold case. For example, the upper bound is $\mathcal{K}_{M,V,x}(N) \leq \mathcal{K}^0_\infty(x) - \frac{1}{N}\|\,\mathrm{grad}\, V\|^2$ with

$$\mathcal{K}^0_\infty(x) = \mathrm{Ric}_x\left(\frac{\mathrm{grad}\, V}{\|\,\mathrm{grad}\, V\|}, \frac{\mathrm{grad}\, V}{\|\,\mathrm{grad}\, V\|}\right) + \frac{\mathrm{grad}\, V(x)}{\|\,\mathrm{grad}\, V(x)\|}\left(\|\,\mathrm{grad}\, V\|\right).$$

We also show that the Cartesian product of two weighted manifolds $(M_i^{n_i}, g_i, e^{-V_i} d\mathrm{vol}_{g_i})$, $i \in \{1,2\}$ has the Bakry-Émery curvature function

$$\mathcal{K}_{M_1 \times M_2, V_1 \oplus V_2, (x_1,x_2)} = \mathcal{K}_{M_1,V_1,x_1} * \mathcal{K}_{M_2,V_2,x_2}. \tag{1.4}$$

Furthermore, we may define the *generalised scalar curvature* for a weighted Riemannian manifold $(M, g, e^{-V} d\mathrm{vol})$ to be the trace of the Ricci tensor

$$S_{M,V,x}(N) := \mathrm{tr}\, \mathrm{Ric}_{N+n,V}, \ \forall\, N \in (0,\infty]. \tag{1.5}$$

In Example 7.4, we investigate curvature sharpness properties of weighted 2-spheres and derive explicit formulas for the curvatures $\mathcal{K}_{M,V,x}$ and $S_{M,V,x}$. At the end of Section 7, we also discuss an interesting connection between curvature sharpness and Ricci solitons (see Theorem 7.5).

In Section 8, we prove the following curvature results related to the geometric structure of $B_2(x)$. First, we define for a graph G an analogue to the generalised scalar curvature, namely

$$S_{G,x}(N) := \mathrm{tr}\, A_N, \ \forall\, N \in (0,\infty].$$

In contrast to Ricci curvature, this scalar curvature can be formulated explicitly for non-weighted graphs in terms of the vertex degrees, the number of triangles and the size of $S_2(x)$.

Let us denote $S_1(x) = \{y_1, \ldots, y_{d_x}\}$. At a vertex x in a non-weighted graph, we define the out-degree $d^+_{y_i}$ of $y_i \in S_1(x)$ to be the number of neighbours of y_i in $S_2(x)$ and the in-degree d^-_z of $z \in S_2(x)$ to be the number of neighbors of z in $S_1(x)$.

Proposition 1.13. *Let $G = (V, w, \nu)$ be a non-weighted graph. Then* *(i) The curvature matrix at a vertex $x \in V$ is given by*

$$A_\infty(x) = -2\Delta_{S_1(x)} - 2\Delta_{S_1'(x)} + J + \frac{3-d_x}{2}\mathrm{Id} - \frac{1}{2}\operatorname{diag}((d_{y_1}^+, \dots, d_{y_{d_x}}^+)^\top), \quad (1.6)$$

where J is the $d_x \times d_x$ all-one matrix, $\Delta_{S_1(x)}$ is the Laplacian matrix of the subgraph of G induced by $S_1(x)$ and $\Delta_{S_1'(x)}$ is the Laplacian matrix of the weighted graph with vertex set $S_1(x)$, vertex measure $\mu \equiv 1$, and edge weights $w_{y_iy_j}^{S_1'(x)} = \sum_{z \in S_2(x)} \frac{w_{y_iz}w_{y_jz}}{d_z^-}$ for $i \neq j$ and 0 otherwise.

(ii) The generalised scalar curvature at a vertex $x \in V$ is given by

$$S_{G,x}(N) = d_x - \frac{d_x^2}{2} + \frac{3}{2}\sum_{y \in S_1(x)} d_y + \sharp_\triangle(x) - 2|S_2(x)| - \frac{2}{N}d_x, \quad (1.7)$$

where $\sharp_\triangle(x)$ denotes the number of triangles (3-cycles) containing the vertex x. In particular, for a d-regular tree, we have $S_{G,x}(N) = d(3-d) - \frac{2d}{N}$.

It follows from (1.7) that the scalar curvature is larger in the presence of more triangles or a smaller two-sphere. Secondly, we provide a sufficient criterion for curvature sharpness.

Theorem 1.14. *Let $G = (V, w, \mu)$ be a weighted graph. A vertex $x \in V$ is N-curvature sharp for some $N \in (0, \infty]$ if the following two homogeneity properties of x are satisfied:*

- *x is S_1-in regular: $p^-(y) = p_{yx}$ is independent of $y \in S_1(x)$,*
- *x is S_1-out regular: $p^+(y) = \sum_{z \in S_2(x)} p_{yz}$ is independent of $y \in S_1(x)$.*

In the case of the non-weighted graphs, the S_1-in regularity is always satisfied ($p^-(y) = 1$), and we even have equivalence between S_1-out regularity and N-curvature sharpness for some $N \in (0, \infty]$ [12, Corollary 5.10]. In fact, one can check directly from (1.6) the following fact in the case of non-weighted graphs: $\mathbf{v}_0$ is an eigenvector of A_∞ if and only if x is S_1-out regular. Therefore, our Proposition 1.7(i) is a substantial extension of [12, Corollary 5.10] in the case of general weighted graphs..

Our final result states that the curvature is nondecreasing under certain graph modifications.

Theorem 1.15. *Let $G = (V, w, \mu)$ be a weighted graph and fix a vertex $x \in V$. Assume that x is S_1-in regular, i.e., $p^-(y) = p_{yx}$ is independent of $y \in S_1(x)$. Consider a modified weighted graph $\widetilde{G}$ obtained from G by one of the following operations:*

(O1) Increase the edge-weight between a fixed pair $y, y' \in S_1(x)$ with $y \neq y'$ by $\tilde{w}_{yy'} = w_{yy'} + C_1$ for any constant $C_1 > 0$.

(O2) Delete a vertex $z_0 \in S_2(x)$ and remove all of its incident edges, i.e., $\tilde{w}_{yz_0} = 0$ for all $y \in S_1(x)$. Increase the edge-weight between all pairs $y, y' \in S_1(x)$ with $y \neq y'$ by

$$\tilde{w}_{yy'} = w_{yy'} + C_2 w_{yz_0} w_{z_0y'} \quad (1.8)$$

with any constant $C_2 \geq \dfrac{p^-(y)}{\mu_x p_{xz_0}^{(2)}}$.

Then $\mathcal{K}_{\widetilde{G},x}(N) \geq \mathcal{K}_{G,x}(N)$ *for any* $N \in (0, \infty]$.

The part (O2) of the above theorem confirms Conjecture 6.13 in [12] in the case of non-weighted graphs where we consider $\tilde{w}_{yy'} = w_{yy'} + 1$ for all pairs $y, y' \in S_1(x)$ of neighbours of z_0. In this special case, the constant $C_2 = 1$ is bigger or equal to the threshold

$$\frac{p^-(y)}{\mu_x p^{(2)}_{xz_0}} = \frac{1}{p^{(2)}_{xz_0}} =: \frac{1}{\text{in-degree of } z_0}.$$

In fact, the S_1-in regularity condition at x can be weakened to S_1-in regularity at x for the involved vertices in $S_1(x)$. In the operation (O1) we only require $p_{yx} = p_{y'x}$, and in (O2) we require p_{yx} is constant for all $y \in S_1(x)$ such that $w_{yz_0} \neq 0$.

Note: *After the submission of our first arXiv version, we became aware of the work by Siconolfi [50, 51] in which the* ∞*-Bakry-Émery curvature* $\mathcal{K}_{G,x}(\infty)$ *is also formulated as an eigenvalue problem in the special case of non-weighted graphs.*

2 Curvature reformulation

In this section, we prove the eigenvalue reformulation of the curvature (Theorem 1.2). Recall the optimization problem which formulates the Bakry-Émery curvature $\mathcal{K}_{G,x}(N)$,

$$\begin{aligned} &\text{maximize } K && (P)\\ &\text{subject to } \Gamma_2(x) - \frac{1}{N}\Delta(x)\Delta(x)^\top - K\Gamma(x) \succeq 0, \end{aligned}$$

This curvature is a local concept and uniquely determined by the structure of the two-ball $B_2(x)$. In particular, the symmetric matrix $\Gamma_2(x)$ is of size $|B_2(x)|$, and the symmetric matrices $\Delta(x)\Delta(x)^\top$ and $\Gamma(x)$ are of sizes $|B_1(x)|$ (and trivially extended by zeros to matrices of sizes $|B_2(x)|$); see Appendix A for details.

Schmuckenschläger [49] observed that the size of these matrices can be reduced by one: since $\Gamma_2(f), \Gamma(f), \Delta f$ all vanish for constant functions f, the curvature-dimension inequality $CD(\mathcal{K}, N)$ remains valid after shifting f by an additive constant. It is therefore sufficient to verify (1.1) for all functions $f : V \to \mathbb{R}$ with $f(x) = 0$. This observation allows us remove from these matrices the row and column corresponding to the vertex x, and we are able to reformulate the above problem (P) as

$$\begin{aligned} &\text{maximize } K && (P')\\ &\text{subject to } M_{K,N}(x) := \left(\Gamma_2(x) - \frac{1}{N}\Delta(x)^T\Delta(x) - K\Gamma(x)\right)_{S_1\cup S_2, S_1\cup S_2} \succeq 0, \end{aligned}$$

Next we recall the concept of the Schur complement, which allows us to further reduce the size of the involved symmetric matrices in (P').

Lemma 2.1 (Schur complement). *Consider a real symmetric matrix* $M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}$, *where* M_{11} *and* M_{22} *are square submatrices, and assume that* $M_{22} \succ 0$. *The Schur complement* M/M_{22} *is defined as*

$$M/M_{22} := M_{11} - M_{12}M_{22}^{-1}M_{21}. \tag{2.1}$$

Then $M/M_{22} \succeq 0$ if and only if $M \succeq 0$.

The proof of this lemma can be found in, e.g., [16, Proposition 2.1] or [12, Proposition 5.13]. We aim to apply this lemma for the symmetric matrix $M_{K,N}(x)$ given in (P'). Since $\Delta(x)$ and $\Gamma(x)$ have zero entries in the $S_2(x)$-structure, it means the matrix $M_{K,N}(x)$ has the following block structure:

$$M_{K,N}(x) = \begin{pmatrix} \Gamma_2(x)_{S_1,S_1} - \frac{1}{N}\Delta(x)_{S_1}\Delta(x)_{S_1}^\top - K\Gamma(x)_{S_1,S_1} & \Gamma_2(x)_{S_1,S_2} \\ \Gamma_2(x)_{S_2,S_1} & \Gamma_2(x)_{S_2,S_1} \end{pmatrix}.$$

By folding $M_{K,N}(x)$ into the upper left block, the Schur complement is given by

$$\begin{aligned} &M_{K,N}(x)/\Gamma_2(x)_{S_2,S_2} \\ &= \Gamma_2(x)_{S_1,S_1} - \frac{1}{N}\Delta(x)_{S_1}\Delta(x)_{S_1}^\top - K\Gamma(x)_{S_1,S_1} - \Gamma_2(x)_{S_1,S_2}\Gamma_2(x)_{S_2,S_2}^{-1}\Gamma_2(x)_{S_2,S_1} \\ &= Q(x) - \frac{1}{N}\Delta(x)_{S_1}\Delta(x)_{S_1}^\top - K\Gamma(x)_{S_1,S_1}, \end{aligned}$$

where $Q(x) := \Gamma_2(x)_{\hat{1}}/\Gamma_2(x)_{S_2,S_2}$ denotes the folding of $\Gamma_2(x)_{\hat{1}} = \begin{pmatrix} \Gamma_2(x)_{S_1,S_1} & \Gamma_2(x)_{S_1,S_2} \\ \Gamma_2(x)_{S_2,S_1} & \Gamma_2(x)_{S_2,S_2} \end{pmatrix}$.

The importance of $\Gamma_2(x)_{S_1,S_1}$ for a lower curvature bound was already mentioned in Schmuckenschläger [49, pp.194-195] (where he used the notation A_{II}).

Lemma 2.1 implies that

$$\mathcal{K}_{G,x}(N) = \arg\max_K \left\{ Q(x) - \frac{1}{N}\Delta(x)_{S_1}\Delta(x)_{S_1}^\top - K\Gamma(x)_{S_1,S_1} \succeq 0 \right\}. \tag{2.2}$$

We recall from Appendix A that $\Gamma(x)_{S_1,S_1} = \frac{1}{2}\operatorname{diag}(\Delta(x)_{S_1})$ and $\Delta(x)_{S_1} = (p_{xy_1}\ p_{xy_2}\ \dots\ p_{xy_m})^\top$, where $S_1(x) = \{y_1, y_2, \dots, y_m\}$.

Denote the vector $\mathbf{v}_0 := \mathbf{v}_0(x) = (\sqrt{p_{xy_1}}\ \sqrt{p_{xy_2}}\ \dots\ \sqrt{p_{xy_m}})^\top$. The maximum argument in (2.2) does not change under the multiplication by $\operatorname{diag}(\mathbf{v}_0)^{-1} \succ 0$ both from left and right sides, that is,

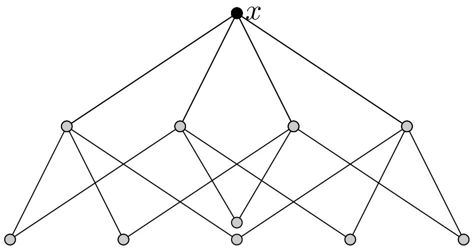
$$\mathcal{K}_{G,x}(N) = \arg\max_K \left\{ \operatorname{diag}(\mathbf{v}_0)^{-1} Q(x) \operatorname{diag}(\mathbf{v}_0)^{-1} - \frac{1}{N}\mathbf{v}_0\mathbf{v}_0^\top - \frac{K}{2}\mathrm{Id} \succeq 0 \right\}. \tag{2.3}$$

In other words,

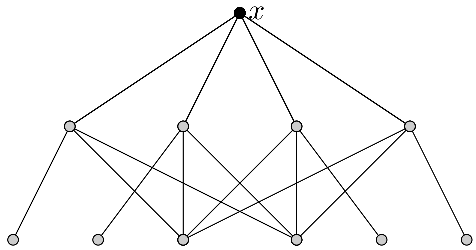
$$\begin{aligned} \mathcal{K}_{G,x}(N) &= \lambda_{\min}\left(2\operatorname{diag}(\mathbf{v}_0)^{-1} Q(x) \operatorname{diag}(\mathbf{v}_0)^{-1} - \frac{2}{N}\mathbf{v}_0\mathbf{v}_0^\top\right) \\ &= \lambda_{\min}\left(A_\infty - \frac{2}{N}\mathbf{v}_0\mathbf{v}_0^\top\right) = \lambda_{\min}(A_N), \end{aligned}$$

where $A_\infty = A_\infty(x)$ and $A_N = A_N(x)$ are defined in (1.2), and $\lambda_{\min}(A_N)$ denotes the smallest eigenvalue of A_N. This finishes the proof of Theorem 1.2.

Remark 2.2. It follows from the Appendix (A.11)-(A.13) that the curvature matrix at a vertex x is completely determined by the weighted structure of the *incomplete two-ball* around x, namely $B_2^{\mathrm{inc}}(x)$, which is obtained from the induced subgraph of $B_2(x)$ by



(a) The $B_2^{\mathrm{inc}}(x)$-structure of G_1



(b) The $B_2^{\mathrm{inc}}(x)$-structure of G_2

Figure 1: Two graphs G_1 and G_2 with different $B_2^{\mathrm{inc}}(x)$-structures share the same curvature matrix. For example, G_1 can be the 4-dimensional cube $\mathcal{Q}^4$.

removing all edges connecting vertices within $S_2(x)$. It is interesting to note however that two graphs can share the same curvature matrix, even when they have non-isomorphic $B_2^{\mathrm{inc}}(x)$. For example, both graphs G_1 and G_2, whose $B_2^{\mathrm{inc}}(x)$ are as in Figure 1, have their curvature matrix at x equal to $A_N^{G_1}(x) = 2\mathrm{Id}_4 - \frac{2}{N}J_4 = A_N^{G_2}(x)$.

On the other hand, the curvature matrix $A_\infty(x)$ contains more information than the curvature function $\mathcal{K}_{G,x}$, and $A_\infty(x)$ cannot be recovered from $\mathcal{K}_{G,x}$. For example, it is shown below that the non-weighted cube $\mathcal{Q}^3$ and complete bipartite graph $K_{3,3}$ share the same curvature function, while having different curvature matrices.

For any vertex x in $G = \mathcal{Q}^3$:

$$A_N^G(x) = \begin{pmatrix} 2 & & \\ & 2 & \\ & & 2 \end{pmatrix} - \frac{2}{N}J_3,$$

$$\sigma(A_N^G(x)) = \{2 - \frac{6}{N}, 2, 2\},$$

$$\mathcal{K}_{G,x}(N) = 2 - \frac{6}{N}.$$

For any vertex x in $H = K_{3,3}$:

$$A_N^H(x) = \begin{pmatrix} 8/3 & -1/3 & -1/3 \\ -1/3 & 8/3 & -1/3 \\ -1/3 & -1/3 & 8/3 \end{pmatrix} - \frac{2}{N}J_3,$$

$$\sigma(A_N^H(x)) = \{2 - \frac{6}{N}, 3, 3\},$$

$$\mathcal{K}_{H,x}(N) = 2 - \frac{6}{N}.$$

3 Properties of the curvature function $\mathcal{K}_{G,x}$

This section is devoted to the proof of Theorem 1.3 about properties of the curvature function $\mathcal{K}_{G,x} : (0,\infty] \to \mathbb{R}$, which will be divided into small steps.

Proposition 3.1. *The curvature function $\mathcal{K}_{G,x} : (0,\infty] \to \mathbb{R}$ is continuous, monotone increasing and concave with $\lim_{N\to 0} \mathcal{K}_{G,x}(N) = -\infty$ and $\lim_{N\to\infty} \mathcal{K}_{G,x}(N) < \infty$.*

Proof. It is known that the zeros of a polynomial are continuous functions of the coefficients of the polynomial (see, e.g., [40, Theorem (1,4)]). In particular for the characteristic polynomial in λ, namely $\det(A_N - \lambda\mathrm{Id})$, it means the ordered set of eigenvalues of A_N, respecting their multiplicities, are continuous in N. In particular, $\mathcal{K}_{G,x}(N) = \lambda_{\min}(A_N)$ is continuous in N.

Monotonicity and concavity of $\mathcal{K}_{G,x}$ employ the crucial fact that, for symmetric matrices A and B,

$$\lambda_{\min}(A+B) = \inf_{v\neq 0} \frac{v^\top (A+B)v}{v^\top v} \geq \inf_{v\neq 0} \frac{v^\top Av}{v^\top v} + \inf_{v\neq 0} \frac{v^\top Bv}{v^\top v} = \lambda_{\min}(A) + \lambda_{\min}(B),$$

and the inequality holds with equality iff A and B share an eigenvector corresponding to their minimal eigenvalues. Recall also that $\mathbf{v}_0\mathbf{v}_0^\top$ is a rank one matrix with the only nontrivial eigenvalue $\mathbf{v}_0^\top\mathbf{v}_0 > 0$, so $\lambda_{\max}(\mathbf{v}_0\mathbf{v}_0^\top) = \mathbf{v}_0^\top\mathbf{v}_0$ and $\lambda_{\min}(\mathbf{v}_0\mathbf{v}_0^\top) = 0$.

For $0 < N' < N \leq \infty$, we have

$$\begin{aligned}\lambda_{\min}(A_N) &= \lambda_{\min}\left(A_{N'} + \Big(\frac{2}{N'} - \frac{2}{N}\Big)\mathbf{v}_0\mathbf{v}_0^\top\right)\\ &\geq \lambda_{\min}(A_{N'}) + \lambda_{\min}\Big(\underbrace{(\frac{2}{N'} - \frac{2}{N})}_{>0}\mathbf{v}_0\mathbf{v}_0^\top\Big) = \lambda_{\min}(A_{N'}),\end{aligned} \tag{3.1}$$

Similarly, for $0 < N' < N \leq \infty$ and $\alpha \in (0,1)$, we have

$$\begin{aligned}\lambda_{\min}(A_{\alpha N+(1-\alpha)N'}) &= \lambda_{\min}\Big(\alpha A_N + (1-\alpha)A_{N'} + 2\underbrace{(\frac{\alpha}{N} + \frac{1-\alpha}{N'} - \frac{1}{\alpha N + (1-\alpha)N'})}_{>0}\mathbf{v}_0\mathbf{v}_0^\top\Big)\\ &\geq \alpha\lambda_{\min}(A_N) + (1-\alpha)\lambda_{\min}(A_{N'}),\end{aligned}$$

To derive $\mathcal{K}_{G,x}(\infty) = \lim_{N\to\infty}\mathcal{K}_{G,x}(N) < \infty$ and $\lim_{N\to 0}\mathcal{K}_{G,x}(N) = -\infty$, we argue that

$$\lambda_{\min}(A_N) = \lambda_{\min}\left(A_\infty - \frac{2}{N}\mathbf{v}_0\mathbf{v}_0^\top\right) \to \lambda_{\min}(A_\infty) \qquad \text{as } N\to\infty,$$

and

$$\lambda_{\min}(A_N) \leq \|A_\infty\| + \lambda_{\min}\big(-\frac{2}{N}\mathbf{v}_0\mathbf{v}_0^\top\big) = \|A_\infty\| - \frac{2}{N}\mathbf{v}_0^\top\mathbf{v}_0 \to -\infty \qquad \text{as } N\to 0,$$

where $\|\cdot\|$ denotes the operator norm. □

Lemma 3.2. *If $\lambda_{\min}(A_{N'})$ is not simple for some $N' \in (0,\infty]$, then $\lambda_{\min}(A_N) = \lambda_{\min}(A_{N'})$ for all $N \in [N',\infty]$. In other words, $\mathcal{K}_{G,x}$ is constant on $[N',\infty]$.*

Proof of Lemma 3.2. Assume that $\lambda_{\min}(A_{N'})$ is not simple, that is, the minimal eigenspace $E_{\min}(A_{N'})$ has dimension at least 2. We first argue that there exists a nonzero $w \in E_{\min}(A_{N'})$ such that $w \perp \mathbf{v}_0$. Consider any two linearly independent vectors $v_1 = a_1\mathbf{v}_0 + b_1w_1$ and $v_2 = a_2\mathbf{v}_0 + b_2w_2$ in $E_{\min}(A_{N'})$ with $w_1 \perp \mathbf{v}_0$ and $w_2 \perp \mathbf{v}_0$. In case $a_1 = 0$ or $a_2 = 0$, we immediately obtain such a vector w. In case $a_1 \neq 0$ and $a_2 \neq 0$, the vector $\frac{1}{a_1}v_1 - \frac{1}{a_2}v_2$ represents such a vector w.

Since $w \perp \mathbf{v}_0$, it lies in the minimal eigenspace $E_{\min}(\mathbf{v}_0\mathbf{v}_0^\top)$ whose minimal eigenvalue is zero. This means $w \in E_{\min}(A_{N'}) \cap E_{\min}(\mathbf{v}_0\mathbf{v}_0^\top)$, so the inequality (3.1) holds with equality, i.e., $\lambda_{\min}(A_N) = \lambda_{\min}(A_{N'})$ for all $N \in [N',\infty]$. □

Lemma 3.3. *If $\lambda_{\min}(A_N)$ is simple for some $N \in (0,\infty]$, then $\mathcal{K}_{G,x}$ is analytic in a small neighbourhood of N.*

Proof. The idea is to prove analyticity by using the implicit function theorem. More precisely, we aim to apply [30, Theorem 6.1.2]. Consider the matrix-valued function $A(t) = A_{1/t}$, and denote $\lambda_0(t) \leq \lambda_1(t) \leq ... \leq \lambda_{m-1}(t)$ to be all eigenvalues of $A(t)$. Let $t_0 = \frac{1}{N}$ and assume that $\lambda_0(t_0) = \lambda_{\min}(A_N)$ is simple. Consider the following polynomial in t and λ:

$$F(t, \lambda) := \det(A(t_0 + t) - (\lambda_0(t_0) + \lambda)\mathrm{Id}) = \sum_{i,j} a_{i,j} t^i \lambda^j.$$

The characteristic polynomial factorization gives

$$F(0, \lambda) = \det(A(t_0) - (\lambda_0(t_0) + \lambda)\mathrm{Id}) = \prod_{i=0}^{m-1} (\lambda_i(t_0) - (\lambda_0(t_0) + \lambda)) = \lambda \prod_{i=1}^{m-1} (\lambda_i(t_0) - \lambda_0(t_0) - \lambda),$$

which means $a_{0,0} = 0$, and $a_{0,1} \neq 0$ since $\lambda_0(t_0) \neq \lambda_i(t_0)$ for $i \geq 1$. The analytic implicit function theorem asserts that there exists an analytic function $\lambda(t)$ around $t = 0$ such that $\lambda(0) = 0$ and $F(t, \lambda(t)) = 0$ for all t near 0, that is, $\lambda_0(t_0) + \lambda(t)$ is an eigenvalue of $A(t_0 + t)$. Moreover, the assumption that $\lambda_0(t_0)$ is a simple and smallest eigenvalue of $A(t_0)$ implies that $\lambda_0(t_0) + \lambda(t)$ stays the smallest eigenvalue of $A(t_0 + t)$ for t near 0. □

Lemma 3.4. *If $\lambda_{\min}(A_{N_1})$ is not simple for some $N_1 \in (0, \infty]$, then there exists the smallest such N_1, and consequently $K_{G,x}$ is analytic, strictly monotone increasing and strictly concave on $(0, N_1]$, and constant on $[N_1, \infty]$.*

Proof. Consider the set

$$\mathcal{N}_{\mathrm{ns}} := \{N \in (0, \infty] : \ \lambda_{\min}(A_N) \text{ is not simple}\},$$

and denote $N_1 := \inf \mathcal{N}_{\mathrm{ns}}$.

We know from Lemma 3.2 that $\mathcal{K}_{G,x}$ is constant on $[N, \infty]$ for all $N \in \mathcal{N}_{\mathrm{ns}}$. Therefore, $\mathcal{K}_{G,x}$ is constant on $(N_1, \infty]$. Note that $N_1 > 0$; otherwise $\mathcal{K}_{G,x}$ is constant on the whole interval $(0, \infty]$, which contradicts to the fact from Proposition 3.1 that $\lim_{N \to 0} \mathcal{K}_{G,x}(N) = -\infty$.

If $\lambda_{\min}(A_{N_1})$ were simple, then $\lambda_{\min}(A_N)$ would also be simple for all N in a small neighbourhood of N_1. This contradicts to the definition of N_1. Therefore, $\lambda_{\min}(A_{N_1})$ is not simple, and $N_1 = \min \mathcal{N}_{\mathrm{ns}}$.

Since $\lambda_{\min}(A_N)$ is simple for all $N \in (0, N_1)$, we know from Lemma 3.3 that $\mathcal{K}_{G,x}$ is analytic on $(0, N_1)$. Recall also from Proposition 3.1 that $\mathcal{K}_{G,x}$ is concave and monotone increasing. If $\mathcal{K}_{G,x}$ were not strictly concave on $(0, N_1)$, this would mean $\mathcal{K}_{G,x}$ is linear on some interval $[a, b] \subset (0, N_1)$. Then the analyticity of $\mathcal{K}_{G,x}$ on $(0, N_1)$ would then imply that $\mathcal{K}_{G,x}$ is linear on the entire interval $(0, N_1)$, which contradicts to the fact that $\lim_{N \to 0} \mathcal{K}_{G,x}(N) = -\infty$. Thus $\mathcal{K}_{G,x}$ is indeed strictly concave on $(0, N_1)$, and consequently it is strictly monotone increasing on $(0, N_1)$. This finishes the proof of Lemma 3.4. □

By combining Proposition 3.1 and Lemmas 3.3 and 3.4, we can conclude Theorem 1.3 with the description of the threshold $N_1 \in (0, \infty]$, namely $N_1 = \min\{N \in (0, \infty] : \lambda_{\min}(A_N) \text{ is not simple}\}$ (and $N = \infty$ in case this set is empty).

Let us end this section with the proof of Proposition 1.4 about the uniqueness of the threshold N_0 such that $\mathcal{K}_{G,x}(N_0) = 0$, which is asserted by the intermediate value theorem for the continuous curvature function $\mathcal{K}_{G,x} : (0, \infty] \to \mathbb{R}$.

Proof of Proposition 1.4. Since $\mathcal{K}_{G,x}(\infty) > 0$ (by assumption) and $\lim_{N\to 0}\mathcal{K}_{G,x}(N) = -\infty$, the intermediate value theorem asserts that there exists an $N_0 \in (0,\infty)$ such that $\mathcal{K}_{G,x}(N_0) = 0$. This implies $\det A_{N_0} = 0$.

Furthermore, $\mathcal{K}_{G,x}(\infty) > 0$ means $\det A_\infty > 0$ and A_∞ is invertible. The matrix determinant formula then gives

$$0 = \det A_{N_0} = \det(A_\infty - \frac{2}{N_0}\mathbf{v}_0\mathbf{v}_0^\top) = (1 - \frac{2}{N_0}\mathbf{v}_0^\top A_\infty^{-1}\mathbf{v}_0)\det A_\infty. \tag{3.2}$$

Therefore, N_0 is uniquely given by $N_0 = 2\mathbf{v}_0^\top A_\infty^{-1}\mathbf{v}_0$. □

4 Curvature bounds and curvature sharpness

Proof of Theorem 1.5. We derive the lower curvature bound via the Rayleigh quotient as follows:

$$\mathcal{K}_{G,x}(N) = \inf_{v\neq 0}\frac{v^\top(A_\infty - \frac{2}{N}\mathbf{v}_0\mathbf{v}_0^\top)v}{v^\top v} \geq \inf_{v\neq 0}\frac{v^\top A_\infty v}{v^\top v} - \frac{2}{N}\sup_{v\neq 0}\frac{v^\top\mathbf{v}_0\mathbf{v}_0^\top v}{v^\top v} = \mathcal{K}_{G,x}(\infty) - \frac{2}{N}\mathbf{v}_0^\top\mathbf{v}_0,$$

where $\mathbf{v}_0^\top\mathbf{v}_0 = \sum_{y\in S_1(x)} p_{xy} = \frac{d_x}{\mu_x}$.

On the other hand, the upper curvature bound can be derived as

$$\mathcal{K}_{G,x}(N) \leq \frac{\mathbf{v}_0^\top A_N\mathbf{v}_0}{\mathbf{v}_0^\top\mathbf{v}_0} = \frac{\mathbf{v}_0^\top(A_\infty - \frac{2}{N}\mathbf{v}_0\mathbf{v}_0^\top)\mathbf{v}_0}{\mathbf{v}_0^\top\mathbf{v}_0} = \frac{\mathbf{v}_0^\top A_\infty\mathbf{v}_0}{\mathbf{v}_0^\top\mathbf{v}_0} - \frac{2}{N}\mathbf{v}_0^\top\mathbf{v}_0. \tag{4.1}$$

Lemma A.1 in Appendix A confirms that

$$\mathcal{K}_\infty^0(x) := \frac{\mathbf{v}_0^\top A_\infty\mathbf{v}_0}{\mathbf{v}_0^\top\mathbf{v}_0} = \frac{1}{2}\left(\frac{d_x}{\mu_x} + 3\frac{\mu_x}{d_x}p_{xx}^{(2)} - \frac{\mu_x}{d_x}\sum_{z\in S_2(x)} p_{xz}^{(2)}\right).$$

□

Remark 4.1. In the case of non-weighted graphs, the quantity $\mathcal{K}_\infty^0(x)$ reduces to the one in [12, Definition 3.2]. Indeed, we have in that case

$$\mathcal{K}_\infty^0(x) = \frac{1}{2}\left(d_x + 3 - \frac{1}{d_x}\sum_{y\in S_1(x)} d_y^+\right) = 2 + \frac{1}{2}\left(d_x - \frac{1}{d_x}\sum_{y\in S_1(x)} d_y\right) + \frac{\sharp_\triangle(x)}{d_x},$$

where d_y^+ is the out-degree of $y \in S_1(x)$ (i.e., the number of neighbours of y in $S_2(x)$) and $\sharp_\triangle(x)$ denotes the number of triangles containing x.

5 Relations between the spectrum of the curvature matrix A_∞ and the curvature function $\mathcal{K}_{G,x}$

Proof of Proposition 1.7 and Proposition 1.6.
The vertex x is N-curvature sharp if and only if the upper bound (4.1): $\lambda_{\min}(A_N) \leq$

$\frac{\mathbf{v}_0^\top A_N \mathbf{v}_0}{\mathbf{v}_0^\top \mathbf{v}_0}$ holds with equality, which happens if and only if $\mathbf{v}_0$ is in the minimal eigenspace $E_{\min}(A_N)$. In particular, x is ∞-curvature sharp if and only if $\mathbf{v}_0 \in E_{\min}(A_\infty)$. This proves Proposition 1.7 (ii).

Assume x is N_1-curvature sharp for some $N_1 \in (0,\infty]$. Then $A_{N_1}\mathbf{v}_0 = \lambda_{\min}(A_{N_1})\mathbf{v}_0$, which implies $A_\infty \mathbf{v}_0 = (\lambda_{\min}(A_{N_1}) + \frac{2}{N_1}\mathbf{v}_0^\top \mathbf{v}_0)\mathbf{v}_0$, that is, $\mathbf{v}_0$ is an eigenvector of A_∞.

Conversely, assume $\mathbf{v}_0$ is an eigenvector of A_∞, that is, $A_\infty \mathbf{v}_0 = \lambda \mathbf{v}_0$ for some $\lambda \in \mathbb{R}$. Denote the spectrum of A_∞ by $\sigma(A_\infty) = \{\lambda, \lambda_1, ..., \lambda_{m-1}\}$ with $\lambda_1 \leq ... \leq \lambda_{m-1}$. Consider $A_\infty v_i = \lambda_i v_i$ where all eigenvectors v_i of A_∞ (different from $\mathbf{v}_0$) are chosen to be orthogonal to $\mathbf{v}_0$. We then obtain for any N,

$$
\begin{aligned}
A_N \mathbf{v}_0 &= (A_\infty - \frac{2}{N}\mathbf{v}_0\mathbf{v}_0^\top)\mathbf{v}_0 = (\lambda - \frac{2}{N}\mathbf{v}_0^\top \mathbf{v}_0)\mathbf{v}_0;\\
A_N v_i &= (A_\infty - \frac{2}{N}\mathbf{v}_0\mathbf{v}_0^\top)v_i = A_\infty v_i = \lambda_i v_i \qquad \forall 1 \leq i < m,
\end{aligned}
$$

which mean its spectrum is $\sigma(A_N) = \{\lambda - \frac{2}{N}\mathbf{v}_0^\top \mathbf{v}_0, \lambda_1, ..., \lambda_{m-1}\}$.

We choose the threshold $N_1 = \frac{2\mathbf{v}_0^\top \mathbf{v}_0}{\lambda - \lambda_1}$ in case $\lambda \geq \lambda_1$ (and choose $N_1 = \infty$ if $\lambda < \lambda_1$), so that

$$
\lambda_{\min}(A_N) = \begin{cases} \lambda - \frac{2}{N}\mathbf{v}_0^\top \mathbf{v}_0 & \text{if } N \leq N_1,\\ \lambda_1 & \text{if } N \geq N_1. \end{cases}
$$

This means for all $N \leq N_1$, $\mathbf{v}_0 \in E_{\min}(A_N)$, that is, x is curvature sharp on $(0, N_1]$. This proves Proposition 1.7 (i). Furthermore, for all $N \geq N_1$, $\lambda_{\min}(A_N) = \lambda_1 = \lambda_{\min}(A_\infty)$, that is, $\mathcal{K}_{G,x}$ is constant on $[N_1, \infty]$. This proves the two forward statements of Proposition 1.6.

To verify the converse statement in Proposition 1.6, suppose that $\mathcal{K}_{G,x}(N) = c - \frac{2}{N}\frac{d_x}{\mu_x}$ for all $N \in (N', N'')$ and hence at $N = N', N''$ by continuity of $\mathcal{K}_{G,x}$. We observe that

$$
\begin{aligned}
c - \frac{2}{N''}\frac{d_x}{\mu_x} = \lambda_{\min}(A_{N''}) &= \lambda_{\min}\left(A_{N'} + \Big(\frac{2}{N'} - \frac{2}{N''}\Big)\mathbf{v}_0\mathbf{v}_0^\top\right)\\
&= \inf_{v \neq 0}\left(\frac{v^\top A_{N'} v}{v^\top v} + \Big(\frac{2}{N'} - \frac{2}{N''}\Big)\frac{v^\top \mathbf{v}_0\mathbf{v}_0^\top v}{v^\top v}\right)\\
&\leq \inf_{v \neq 0}\frac{v^\top A_{N'} v}{v^\top v} + \Big(\frac{2}{N'} - \frac{2}{N''}\Big)\mathbf{v}_0^\top \mathbf{v}_0\\
&= \lambda_{\min}(A_{N'}) + \Big(\frac{2}{N'} - \frac{2}{N''}\Big)\frac{d_x}{\mu_x} = c - \frac{2}{N''}\frac{d_x}{\mu_x},
\end{aligned}
$$

so the inequality holds with equality, which occurs when $\mathbf{v}_0 \in E_{\min}(A_{N'})$. Consequently, it holds that $\mathbf{v}_0 \in E_{\min}(A_{N''})$. So x is N''-curvature sharp as desired. □

The next result is an interesting observation about the non-smallest eigenvalues of A_N, which is not included in the Introduction.

Corollary 5.1. *If $\mathcal{K}_{G,x}(\infty) > 0$, then all of the non-smallest eigenvalues of A_N are strictly positive for all dimensions $N \in (0, \infty]$.*

Proof. Let $\lambda_i(A_N)$ denote the i-th smallest eigenvalue of A_N (respecting multiplicity). Assume for the sake of contradiction that there exist $N' \in (0,\infty)$ and $i \geq 2$ such that $\lambda_i(A_{N'}) \neq \lambda_{\min}(A_{N'})$ and $\lambda_i(A_{N'}) < 0$. We also know from $\mathcal{K}_{G,x}(\infty) > 0$ that $\lambda_i(A_\infty) > 0$. Since $\lambda_i(A_N)$ is continuous on N, the intermediate value theorem implies that $\lambda_i(A_{\hat{N}_0}) = 0$ for some $\hat{N}_0 \in (N',\infty)$, and hence $\det(A_{\hat{N}_0}) = 0$. The matrix determinant formula $0 = \det A_{\hat{N}_0} = (1 - \frac{2}{\hat{N}_0}\mathbf{v}_0^\top A_\infty^{-1}\mathbf{v}_0)\det A_\infty$ with $\det A_\infty > 0$ (because $\mathcal{K}_{G,x}(\infty) > 0$) asserts that $\hat{N}_0 = 2\mathbf{v}_0^\top A_\infty^{-1}\mathbf{v}_0$, which is the same threshold as N_0 in Proposition 1.4. In other words, $\lambda_{\min}(A_{\hat{N}_0}) = 0 = \lambda_i(A_{\hat{N}_0})$ is not simple. By Lemma 3.4, $\mathcal{K}_{G,x}$ must then be constant on $[\hat{N}_0,\infty)$, which is contradiction to the fact that $\mathcal{K}_{G,x}(\hat{N}_0) = 0 < \mathcal{K}_{G,x}(\infty)$. $\square$

Proposition 1.6 raises the question whether there exists a graph with a vertex x which is not curvature sharp for any finite N but nevertheless its curvature function is constant near infinity. The following example provides the answer.

Example 5.2. We consider the Cartesian product $P_3 \times P_2$, where P_n is the path containing n vertices.

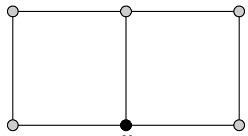


Figure 2: Cartesian product of P_3 and P_2

The curvature matrix at x is given by

$$A_\infty(x) = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1.5 & 1 \\ 0 & 1 & 1.5 \end{pmatrix},$$

and it has the smallest eigenvalue of 0.5. The vector $\mathbf{v}_0 = (1\ 1\ 1)^\top$ is not an eigenvector, but it is perpendicular to the minimal eigenspace $E_{\min}(A_\infty(x)) = \mathrm{span}\,(0\ 1\ -1)^\top$.

The rank one perturbation $A_N(x) = A_\infty(x) - \frac{2}{N}\mathbf{v}_0\mathbf{v}_0^\top = A_\infty(x) - \frac{2}{N}J_3$ has its spectrum equal to $\sigma(A_N(x)) = \{\frac{1}{2},\ \frac{9}{4} - \frac{3}{N} \pm \sqrt{\frac{1}{16} - \frac{1}{2N} + \frac{9}{N^2}}\}$. Therefore, the curvature function at x is given by

$$\mathcal{K}_{P_3\times P_2}(x) = \begin{cases} \frac{9}{4} - \frac{3}{N} - \sqrt{\frac{1}{16} - \frac{1}{2N} + \frac{9}{N^2}} & \text{if } N \in (0, \frac{10}{3}] \\ \frac{1}{2} & \text{if } N \in [\frac{10}{3}, \infty]. \end{cases}$$

6 Curvature of Cartesian product of graphs

Given two weighted graphs G, G' and two fixed positive numbers $\alpha, \beta \in \mathbb{R}^+$, the weighted Cartesian product $G \times_{\alpha,\beta} G'$ is defined with the following weight function and vertex measure: for $x, y \in G$ and $x', y' \in G'$,

$$w_{(x,x')(y,x')} := \alpha w_{xy}\mu_{x'},$$
$$w_{(x,x')(x,y')} := \beta w_{x'y'}\mu_x,$$
$$\mu_{(x,x')} := \mu_x \mu_{x'}.$$

One can translate the above definition into the transition rate p as

$$p_{(x,x')(y,x')} = \alpha \frac{w_{xy}\mu_{x'}}{\mu_x \mu_{x'}} = \alpha p_{xy},$$
$$p_{(x,x')(x,y')} = \beta p_{x'y'},$$
$$\frac{d_{(x,x')}}{\mu_{(x,x')}} = \sum_y p_{(x,x')(y,x')} + \sum_{y'} p_{(x,x')(x,y')} = \alpha \frac{d_x}{\mu_x} + \beta \frac{d_{x'}}{\mu_{x'}}.$$

Here we use the same symbols w, μ, p and d for all graphs G, G' and its product, where the associated graph can be determined from the input vertices. With this idea, we also use the notations $A_\infty(\cdot), A_N(\cdot)$ and $Q(\cdot)$. This simplifies our notations without making them ambiguous.

Proof of Theorem 1.10. Now the central vertex is (x, x') with horizontal neighbours (y, x') for $y \in S_1(x)$ and vertical neighbours (x, y') for $y' \in S_1(x')$. Note also that (y, x') and (x, y') are not adjacent but sharing one common neighbour in S_2, namely (y, y'). On the other hand, the vertex (y, y') has exactly two neighbours in S_1, namely (y, x') and (x, y'). The transition rate on each edge are presented in the following scheme.

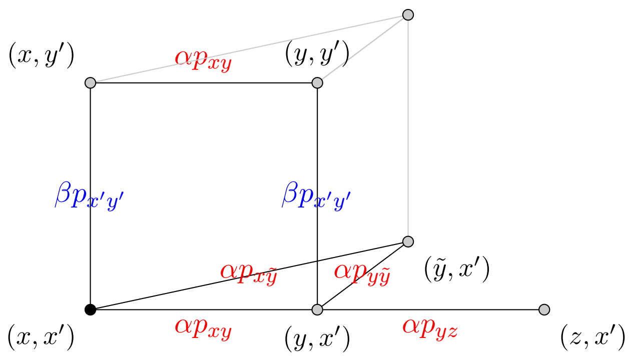


Figure 3: The scheme showing a horizontal neighbour and a vertical neighbour of the central vertex (x, x') in the Cartesian product $G \times_{\alpha,\beta} G'$ and transition rate p on each edge.

For $y \in S_1(x)$, we have from (A.11) that

$$
\begin{aligned}
&4Q((x,x'))_{(y,x')(y,x')} \\
&= 2p^2_{(x,x')(y,x')} + 3p_{(x,x')(y,x')}p_{(y,x')(x,x')} - \frac{d_{(x,x')}}{\mu_{(x,x')}}p_{(x,x')(y,x')} \\
&\quad + 3p_{(x,x')(y,x')}\Big(\sum_{z\in S_2(x)} p_{(y,x')(z,x')} + \sum_{y'\in S_1(x')} p_{(y,x')(y,y')}\Big) \\
&\quad + \sum_{\tilde{y}\in S_1(x)} (3p_{(x,x')(y,x')}p_{(y,x')(\tilde{y},x')} + p_{(x,x')(\tilde{y},x')}p_{(\tilde{y},x')(y,x')}) \\
&\quad - 4\sum_{z\in S_2(x)} \frac{p^2_{(x,x')(y,x')}p^2_{(y,x')(z,x')}}{\sum_{y\in S_1(x)} p_{(x,x')(y,x')}p_{(y,x')(z,x')}} \\
&\quad - 4\sum_{y'\in S_1(x')} \frac{p^2_{(x,x')(y,x')}p^2_{(y,x')(y,y')}}{p_{(x,x')(y,x')}p_{(y,x')(y,y')} + p_{(x,x')(x,y')}p_{(x,y')(y,y')}} \\
&= 2\alpha^2 p^2_{xy} + 3\alpha^2 p_{xy}p_{yx} - (\alpha\frac{d_x}{\mu_x} + \beta\frac{d_{x'}}{\mu_{x'}})(\alpha p_{xy}) + 3\alpha p_{xy}(\sum_{z\in S_2(x)} \alpha p_{yz} + \sum_{y'\in S_1(x')} \beta p_{x'y'}) \\
&\quad + \alpha^2 \sum_{\tilde{y}\in S_1(x)} (3p_{xy}p_{y\tilde{y}} + p_{x\tilde{y}}p_{\tilde{y}y}) - 4\Big(\alpha^2 \sum_{z\in S_2(x)} \frac{p^2_{xy}p^2_{yz}}{p^{(2)}_{xz}} + \sum_{y'\in S_1(x')} \frac{(\alpha p_{xy})^2(\beta p_{x'y'})^2}{2\alpha\beta p_{xy}p_{x'y'}}\Big) \\
&= 4\alpha^2 Q(x)_{yy}.
\end{aligned}
$$

And similarly, $4Q((x,x'))_{(x,y')(x,y')} = 4\beta^2 Q(x)_{y'y'}$ for $y' \in S_1(x')$.

For $y_i \neq y_j \in S_1(x)$, we have from (A.12) that

$$
\begin{aligned}
&4Q((x,x'))_{(y_i,x')(y_j,x')} \\
&= 2p_{(x,x')(y_i,x')}p_{(x,x')(y_j,x')} - 2p_{(x,x')(y_i,x')}p_{(y_i,x')(y_j,x')} - 2p_{(x,x')(y_j,x')}p_{(y_j,x')(y_i,x')} \\
&\quad - 4\sum_{z\in S_2(x)} \frac{p_{(x,x')(y_i,x')}p_{(y_i,x')(z,x')}p_{(x,x')(y_j,x')}p_{(y_j,x')(z,x')}}{\sum_{\tilde{y}\in S_1(x)} p_{(x,x')(\tilde{y},x')}p_{(\tilde{y},x')(z,x')}} \\
&= 2\alpha^2 p_{xy_i}p_{xy_j} - 2\alpha^2 p_{xy_i}p_{y_iy_j} - 2\alpha^2 p_{xy_j}p_{y_jy_i} - 4\sum_{z\in S_2(x)} \frac{\alpha^4 p_{xy_i}p_{y_iz}p_{xy_j}p_{y_jz}}{\sum_{\tilde{y}\in S_1(x)} \alpha^2 p_{x\tilde{y}}p_{\tilde{y}z}} \\
&= 4\alpha^2 Q(x)_{y_iy_j}.
\end{aligned}
$$

And similarly, $4Q((x,x'))_{(x,y'_i)(x,y'_j)} = 4\beta^2 Q(x)_{y'_iy'_j}$ for $y'_i \neq y'_j \in S_1(x')$.

For any $y \in S_1(x)$ and $y' \in S_1(x')$, we have from (A.12) that

$$
\begin{aligned}
&4Q((x,x'))_{(y,x')(x,y')} \\
&= 2p_{(x,x')(y,x')}p_{(x,x')(x,y')} - 4\frac{p_{(x,x')(y,x')}p_{(y,x')(y,y')}p_{(x,x')(x,y')}p_{(x,y')(y,y')}}{p_{(x,x')(y,x')}p_{(y,x')(y,y')} + p_{(x,x')(x,y')}p_{(x,y')(y,y')}} \\
&= 2\alpha\beta p_{xy}p_{x'y'} - 4\frac{(\alpha\beta p_{xy}p_{x'y'})^2}{2\alpha\beta p_{xy}p_{x'y'}} = 0.
\end{aligned}
$$

We can conclude from the above calculation that $Q((x,x')) = \alpha^2 Q(x) \oplus \beta^2 Q(y)$. Note also that the matrix $\operatorname{diag} \mathbf{v}_0((x,x')) = \sqrt{\alpha}\operatorname{diag} \mathbf{v}_0(x) \oplus \sqrt{\beta}\operatorname{diag} \mathbf{v}_0(x')$. Therefore, we derive the curvature matrix as

$$A_\infty((x,x')) = 2\,\mathrm{diag}\,\mathbf{v}_0((x,x'))^{-1} Q((x,x'))\,\mathrm{diag}\,\mathbf{v}_0((x,x'))^{-1} = \alpha A_\infty(x) \oplus \beta A_\infty(x'),$$

as desired. □

Next we prove Theorem 1.12, which will be rephrased in a more abstract way. This will be useful in the next section when we discuss the Ricci curvature of weighted manifolds in an analogous manner.

Theorem 6.1. *For $i \in \{1,2\}$, let A_i be $m_i \times m_i$ symmetric matrices and $\mathbf{v}_i$ be vectors in $\mathbb{R}^{m_i}$. Given fixed weights $\alpha, \beta > 0$, let A and $\mathbf{v}$ be given as*

$$A = \alpha A_1 \oplus \beta A_2 \text{ and } \mathbf{v} = \sqrt{\alpha}\mathbf{v}_1 \oplus \sqrt{\beta}\mathbf{v}_2.$$

For $N \in (0,\infty]$, consider

$$A_i(N) := A_i - \frac{2}{N}\mathbf{v}_i\mathbf{v}_i^\top \text{ and } A(N) := A - \frac{2}{N}\mathbf{v}\mathbf{v}^\top.$$

Then we have

$$\min\{\alpha\lambda_1, \beta\lambda_2\} \le \lambda_{\min}\left(A(N_1+N_2)\right) \le \max\{\alpha\lambda_1, \beta\lambda_2\}, \tag{6.1}$$

where $\lambda_i := \lambda_{\min}\left(A_i(N_i)\right)$.

Proof of Theorem 6.1. Let us first consider the case $N_1, N_2 \in (0,\infty)$. We have the matrix $\mathbf{v}\mathbf{v}^\top = \begin{pmatrix} \alpha\mathbf{v}_1\mathbf{v}_1^\top & \sqrt{\alpha\beta}\mathbf{v}_1\mathbf{v}_2^\top \\ \sqrt{\alpha\beta}\mathbf{v}_2\mathbf{v}_1^\top & \beta\mathbf{v}_2\mathbf{v}_2^\top \end{pmatrix}$. It follows that

$$A(N_1+N_2) = \begin{pmatrix} \alpha A_1(N_1) & \\ & \beta A_2(N_2) \end{pmatrix} + \frac{2}{N_1+N_2} \underbrace{\begin{pmatrix} \alpha\frac{N_2}{N_1}\mathbf{v}_1\mathbf{v}_1^\top & -\sqrt{\alpha\beta}\mathbf{v}_1\mathbf{v}_2^\top \\ -\sqrt{\alpha\beta}\mathbf{v}_2\mathbf{v}_1^\top & \beta\frac{N_1}{N_2}\mathbf{v}_2\mathbf{v}_2^\top \end{pmatrix}}_{=:J}.$$

We want to verify that $J \succeq 0$, which will then imply the left inequality in (6.1).

For any vector $w = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}$ with $w_i \in \mathbb{R}^{m_i}$, we have

$$\begin{aligned} w^\top J w &= \alpha\frac{N_2}{N_1} w_1^\top \mathbf{v}_1\mathbf{v}_1^\top w_1 + \beta\frac{N_1}{N_2} w_2^\top \mathbf{v}_2\mathbf{v}_2^\top w_2 - 2\sqrt{\alpha\beta} w_1^\top \mathbf{v}_1\mathbf{v}_2^\top w_2 \\ &= \left(\sqrt{\alpha\frac{N_2}{N_1}} w_1^\top \mathbf{v}_1 - \sqrt{\beta\frac{N_1}{N_2}} w_2^\top \mathbf{v}_2\right)^2 \ge 0. \end{aligned}$$

Thus $J \succeq 0$. Next we prove the right inequality in (6.1). For $i \in \{1,2\}$, we choose a unit eigenvector $\mathbf{w}_i$ such that $A_i\mathbf{w}_i = \lambda_i\mathbf{w}_i$ where $\lambda_i = \lambda_{\min}\left(A_i(N_i)\right)$, and let $\mathbf{w} := \begin{pmatrix} c_1\mathbf{w}_1 \\ c_2\mathbf{w}_2 \end{pmatrix}$ with arbitrary constants $c_i \ne 0$. It follows from the Rayleigh quotient description that

$$\begin{aligned} \lambda_{\min}\left(A(N_1+N_2)\right) &\le \frac{\mathbf{w}^\top\left(\alpha A_1(N_1) \oplus \beta A_2(N_2)\right)\mathbf{w} + \frac{2}{N_1+N_2}\mathbf{w}^\top J\mathbf{w}}{\mathbf{w}^\top\mathbf{w}} \\ &= \frac{1}{c_1^2+c_2^2}\left(\alpha c_1^2\lambda_1 + \beta c_2^2\lambda_2 + \frac{2}{N_1+N_2}\left(c_1\sqrt{\alpha\frac{N_2}{N_1}}\mathbf{w}_1^\top\mathbf{v}_1 - c_2\sqrt{\beta\frac{N_1}{N_2}}\mathbf{w}_2^\top\mathbf{v}_2\right)^2\right). \end{aligned}$$

We may choose $c_1 = \sqrt{\beta \frac{N_1}{N_2}} \mathbf{w}_2^\top v_2$ and $c_2 = \sqrt{\alpha \frac{N_2}{N_1}} \mathbf{w}_1^\top v_1$ so that the square term above becomes zero. As a result,

$$\lambda_{\min}\left(A(N_1+N_2)\right) \le \frac{\alpha c_1^2 \lambda_1 + \beta c_2^2 \lambda_2}{c_1^2 + c_2^2} \le \max\{\alpha\lambda_1, \beta\lambda_2\},$$

which finishes the proof of (6.1). The case that N_1 or N_2 equals ∞ is not hard to prove by modifying the above argument. □

Now, Theorem 1.12 follows from Theorem 6.1 and the following general fact [12, Proposition 7.3] about star product.

Proposition 6.2 ([12]). *Let $f_1, f_2 : (0, \infty] \to \mathbb{R}$ be continuous monotone non-decreasing functions with $\lim_{N\to 0} = -\infty$. Then a function $F : (0, \infty] \to \mathbb{R}$ satisfies $F = f_1 * f_2$ if and only if it holds for any $N_1, N_2 \in (0, \infty)$ that*

$$\min\{f_1(N_1), f_2(N_2)\} \le F(N_1 + N_2) \le \max\{f_1(N_1), f_2(N_2)\},$$

and $F(\infty) = \lim_{N\to\infty} F(N)$.

7 The case of weighted manifolds

In [12, Section 1.6], the authors briefly draw a comparison between the Bakry-Émery curvature functions of graphs and that of weighted Riemannian manifolds. Here, we discuss this comparison further by investigating the analogous result that the optimal lower Ricci curvature bound at a point on a weighted Riemannian manifold is also the minimal eigenvalue of a rank one perturbation of a curvature matrix.

A *weighted Riemannian manifold* is a triple $(M^n, g, e^{-V} d\mathrm{vol}_g)$, where (M^n, g) is an n-dimensional Riemannian manifold, $d\mathrm{vol}_g$ is the Riemannian volume element, and V is a smooth real valued function on M^n. The *N-Bakry-Émery Ricci tensor* of $(M^n, g, e^{-V} d\mathrm{vol}_g)$ is defined to be

$$\mathrm{Ric}_{N,V} := \mathrm{Ric} + \mathrm{Hess}\, V - \frac{\mathrm{grad}\, V \otimes \mathrm{grad}\, V}{N - n}, \tag{7.1}$$

where Ric is the Ricci curvature tensor of (M^n, g), $\mathrm{Hess}\, V$ is the Hessian of V, and $\mathrm{grad}\, V$ is the gradient of V ([1, 2]). Using the V-Laplacian $\Delta_V := \Delta_g - g(\mathrm{grad}\, V, \mathrm{grad}\,\cdot)$, where Δ_g is the Laplace-Beltrami operator on (M^n, g), one can define the Bakry-Émery curvature-dimension inequality $CD(\mathcal{K}, N)$ (at any point $x \in M$) as in Definition 1.1. Then $CD(\mathcal{K}, N), N \in (n, \infty]$ (at a given point $x \in M$) holds if and only if $\mathrm{Ric}_{N,V} \ge \mathcal{K}$ (at $x \in M$) (see [1, pp. 93–94]).

Definition 7.1. Let $(M^n, g, e^{-V} d\mathrm{vol}_g)$ be a weighted Riemannian manifold. For a given $N \in (n, \infty]$, the Bakry-Émery curvature $\mathcal{K}(M, V, x; N)$ at a point $x \in M$ is defined to be the largest $\mathcal{K}$ such that $CD(\mathcal{K}, N)$ holds at x. The function $\mathcal{K}_{M,V,x} : (0, \infty] \to \mathbb{R}$ given by $\mathcal{K}_{M,V,x}(N) := \mathcal{K}(M, V, x; N + n)$ is called the Bakry-Émery curvature function of $(M^n, g, e^{-V} d\mathrm{vol}_g)$ at x.

Remark 7.2. Recall n is the dimension of the underlying Riemannian manifold. The purpose to define the curvature function $\mathcal{K}_{M,V,x}$ on the interval $(0, \infty]$ instead of on $(n, \infty]$ is to make it compatible with the graph case.

When V is constant, that is, when the curvature-dimension inequality is based on the Laplace-Beltrami operator Δ_g, the dimension parameter N in (7.1) can be equal to n, and the function $\mathcal{K}_{M,V,x}$ is a constant function on $[0,\infty]$ (see [1, pp. 93–94], [3, Appendix C.6]). When V is not constant, $\mathcal{K}_{M,V,x}(N)$ tends to $-\infty$ as N tends to 0.

Next we investigate the shape of the Bakry-Émery curvature function $\mathcal{K}_{M,V,x}$ at x on a weighted Riemannian manifold $(M^n, g, e^{-V}d\mathrm{vol}_g)$. If $\operatorname{grad} V(x) = 0$, then this function $\mathcal{K}_{M,V,x}$ is constant. In the sequel, we consider the case that $\operatorname{grad} V(x) \neq 0$. Since $\mathrm{Ric}_{N,V}$ is a symmetric $(0,2)$-tensor, there exists a linear transformation $\mathcal{A}_{N-n} : T_xM \to T_xM$ from the tangent space T_xM of M at x to itself, such that

$$\mathrm{Ric}_{N,V}(v,v) = g(\mathcal{A}_{N-n}v, v), \text{ for any } v \in T_xM.$$

Therefore, the optimal lower Ricci curvature bound at x can be expressed as the minimal eigenvalue:

$$\mathcal{K}_{M,V,x}(N) := \inf_{v \in S_xM} \mathrm{Ric}_{N+n,V}(v,v) = \lambda_{\min}(\mathcal{A}_N), \text{ for any } N \in (0,\infty],$$

where S_xM stands for the space of unit tangent vectors at x. For any $v, w \in T_xM$, the tensor $\mathrm{Ric}_{N+n,V}$, $N \in (0,\infty]$ can be written independently of the choice of an orthonormal basis $\{e_i\}_{i=1}^n$ of the tangent space T_xM as

$$\begin{aligned}\mathrm{Ric}_{N+n,V}(v,w) &= \mathrm{Ric}(v,w) + \mathrm{Hess}V(v,w) - \frac{v(V)\cdot w(V)}{N} \\ &= \sum_{i=1}^n g(R(v,e_i)e_i, w) + g(\nabla_v \operatorname{grad} V, w) - \frac{1}{N} g(g(\operatorname{grad} V, v)\operatorname{grad} V, w),\end{aligned}$$

where $\nabla_v\cdot$ is the covariant derivative along v, and $R(\cdot,\cdot)\cdot$ is the Riemann curvature tensor. Let us define linear transformations $\mathcal{A}_\infty, \mathcal{B} : T_xM \to T_xM$ as follows: for any $v \in T_xM$,

$$\begin{aligned}\mathcal{A}_\infty v &:= \sum_{i=1}^n R(v,e_i)e_i + \nabla_v \operatorname{grad} V, \\ \mathcal{B}v &:= \frac{1}{2} g(\operatorname{grad} V, v)\operatorname{grad} V.\end{aligned}$$

Therefore, the linear transformation $\mathcal{A}_N : T_xM \to T_xM$ satisfies

$$\mathcal{A}_N = \mathcal{A}_\infty - \frac{2}{N}\mathcal{B}. \tag{7.2}$$

Recall that T_xM equipped with the inner product g is an n-dimensional Euclidean vector space. Let A_∞, A_N be the matrix representation of $\mathcal{A}_\infty, \mathcal{A}_N$ with respect to an orthonormal basis $\{e_i\}_{i=1}^n$ of T_xM. Let $\mathbf{v}_0$ be the n-dimensional coordinate vector of $\frac{1}{\sqrt{2}}\operatorname{grad} V(x)$ with respect to $\{e_i\}_{i=1}^n$. Then we have a matrix version of (7.2):

$$A_N = A_\infty - \frac{2}{N}\mathbf{v}_0\mathbf{v}_0^\top. \tag{7.3}$$

Notice that both A_∞ and A_N are symmetric $n \times n$ matrices. We call A_∞ the *the curvature matrix* at x (with respect to the orthonormal basis $\{e_i\}_{i=1}^n$) of the weighted manifold

$(M, g, e^{-V} d\mathrm{vol}_g)$. The matrix A_N is a rank one perturbation of the curvature matrix A_∞. The Bakry-Émery curvature function satisfies

$$\mathcal{K}_{M,V,x}(N) = \lambda_{\min}(A_N) = \lambda_{\min}(A_\infty - \frac{2}{N}\mathbf{v}_0\mathbf{v}_0^\top). \tag{7.4}$$

Therefore, we reduce the study of the Bakry-Émery curvature functions of weighted Riemannian manifolds to a matrix eigenvalue problem of the same type as in the graph case.

Then, it is direct to check the results (Theorem 1.3, Proposition 1.4, Theorem 1.5, and Propositions 1.6 and 1.7) describing the shape of curvature functions of graphs also holds for the curvature functions of weighted manifolds.

In particular, we mention the quantity $\mathcal{K}_\infty^0(x)$ in the weighted manifold case

$$\begin{aligned}\mathcal{K}_\infty^0(x) :=& \frac{\mathbf{v}_0^\top A_\infty \mathbf{v}_0}{\mathbf{v}_0^\top \mathbf{v}_0} = \frac{g(\mathcal{A}_\infty \operatorname{grad} V, \operatorname{grad} V)}{g(\operatorname{grad} V, \operatorname{grad} V)} \\ =& \operatorname{Ric}_x\left(\frac{\operatorname{grad} V}{\|\operatorname{grad} V\|}, \frac{\operatorname{grad} V}{\|\operatorname{grad} V\|}\right) + \frac{\operatorname{grad} V(x)}{\|\operatorname{grad} V(x)\|}(\|\operatorname{grad} V\|).\end{aligned}$$

Then we have

$$\mathcal{K}_{M,V,x}(N) \leq \frac{\mathbf{v}_0^\top A_N \mathbf{v}_0}{\mathbf{v}_0^\top \mathbf{v}_0} = \mathcal{K}_\infty^0(x) - \frac{1}{N}\|\operatorname{grad} V(x)\|^2. \tag{7.5}$$

We say that x is *N-curvature sharp* if (7.5) holds with equality. Then, for example, one can conclude similarly to Proposition 1.7 that x is ∞-curvature sharp if and only if $\operatorname{grad} V(x)$ is an eigenvector corresponding to the minimal eigenvalue of $\mathcal{A}_\infty$.

Now we discuss the curvature functions of the Cartesian product of weighted Riemannian manifolds. Given two weighted manifolds $(M_i^{n_i}, g_i, e^{-V_i} d\mathrm{vol}_{g_i})$, $i \in \{1, 2\}$, the Cartesian product $(M, g, e^{-V} d\mathrm{vol}_g) = (M_1 \times M_2, g_1 \oplus g_2, e^{-V_1 \oplus V_2} d\mathrm{vol}_{g_1 \oplus g_2})$ has a canonical identification of the tangent space $T_{(x_1,x_2)}M \simeq T_{x_1}M_1 \oplus T_{x_2}M_2$. We observe that $\mathcal{A}_\infty, \mathcal{B}$ of the product is naturally decomposed into the corresponding $\mathcal{A}_\infty, \mathcal{B}$ in each factor, that is,

$$\begin{aligned}\mathcal{A}_\infty^M(v_1 \oplus v_2) &= \sum_{i=1}^{n_1} R(v_1, e_i)e_i \oplus \sum_{j=1}^{n_2} R(v_2, e_i)e_i + \nabla_{v_1} \operatorname{grad} V_1 \oplus \nabla_{v_2} \operatorname{grad} V_2 \\ &= \mathcal{A}_\infty^{M_1}(v_1) \oplus \mathcal{A}_\infty^{M_2}(v_2),\end{aligned}$$

and $\mathcal{B}(v_1 \oplus v_2) = g(\operatorname{grad} V_1 \oplus \operatorname{grad} V_2, v_1 \oplus v_2)(\operatorname{grad} V_1 \oplus \operatorname{grad} V_2)$, for any $v_i \in T_{x_i}M_i$. In the matrix form, we have

$$A_\infty^M = A_\infty^{M_1} \oplus A_\infty^{M_2}, \text{ and } \mathbf{v}_0^M = \mathbf{v}_0^{M_1} \oplus \mathbf{v}_0^{M_2}.$$

Theorem 6.1 is then applicable for manifolds and yields the following theorem.

Theorem 7.3. *The curvature function of the Cartesian product*

$$(M, g, e^{-V} d\mathrm{vol}_g) = (M_1 \times M_2, g_1 \oplus g_2, e^{-V_1 \oplus V_2} d\mathrm{vol}_{g_1 \oplus g_2})$$

satisfies the following inequalities:

$$\min\{\lambda_{\min}(\mathcal{A}_{N_1}^{M_1}), \lambda_{\min}(\mathcal{A}_{N_2}^{M_2})\} \leq \lambda_{\min}(\mathcal{A}_{N_1+N_2}^M) \leq \max\{\lambda_{\min}(\mathcal{A}_{N_1}^{M_1}), \lambda_{\min}(\mathcal{A}_{N_2}^{M_2})\},$$

and consequently, $\mathcal{K}_{M,V,(x_1,x_2)} = \mathcal{K}_{M_1,V_1,x_1} * \mathcal{K}_{M_2,V_2,x_2}$.

We conclude this section with the following example of a weighted Riemannian manifold with ∞-curvature sharp points.

Example 7.4 (weighted 2-sphere). Let $M = S^2(r)$ be the two-dimensional sphere of radius r with coordinates $\mathbf{x}(\theta,\phi) = (r\cos\theta\cos\phi, r\sin\theta\cos\phi, r\sin\phi)$ for $\theta \in (0,2\pi)$ and $\phi \in (-\pi/2,\pi/2)$, and the corresponding metric $g = r^2(\cos^2(\phi)d\theta\otimes d\theta + d\phi\otimes d\phi)$. Let $V : M \to \mathbb{R}$ be a smooth height function, i.e., $V(\mathbf{x}(\theta,\phi)) = h(\phi)$ for some smooth function h. Consider the weighted manifold $(M, g, e^{-V}d\mathrm{vol}_g)$ and a point $p \in M$ with $\operatorname{grad} V(p) \neq 0$.

The tangent space T_pM is spanned by $\operatorname{grad} V(p)$ and the tangent vector $\mathbf{x}_\theta(p) \in T_pM$, which satisfy $g(\mathbf{x}_\theta(p), \operatorname{grad} V(p)) = 0$. We first check that both the tangent vector $\operatorname{grad} V(p)$ and $\mathbf{x}_\theta(p)$ are in fact eigenvectors of $\mathcal{A}_N$ (based at p).

Consider the geodesic $\alpha := \mathbf{x}(\theta_0,\cdot) : (-\pi/2,\pi/2) \to S^2(r)$ which passes through $p = \alpha(t) = \mathbf{x}(\theta_0, t)$. The tangent vector $\operatorname{grad} V(p)$ is parallel to $\alpha'(t)$, so we may write $\operatorname{grad} V(p) = k(t)\alpha'(t)$ for some smooth function $k : (-\pi/2,\pi/2) \to \mathbb{R}$. It follows that at $p \in M$

$$\nabla_{\operatorname{grad} V} \operatorname{grad} V = \nabla_{k\alpha'} k\alpha' = k\nabla_{\alpha'} k\alpha' = k^2 \underbrace{\nabla_{\alpha'}\alpha'}_{=0} + kk'\alpha' = k' \operatorname{grad} V,$$

and hence,

$$\begin{aligned}\mathcal{A}_N \operatorname{grad} V &= \sum_{i=1}^{2} R(\operatorname{grad} V, e_i)e_i + \nabla_{\operatorname{grad} V} \operatorname{grad} V - \frac{g(\operatorname{grad} V, \operatorname{grad} V)}{N} \operatorname{grad} V \\ &= \left(\frac{1}{r^2} + k' - \frac{k^2 r^2}{N}\right) \operatorname{grad} V.\end{aligned}$$

On the other hand, we have $g_p(\nabla_{\mathbf{x}_\theta} \operatorname{grad} V, \operatorname{grad} V) = 0$, and

$$g_p\left(\nabla_{\mathbf{x}_\theta} \operatorname{grad} V, \frac{\mathbf{x}_\theta}{\|\mathbf{x}_\theta\|}\right) = -\|x_\theta\| g_p\left(\operatorname{grad} V, \nabla_{\frac{\mathbf{x}_\theta}{\|\mathbf{x}_\theta\|}} \frac{\mathbf{x}_\theta}{\|\mathbf{x}_\theta\|}\right) = -\|x_\theta\| g_p\left(\operatorname{grad} V, k_g \frac{\mathbf{x}_\phi}{\|\mathbf{x}_\phi\|}\right),$$

where $k_g = \frac{1}{r}\tan(t)$ is the geodesic curvature of the parallel circles with the unit tangent vector $\frac{\mathbf{x}_\theta}{\|\mathbf{x}_\theta\|}(p)$, and $\frac{\mathbf{x}_\phi}{\|\mathbf{x}_\phi\|}(p) = \frac{\alpha'(t)}{\|\alpha'(t)\|} = \frac{\alpha'(t)}{r}$. It follows that

$$\nabla_{\mathbf{x}_\theta(p)} \operatorname{grad} V = -g\left(\operatorname{grad} V(p), \frac{\alpha'(t)}{r}\right)\frac{1}{r}\tan(t)\mathbf{x}_\theta(p) = -k(t)\tan(t)\mathbf{x}_\theta(p).$$

Therefore, we have

$$\begin{aligned}\mathcal{A}_N \mathbf{x}_\theta(p) &= \sum_{i=1}^{2} R(\mathbf{x}_\theta, e_i)e_i + \nabla_{\mathbf{x}_\theta} \operatorname{grad} V - \frac{g(\operatorname{grad} V(p), \mathbf{x}_\theta)}{N} \operatorname{grad} V(p) \\ &= \left(\frac{1}{r^2} - k(t)\tan(t)\right)\mathbf{x}_\theta(p).\end{aligned}$$

It means that both $\operatorname{grad} V(p)$ and $\mathbf{x}_\theta(p)$ are eigenvectors of $\mathcal{A}_N$. Then the Bakry-Émery curvature and the generalised scalar curvature at p are given by

$$\begin{aligned}\mathcal{K}_{M,V,p}(N) &= \min\left\{\frac{1}{r^2} + k'(t) - \frac{k(t)^2 r^2}{N}, \frac{1}{r^2} - k(t)\tan(t)\right\}, \\ S_{M,V,p}(N) &= \frac{2}{r^2} - k(t)\tan(t) + k'(t) - \frac{k(t)^2 r^2}{N}.\end{aligned}$$

Recall that the point $p = \alpha(t)$ is ∞-curvature sharp if and only if $\operatorname{grad} V(p)$ corresponds to the minimal eigenvalue of $\mathcal{A}_\infty$, which occurs precisely when $k'(t) \leq -\tan(t)k(t)$. In the special case when $k : (-\pi/2, \pi/2) \to \mathbb{R}$ is even, either the point $p = \alpha(t)$ or its mirror $p' = \alpha(-t)$ (or both) is ∞-curvature sharp. In particular, if $k(\cdot) = c\cos(\cdot)$ on the whole interval $(-\pi/2, \pi/2)$ for some $c \neq 0$ (which means $V(x, y, z) = az + b$ with $a = cr$ and $b \in \mathbb{R}$), then we have $k' = -\tan(\cdot)k$ and hence p is ∞-curvature sharp. In fact, every point of M except for the south and north poles (i.e., when $\phi = -\pi/2, \pi/2$) is ∞-curvature sharp. At the south and north poles, the curvature functions are constant. Moreover, this choice of k provides a non-constant potential function V for the round sphere as a gradient Ricci soliton.

A complete Riemannian manifold (M, g) is called a gradient Ricci soliton with a potential function V if $\mathrm{Ric}_{V,\infty} = \lambda g$ for some constant λ (see, e.g., [53, Definition 1.2.3]).

Theorem 7.5. *Every gradient Ricci soliton (M, g) with a potential function V leads to a weighted Riemannian manifold $(M, g, e^{-V}\mathrm{dvol}_g)$ which is ∞-curvature sharp at every point $x \in M$ with* $\operatorname{grad} V(x) \neq 0$.

Proof. Being a gradient Ricci soliton means, for every point $x \in M$, $\mathcal{A}_\infty(x) = \lambda \mathrm{Id}$. In particular, if $\operatorname{grad} V(x)$ is nonzero, then it is an eigenvector corresponding to the smallest eigenvalue of $\mathcal{A}_\infty(x)$, and therefore x is ∞-curvature sharp by Theorem 1.7(ii). □

8 Geometric structure of $B_2(x)$ and curvature properties

In this section, we present the proofs of the three results (Proposition 1.13, and Theorems 1.14 and 1.15) about the curvature at x which are related to the geometric structure of the $B_2(x)$.

Proof of Propositions 1.13. The computations for the matrix A_∞ and

$$S_{G,x}(N) = \mathrm{tr}(A_\infty - \frac{2}{N}\mathbf{v}_0\mathbf{v}_0^\top) = S_{G,x}(\infty) - \frac{2}{N}\frac{d_x}{\mu_x}$$

are given in Appendix (A.18) and (A.14). In the particular case of non-weighted graphs, the terms in (A.18) and (A.14) are simplified by $\mu_x = 1$ and $p_{uv} \in \{0, 1\}$, which directly gives the desired result. □

Proof of Theorem 1.14. In view of Proposition 1.7, we need to show that $\mathbf{v}_0$ is an eigenvector of A_∞ under the S_1-in and S_1-out regularity assumption: $p^-(y) := p_{yx}$ and $p^+(y) := \sum_{z \in S_2(x)} p_{yz}$ are independent of $y \in S_1(x)$.

The vector $\mathbf{v}_0 = \begin{pmatrix}\sqrt{p_{xy_1}} & \sqrt{p_{xy_2}} & \cdots & \sqrt{p_{xy_m}}\end{pmatrix}^\top$ is an eigenvector of A_∞ if and only if $\lambda \mathbf{v}_0 = A_\infty \mathbf{v}_0 = 2\,\mathrm{diag}(\mathbf{v}_0)^{-1} Q\,\mathrm{diag}(\mathbf{v}_0)^{-1}$ for some $\lambda \in \mathbb{R}$, or equivalently,

$$2Q\mathbb{1}_m = \lambda \begin{pmatrix}p_{xy_1} & p_{xy_2} & \cdots & p_{xy_m}\end{pmatrix}^\top,$$

that is, $\frac{1}{p_{xy_i}} \sum_{j=1}^m Q_{y_i y_j} = \frac{1}{2}\lambda$ is independent of $i \in [m] := \{1, 2, \ldots, m\}$.

A direct calculation using the formula (A.15) yields, for any $i \in [m]$,

$$\begin{aligned}\frac{1}{p_{xy_i}}\sum_{j=1}^{m} Q_{y_iy_j} &= \frac{1}{4}\frac{d_x}{\mu_x} + \frac{3}{4}p_{y_ix} - \frac{1}{4}\sum_{z\in S_2(x)} p_{y_iz} + \sum_{j=1}^{m}\left(\frac{1}{4}p_{y_iy_j} - \frac{1}{4}\frac{p_{xy_j}p_{y_jy_i}}{p_{xy_i}}\right)\\ &= \frac{1}{4}\frac{d_x}{\mu_x} + \frac{3}{4}p_{y_ix} - \frac{1}{4}\sum_{z\in S_2(x)} p_{y_iz} + \frac{1}{4}\sum_{j=1}^{m} p_{y_iy_j}\underbrace{\left(1 - \frac{p_{y_jx}}{p_{y_ix}}\right)}_{=0},\end{aligned}$$

which is independent of i, given that x is S_1-in and S_1-out regular. □

Proof of Theorem 1.15. We denote by $\widetilde{Q}$, $\widetilde{A}_\infty$ and $\widetilde{A}_N$ the corresponding matrices Q, A_∞ and A_N centered at the vertex x of the modified graph $\widetilde{G} = (V, \tilde{w}, \mu)$. We aim to prove that $\mathcal{K}_{\widetilde{G},x}(N) \geq \mathcal{K}_{G,x}(N)$, that is, $\lambda_{\min}(\widetilde{A}_N) \geq \lambda_{\min}(A_N)$. It suffices to show that $\widetilde{A}_N - A_N$ is positive semidefinite, since it would then imply that $\lambda_{\min}(\widetilde{A}_N) \geq \lambda_{\min}(\widetilde{A}_N - A_N) + \lambda_{\min}(A_N) \geq \lambda_{\min}(A_N)$.

Note that the vector $\mathbf{v}_0 = (\sqrt{p_{xy_1}}\ \sqrt{p_{xy_2}}\ \cdots\ \sqrt{p_{xy_m}})^\top$ is unchanged under this graph modification, so we have $\widetilde{A}_N - A_N = 2\,\mathrm{diag}(\mathbf{v}_0)^{-1}(\widetilde{Q} - Q)\,\mathrm{diag}(\mathbf{v}_0)^{-1}$. To prove that $\widetilde{A}_N - A_N \succeq 0$ is equivalent to showing that $\widetilde{Q} - Q \succeq 0$.

Operation (O1): The modification $\tilde{w}_{yy'} = w_{yy'} + C_1$ for a constant $C_1 > 0$ means $\tilde{p}_{yy'} - p_{yy'} = \frac{C_1}{\mu_y}$ and $\tilde{p}_{y'y} - p_{y'y} = \frac{C_1}{\mu_{y'}}$. We then derive from the formulae (A.11) and (A.12) that the matrix $\widetilde{Q} - Q$ have four nontrivial entries:

$$\begin{aligned}(\widetilde{Q} - Q)_{yy} &= \frac{1}{4}\left(3p_{xy}(\tilde{p}_{yy'} - p_{yy'}) + p_{xy'}(\tilde{p}_{y'y} - p_{y'y})\right)\\ &= \frac{C_1}{4}\left(3\frac{p_{xy}}{\mu_y} + \frac{p_{xy'}}{\mu_{y'}}\right) = \frac{C_1}{4\mu_x}(3p_{yx} + p_{y'x}),\end{aligned}$$

and similarly, $(\widetilde{Q}-Q)_{y'y'} = \frac{C_1}{4\mu_x}(p_{yx}+3p_{y'x})$ and $(\widetilde{Q}-Q)_{yy'} = (\widetilde{Q}-Q)_{y'y} = -\frac{C_1}{2\mu_x}(p_{yx}+p_{y'x})$.

Consequently, the matrix $\widetilde{Q} - Q$ has two nontrivial eigenvalues, corresponding to those of the following 2×2 matrix

$$\begin{pmatrix} (\widetilde{Q} - Q)_{yy} & (\widetilde{Q} - Q)_{yy'} \\ (\widetilde{Q} - Q)_{y'y} & (\widetilde{Q} - Q)_{y'y'} \end{pmatrix} = \frac{C}{4\mu_x}\begin{pmatrix} 3p_{yx} + p_{y'x} & -2p_{yx} - 2p_{y'x} \\ -2p_{yx} - 2p_{y'x} & p_{yx} + 3p_{y'x} \end{pmatrix}.$$

This matrix has eigenvalues $p_{yx}+p_{y'x}\pm\sqrt{2p_{yx}^2 + 2p_{y'x}^2}$, and it becomes positive semidefinite when we assume $p_{yx} = p_{y'x}$.

Operation (O2): Note that the edge-weight modification $\tilde{w}_{yy'} = w_{yy'} + C_2 w_{yz_0}w_{z_0y'}$ for all different $y, y' \in S_1(x)$ means $\tilde{p}_{yy'} - p_{yy'} = C_2 p_{yz_0}p_{z_0y'}\mu_{z_0}$.

For $y_i, y_j \in S_1(x)$ such that $y_i \neq y_j$, the formula (A.12) gives

$$\begin{aligned}
(\widetilde{Q} - Q)_{y_i y_j} &= -\frac{1}{2} p_{xy_i} (\tilde{p}_{y_i y_j} - p_{y_i y_j}) - \frac{1}{2} p_{xy_j} (\tilde{p}_{y_j y_i} - p_{y_j y_i}) + \frac{p_{xy_i} p_{y_i z_0} p_{xy_j} p_{y_j z_0}}{p^{(2)}_{xz_0}} \qquad (8.1) \\
&= -\frac{1}{2} p_{xy_i} \cdot C_2 p_{y_i z_0} p_{z_0 y_j} \mu_{z_0} - \frac{1}{2} p_{xy_j} \cdot C_2 p_{y_j z_0} p_{z_0 y_i} \mu_{z_0} + \frac{p_{xy_i} p_{y_i z_0} p_{xy_j} p_{y_j z_0}}{p^{(2)}_{xz_0}} \\
&= -C_2 p_{xy_i} p_{y_i z_0} p_{z_0 y_j} \mu_{z_0} + \frac{p_{xy_i} p_{y_i z_0} p_{xy_j} p_{y_j z_0}}{p^{(2)}_{xz_0}} \\
&= -p_{xy_i} p_{y_i z_0} p_{z_0 y_j} \left(C_2 \mu_{z_0} - \frac{p_{xy_j} p_{y_j z_0}}{p_{z_0 y_j} p^{(2)}_{xz_0}} \right),
\end{aligned}$$

where the third equation is due to $p_{xy_i} p_{y_i z_0} p_{z_0 y_j} = p_{xy_j} p_{y_j z_0} p_{z_0 y_i}$ which can be checked by

$$\frac{p_{xy_i} p_{y_i z_0} p_{z_0 y_j}}{p_{xy_j} p_{y_j z_0} p_{z_0 y_i}} = \frac{w_{xy_i} w_{y_i z_0} w_{z_0 y_j}}{\mu_x \mu_{y_i} \mu_{z_0}} \cdot \frac{\mu_x \mu_{y_j} \mu_{z_0}}{w_{xy_j} w_{y_j z_0} w_{z_0 y_i}} = \frac{w_{xy_i} \mu_{y_j}}{\mu_{y_i} w_{xy_j}} = \frac{p_{y_i x}}{p_{y_j x}} = \frac{p^-(y)}{p^-(y)} = 1.$$

For $y_i \in S_1(x)$, the formula (A.11) gives

$$\begin{aligned}
(\widetilde{Q} - Q)_{y_i y_i} &= -\frac{3}{4} p_{xy_i} p_{y_i z_0} + \frac{1}{4} \sum_{y_j \neq y_i} \big(3 p_{xy_i} (\tilde{p}_{y_i y_j} - p_{y_i y_j}) + p_{xy_j} (\tilde{p}_{y_j y_i} - p_{y_j y_i}) \big) + \frac{p^2_{xy_i} p^2_{y_i z_0}}{p^{(2)}_{xz_0}} \qquad (8.2) \\
&= -\frac{3}{4} p_{xy_i} p_{y_i z_0} + \sum_{y_j \neq y_i} \left(\frac{3 C_2 \mu_{z_0}}{4} p_{xy_i} p_{y_i z_0} p_{z_0 y_j} + \frac{C_2 \mu_{z_0}}{4} p_{xy_j} p_{y_j z_0} p_{z_0 y_i} \right) + \frac{p^2_{xy_i} p^2_{y_i z_0}}{p^{(2)}_{xz_0}} \\
&= -\frac{3}{4} p_{xy_i} p_{y_i z_0} + C_2 \mu_{z_0} \sum_{y_j \neq y_i} p_{xy_i} p_{y_i z_0} p_{z_0 y_j} + \frac{p^2_{xy_i} p^2_{y_i z_0}}{p^{(2)}_{xz_0}} \\
&= p_{xy_i} p_{y_i z_0} \left(-\frac{3}{4} + C_2 \mu_{z_0} \sum_{y_j \neq y_i} p_{z_0 y_j} + \frac{p_{xy_i} p_{y_i z_0}}{p^{(2)}_{xz_0}} \right).
\end{aligned}$$

Combining (8.2) and (8.1), we derive the sum of entries in i-th row as

$$\begin{aligned}
(\widetilde{Q} - Q)_{y_i y_i} + \sum_{j \neq i} (\widetilde{Q} - Q)_{y_i y_j} &= p_{xy_i} p_{y_i z_0} \left(-\frac{3}{4} + \frac{p_{xy_i} p_{y_i z_0}}{p^{(2)}_{xz_0}} + \sum_{j \neq i} \frac{p_{xy_j} p_{y_j z_0}}{p^{(2)}_{xz_0}} \right) \\
&= p_{xy_i} p_{y_i z_0} \left(-\frac{3}{4} + \frac{1}{p^{(2)}_{xz_0}} \sum_{y \in S_1(x)} p_{xy} p_{yz_0} \right) \\
&= \frac{1}{4} p_{xy_i} p_{y_i z_0} > 0.
\end{aligned}$$

(Note that the terms involving C_2 are cancelled out in the above expression.)

Under the assumption that $C_2 \mu_{z_0} \geq \frac{p_{xy_j} p_{y_j z_0}}{p_{z_0 y_j} p^{(2)}_{xz_0}}$ for all $j \neq i$, we can guarantee in (8.1) that $(\widetilde{Q} - Q)_{y_i y_j} \leq 0$. It then follows that

$$(\widetilde{Q} - Q)_{y_i y_i} > -\sum_{j \neq i} (\widetilde{Q} - Q)_{y_i y_j} = \sum_{j \neq i} \left| (\widetilde{Q} - Q)_{y_i y_j} \right|,$$

which shows $\widetilde{Q} - Q$ is diagonally dominant and hence $\widetilde{Q} - Q \succeq 0$.

Finally, we remark that the assumption $C_2\mu_{z_0} \geq \frac{p_{xy_j}p_{y_jz_0}}{p_{z_0y_j}p^{(2)}_{xz_0}}$ can be re-written as the assumption given in Theorem 1.15, namely $C_2 \geq \frac{p^-(y)}{\mu_x p^{(2)}_{xz_0}}$ due to the following identity:

$$\frac{p_{xy_j}p_{y_jz_0}}{p_{z_0y_j}p^{(2)}_{xz_0}} \cdot \frac{1}{\mu_{z_0}} = \frac{w_{xy_j}w_{y_jz_0}}{\mu_x\mu_{y_j}w_{z_0y_j}p^{(2)}_{xz_0}} = \frac{p_{y_jx}}{\mu_x p^{(2)}_{xz_0}} = \frac{p^-(y)}{\mu_x p^{(2)}_{xz_0}}.$$

□

A Explicit Structure of relevant matrices

In this section we collect the explicit expressions of matrices $\left(\Delta(x)\Delta(x)^\top\right)_{\hat{1}}$, $\Gamma(x)_{\hat{1}}$, $\Gamma_2(x)_{\hat{1}}$, $Q(x)$ and $A_\infty(x)$, all of which are important ingredients to our curvature calculation in Theorem 1.2. These expressions will be given in (A.1), (A.2), (A.5)-(A.9), (A.11)-(A.12) and (A.13), respectively.

We fix the central vertex $x \in V$ and let $m = |S_1(x)|$ and $n = |S_2(x)|$ be the size of 1-sphere and 2-sphere around x, respectively. The vertices in $S_1(x)$ and $S_2(x)$ are indexed by

$$S_1(x) = \{y_1, y_2, ..., y_m\}; \qquad S_2(x) = \{z_1, z_2, ..., z_n\}.$$

The linear operator $\Delta(\cdot)(x)$ and the bilinear forms $\Gamma(\cdot,\cdot)(x), \Gamma_2(\cdot,\cdot)(x)$ can be represented by a vector $\Delta(x)$ and matrices $\Gamma(x), \Gamma_2(x)$ as follows:

$$\Delta f(x) = \Delta(x)^\top \vec{f},$$
$$\Gamma(f,g)(x) = \vec{f}^\top \Gamma(x)\vec{g},$$
$$\Gamma_2(f,g)(x) = \vec{f}^\top \Gamma_2(x)\vec{g}.$$

In the first two equations, $\vec{f}$ and $\vec{g}$ are vector representations indexed by vertices in $B_1(x)$ as

$$\vec{f} = \begin{pmatrix} f(x) & f(y_1) & \cdots & f(y_m) \end{pmatrix}^\top,$$

and similarly for $\vec{g}$. In the last equation, $\vec{f}$ and $\vec{g}$ are vector representations indexed by vertices in $B_2(x)$ as

$$\vec{f} = \begin{pmatrix} f(x) & f(y_1) & \cdots & f(y_m) & f(z_1) & \cdots & f(z_n) \end{pmatrix}^\top,$$

and similarly for $\vec{g}$.

More explicitly, the defining equation $\Delta f(x) = \sum_{y\in S_1(x)} p_{xy}(f(y) - f(x))$ is translated to

$$\Delta(x) = \begin{pmatrix} -\frac{d_x}{\mu_x} & p_{xy_1} & p_{xy_2} & \cdots & p_{xy_m} \end{pmatrix}^\top,$$

and $\Delta(x)_{S_1} = \begin{pmatrix} p_{xy_1} & p_{xy_2} & \cdots & p_{xy_m} \end{pmatrix}^\top$ when restricted to the vertices in $S_1(x)$.

Hence we derive that

$$\left(\Delta(x)\Delta(x)^\top\right)_{\hat{1}} = \Delta(x)_{S_1}\Delta(x)_{S_1}^\top = \begin{pmatrix} p_{xy_1}^2 & p_{xy_1}p_{xy_2} & \cdots & p_{xy_1}p_{xy_m} \\ p_{xy_2}p_{xy_1} & p_{xy_2}^2 & \cdots & p_{xy_2}p_{xy_m} \\ \vdots & \vdots & \ddots & \vdots \\ p_{xy_m}p_{xy_1} & p_{xy_m}p_{xy_2} & \cdots & p_{xy_m}^2 \end{pmatrix}. \tag{A.1}$$

The defining equation $2\Gamma(f,g) = \Delta(f\cdot g) - f\cdot\Delta g - \Delta f\cdot g$ means

$$\begin{aligned} 2\Gamma(f,g)(x) &= \sum_{y\in S_1(x)} p_{xy}[(f(y)g(y)-f(x)g(x)) - f(x)(g(y)-g(x)) - (f(y)-f(x))g(x)] \\ &= \sum_{y\in S_1(x)} p_{xy}(f(y)-f(x))(g(y)-g(x)) \\ &= \sum_{y\in S_1(x)} p_{xy}[f(x)g(x) - f(x)g(y) - f(y)g(x) + f(y)g(y)], \end{aligned}$$

which can be translated to

$$\Gamma(x) = \frac{1}{2}\begin{pmatrix} \frac{d_x}{\mu_x} & -p_{xy_1} & -p_{xy_2} & \cdots & -p_{xy_m} \\ -p_{xy_1} & p_{xy_1} & & & \\ -p_{xy_2} & & p_{xy_2} & & \\ \vdots & & & \ddots & \\ -p_{xy_m} & & & & p_{xy_m} \end{pmatrix}.$$

In particular, after removing the first row and column corresponding to the vertex x, we simply have

$$\Gamma(x)_{\hat{1}} = \Gamma(x)_{S_1,S_1} = \frac{1}{2}\mathrm{diag}\begin{pmatrix} p_{xy_1} & p_{xy_2} & \cdots & p_{xy_m} \end{pmatrix} = \frac{1}{2}\mathrm{diag}\left(\Delta(x)_{S_1}\right). \tag{A.2}$$

Now we discuss the structure of the matrix $\Gamma_2(x)$. After removing the first row and column corresponding to x, the matrix $\Gamma_2(x)_{\hat{1}}$ has the following block structure in $S_1(x)\sqcup S_2(x)$:

$$\Gamma_2(x)_{\hat{1}} = \Gamma_2(x)_{S_1\cup S_2, S_1\cup S_2} = \begin{pmatrix} \Gamma_2(x)_{S_1,S_1} & \Gamma_2(x)_{S_1,S_2} \\ \Gamma_2(x)_{S_2,S_1} & \Gamma_2(x)_{S_2,S_2} \end{pmatrix}. \tag{A.3}$$

The defining equation $2\Gamma_2(f,g) = \Delta(\Gamma(f,g)) - \Gamma(f,\Delta g) - \Gamma(g,\Delta f)$ yields

$$\begin{aligned} 4\Gamma_2(f,g)(x) = &\sum_{y\in S_1(x)} p_{xy}\left[2\Gamma(f,g)(y) - (f(y)-f(x))\Delta g(y) - (g(y)-g(x))\Delta f(y)\right] \\ &- \frac{2d_x}{\mu_x}\Gamma(f,g)(x) + 2\Delta f(x)\Delta g(x). \end{aligned}$$

Let us denote by $I(\cdot,\cdot)(x)$ the bilinear form defined via

$$I(f,g)(x) := \sum_{y\in S_1(x)} p_{xy}\left[2\Gamma(f,g)(y) - (f(y)-f(x))\Delta g(y) - (g(y)-g(x))\Delta f(y)\right],$$

and the matrix representing it by $I(x)$. Then we have

$$4\Gamma_2(x) = I(x) - \frac{2d_x}{\mu_x}\Gamma(x) + 2\Delta(x)\Delta(x)^\top,$$

and hence

$$4\Gamma_2(x)_{\hat{1}} = I(x)_{\hat{1}} - \frac{2d_x}{\mu_x}\Gamma(x)_{\hat{1}} + 2\left(\Delta(x)\Delta(x)^\top\right)_{\hat{1}}. \tag{A.4}$$

In order to derive $I(x)_{\hat{1}}$, we only need to compute the expression of $I(f,g)(x)$ for functions f and g satisfying $f(x) = g(x) = 0$:

$$\begin{aligned}
&I(f,g)(x) \\
=& \sum_{y\in S_1(x)} p_{xy}\left[2\Gamma(f,g)(y) - f(y)\Delta g(y) - g(y)\Delta f(y)\right] \\
=& \sum_{y\in S_1(x)}\sum_{z\in S_1(y)} p_{xy}p_{yz}\left[(f(z)-f(y))(g(z)-g(y)) - f(y)(g(z)-g(y)) - g(y)(f(z)-f(y))\right] \\
=& \sum_{y\in S_1(x)}\sum_{z\in S_1(y)} p_{xy}p_{yz}\left[f(z)g(z) - 2f(z)g(y) - 2f(y)g(z) + 3f(y)g(y)\right] \\
=& \sum_{y\in S_1(x)}\sum_{z\in S_2(x)} p_{xy}p_{yz}\left[f(z)g(z) - 2f(z)g(y) - 2f(y)g(z) + 3f(y)g(y)\right] \\
&+ \sum_{y\in S_1(x)}\sum_{y'\in S_1(x)} p_{xy}p_{yy'}\left[f(y')g(y') - 2f(y')g(y) - 2f(y)g(y') + 3f(y)g(y)\right] \\
&+ \sum_{y\in S_1(x)} p_{xy}p_{yx}\cdot 3f(y)g(y) \\
=& \sum_{y\in S_1(x)}\left[3p_{xy}p_{yx} + 3p_{xy}\sum_{z\in S_2(x)} p_{yz} + 3p_{xy}\sum_{y'\in S_1(x)} p_{yy'} + \sum_{y'\in S_1(x)} p_{xy'}p_{y'y}\right] f(y)g(y) \\
&- \sum_{y\in S_1(x)}\sum_{y'\in S_1(x)} 2p_{xy}p_{yy'}(f(y')g(y) + f(y)g(y')) \\
&- \sum_{y\in S_1(x)}\sum_{z\in S_2(x)} 2p_{xy}p_{yz}(f(y)g(z) + g(y)f(z)) + \sum_{z\in S_2(x)} p^{(2)}_{xz} f(z)g(z).
\end{aligned}$$

In the above, we use the notation

$$p^{(2)}_{xz} := \sum_{y\in S_1(x)} p_{xy}p_{yz}.$$

Therefore we have the expression of the matrix $I(x)_{\hat{1}}$ as below. For any $y \in S_1(x)$,

$$I(x)_{yy} = 3p_{xy}p_{yx} + 3p_{xy}\sum_{z\in S_2(x)} p_{yz} + 3p_{xy}\sum_{y'\in S_1(x)} p_{yy'} + \sum_{y'\in S_1(x)} p_{xy'}p_{y'y}.$$

For any $y_i, y_j \in S_1(x)$ such that $y_i \neq y_j$,

$$I(x)_{y_iy_j} = -2p_{xy_i}p_{y_iy_j} - 2p_{xy_j}p_{y_jy_i}.$$

For any $y \in S_1(x)$ and $z \in S_2(x)$,

$$I(x)_{yz} = I(x)_{zy} = -2p_{xy}p_{yz},\ I(x)_{zz} = p^{(2)}_{xz}.$$

For any $z_i, z_j \in S_2(x)$ such that $z_i \neq z_j$,

$$I(x)_{z_iz_j} = 0.$$

Combining the above expressions for $I(x)_{\hat{1}}$ with (A.1),(A.2) and (A.4) yields the expressions for $\Gamma_2(x)_{\hat{1}}$ as below.

For any $y \in S_1(x)$,

$$(4\Gamma_2(x))_{yy} = 2p_{xy}^2 + 3p_{xy}p_{yx} - \frac{d_x}{\mu_x}p_{xy} + 3p_{xy}\sum_{z\in S_2(x)} p_{yz} + \sum_{y'\in S_1(x)} \left(3p_{xy}p_{yy'} + p_{xy'}p_{y'y}\right). \tag{A.5}$$

For any $y_i, y_j \in S_1(x)$ such that $y_i \neq y_j$,

$$(4\Gamma_2(x))_{y_iy_j} = 2p_{xy_i}p_{xy_j} - 2p_{xy_i}p_{y_iy_j} - 2p_{xy_j}p_{y_jy_i}, \tag{A.6}$$

and, for any $z \in S_2(x)$,

$$(4\Gamma_2(x))_{yz} = (4\Gamma_2(x))_{zy} = -2p_{xy}p_{yz}; \tag{A.7}$$

$$(4\Gamma_2(x))_{zz} = p_{xz}^{(2)}, \tag{A.8}$$

and for any $z_i, z_j \in S_2(x)$ such that $z_i \neq z_j$,

$$(4\Gamma_2(x))_{z_iz_j} = 0. \tag{A.9}$$

The Schur's complement

$$Q(x) := \Gamma_2(x)_{\hat{1}}/\Gamma_2(x)_{S_2,S_2} = \Gamma_2(x)_{S_1,S_1} - \Gamma_2(x)_{S_1,S_2}\Gamma_2(x)_{S_2,S_2}^{-1}\Gamma_2(x)_{S_2,S_1}$$

is the result of folding the matrix in (A.3) into the upper-left block.

For all $y_i, y_j \in S_1(x)$ (with possibly $i = j$), the (y_i, y_j)-entry of $\Gamma_2(x)_{S_1,S_2}\Gamma_2(x)_{S_2,S_2}^{-1}\Gamma_2(x)_{S_2,S_1}$ can be computed from (A.7), (A.8) and (A.9) as

$$\left(\Gamma_2(x)_{S_1,S_2}\Gamma_2(x)_{S_2,S_2}^{-1}\Gamma_2(x)_{S_2,S_1}\right)_{y_iy_j} = \sum_{z\in S_2(x)} \frac{p_{xy_i}p_{y_iz}\cdot p_{xy_j}p_{y_jz}}{p_{xz}^{(2)}}. \tag{A.10}$$

Combining the above equation with (A.5) and (A.6), we obtain the entries of $Q(x)$ as follows.

For $y \in S_1(x)$,

$$Q(x)_{yy} = \frac{1}{2}p_{xy}^2 + \frac{3}{4}p_{xy}p_{yx} - \frac{1}{4}\frac{d_x}{\mu_x}p_{xy} + \frac{3}{4}p_{xy}\sum_{z\in S_2(x)} p_{yz} + \frac{1}{4}\sum_{y'\in S_1(x)}\left(3p_{xy}p_{yy'} + p_{xy'}p_{y'y}\right) - \sum_{z\in S_2(x)}\frac{p_{xy}^2p_{yz}^2}{p_{xz}^{(2)}}. \tag{A.11}$$

For $y_i, y_j \in S_1(x)$ such that $y_i \neq y_j$,

$$Q(x)_{y_iy_j} = \frac{1}{2}p_{xy_i}p_{xy_j} - \frac{1}{2}p_{xy_i}p_{y_iy_j} - \frac{1}{2}p_{xy_j}p_{y_jy_i} - \sum_{z\in S_2(x)}\frac{p_{xy_i}p_{y_iz}p_{xy_j}p_{y_jz}}{p_{xz}^{(2)}}. \tag{A.12}$$

The curvature matrix $A_\infty(x) = 2\,\mathrm{diag}(\mathbf{v}_0)^{-1} Q(x)\,\mathrm{diag}(\mathbf{v}_0)^{-1}$ with

$$\mathbf{v}_0(x) := (\sqrt{p_{xy_1}}\ \sqrt{p_{xy_2}}\ \cdots\ \sqrt{p_{xy_m}})^\top$$

has its entries equal to

$$A_\infty(x)_{y_iy_j} = \frac{2}{\sqrt{p_{xy_i}p_{xy_j}}} Q(x)_{y_iy_j} \tag{A.13}$$

for all $y_i, y_j \in S_1(x)$ (with possibly $i = j$).

The generalised scalar curvature $S_{G,x}(N) = \mathrm{tr}(A_\infty - \frac{2}{N}\mathbf{v}_0\mathbf{v}_0^\top) = S_{G,x}(\infty) - \frac{2}{N}\frac{d_x}{\mu_x}$ can then be computed from (A.11) as below:

$$\begin{aligned} S_{G,x}(\infty) = {} & \left(1 - \frac{m}{2}\right)\frac{d_x}{\mu_x} + \frac{3}{2}\sum_{y\in S_1(x)} p_{yx} + \frac{3}{2}\sum_{y\in S_1(x)}\sum_{z\in S_2(x)} p_{yz} \\ & + \frac{1}{2}\sum_{y\in S_1(x)}\sum_{y'\in S_1(x)}\left(3p_{yy'} + \frac{p_{xy'}p_{y'y}}{p_{xy}}\right) - 2\sum_{y\in S_1(x)}\sum_{z\in S_2(x)} p_{xy}\frac{p_{yz}^2}{p_{xz}^{(2)}}. \end{aligned} \tag{A.14}$$

Next we analyse the structure of the matrix $Q(x)$ via certain Laplacians, extending results in [12, Section 8]. Let $\Delta_{S_1(x)}$ be the Laplacian of the weighted graph with the vertex set $\{y_1, y_2, \ldots, y_m\}$, the vertex measure $\mu \equiv 1$, and the symmetric edge-weight function given by

$$w_{y_iy_j}^{S_1(x)} := \frac{1}{2}p_{xy_i}p_{y_iy_j} + \frac{1}{2}p_{xy_j}p_{y_jy_i}.$$

That is, for any function $f : \{y_1, y_2, \ldots, y_m\} \to \mathbb{R}$, we have

$$\Delta_{S_1(x)} f(y_i) = \sum_{j\in[m]} w_{y_iy_j}^{S_1(x)}(f(y_j) - f(y_i)),$$

where we use the notation $[m] := \{1, 2, \ldots, m\}$. We observe that

$$\sum_{j\in[m]} w_{y_iy_j}^{S_1(x)} = \frac{1}{2}p_{xy_i}\sum_{y_j\in S_1(x)} p_{y_iy_j} + \frac{1}{2}\sum_{y_j\in S_1(x)} p_{xy_j}p_{y_jy_i}.$$

We then derive from (A.5) and (A.6) that

$$\Gamma_2(x)_{S_1,S_1} = -\Delta_{S_1(x)} + \frac{1}{2}\left(\Delta(x)\Delta(x)^\top\right)_{\hat{1}} - \frac{1}{4}\frac{d_x}{\mu_x}\mathrm{diag}(\Delta(x)_{S_1}) + \mathrm{diag}(\mathbf{w}_1(x)), \tag{A.15}$$

where $\Delta_{S_1(x)}$ stands here for the corresponding Laplacian matrix and $\mathbf{w}_1(x)$ denotes the m-dimensional vector with the i-th entry given by

$$\frac{3}{4}p_{xy_i}(p^-(y_i) + p^+(y_i)) + \frac{1}{4}\sum_{y'\in S_1(x)}(p_{xy_i}p_{y_iy'} - p_{xy'}p_{y'y_i}).$$

In the above we use the notations $p^-(y) = p_{yx}$ and $p^+(y) = \sum_{z\in S_2(x)} p_{yz}$ for $y \in S_1(x)$.

Let $\Delta_{S_1'(x)}$ be the Laplacian on the weighted graph with the vertex set $\{y_1, y_2, \ldots, y_m\}$, the vertex measure $\mu \equiv 1$, and the symmetric edge-weight function given by

$$w_{y_iy_j}^{S_1'(x)} := \sum_{z\in S_2(x)} \frac{p_{xy_i}p_{y_iz}p_{xy_j}p_{y_jz}}{p_{xz}^{(2)}} \text{ for } i \neq j, \text{ and } 0 \text{ otherwise.}$$

As an operator, we have for any function $f : \{y_1, y_2, \ldots, y_m\} \to \mathbb{R}$,

$$\Delta_{S_1'(x)} f(y_i) = \sum_{j\in[m]} w_{y_iy_j}^{S_1'(x)} (f(y_j) - f(y_i)).$$

Observe that

$$\sum_{j\in[m]} w_{y_iy_j}^{S_1'(x)} = p_{xy_i} p^+(y_i) - \sum_{z\in S_2(x)} \frac{p_{xy_i}^2 p_{y_iz}^2}{p_{xz}^{(2)}}.$$

We then derive form (A.10) that

$$\Gamma_2(x)_{S_1,S_2} \Gamma_2(x)_{S_2,S_2}^{-1} \Gamma_2(x)_{S_2,S_1} = \Delta_{S_1'(x)} + \mathrm{diag}((p_{xy_1} p^+(y_1) \cdots p_{xy_m} p^+(y_m))^\top). \quad \text{(A.16)}$$

Combing (A.15) and (A.16), we arrive at

$$Q(x) = -\Delta_{S_1''(x)} + \frac{1}{2}\left(\Delta(x)\Delta(x)^\top\right)_{\hat{1}} - \frac{1}{4}\frac{d_x}{\mu_x} \mathrm{diag}(\Delta(x)_{S_1}) + \mathrm{diag}(\mathbf{w}(x)), \quad \text{(A.17)}$$

where $\Delta_{S_1''(x)} := \Delta_{S_1(x)} + \Delta_{S_1'(x)}$ and $\mathbf{w}(x)$ is the m-dimensional vector with the i-th entry given by

$$\frac{3}{4} p_{xy_i} p^-(y_i) - \frac{1}{4} p_{xy_i} p^+(y_i) + \frac{1}{4} \sum_{y'\in S_1(x)} (p_{xy_i} p_{y_iy'} - p_{xy'} p_{y'y_i}).$$

In terms of the Laplacian $\Delta_{S_1''(x)}$, we have the following identity from (A.17)

$$\begin{aligned} A_\infty(x) =& -2\,\mathrm{diag}(\mathbf{v}_0)^{-1} \Delta_{S_1''(x)} \mathrm{diag}(\mathbf{v}_0)^{-1} + \mathbf{v}_0 \mathbf{v}_0^\top - \frac{1}{2}\frac{d_x}{\mu_x} \mathrm{Id} \\ &+ \frac{1}{2} \mathrm{diag}\left[\begin{pmatrix} 3p^-(y_1) - p^+(y_1) + \sum_{y'\in S_1(x)} \frac{p_{xy_1}p_{y_1y'} - p_{xy'}p_{y'y_1}}{p_{xy_1}} \\ \vdots \\ 3p^-(y_m) - p^+(y_m) + \sum_{y'\in S_1(x)} \frac{p_{xy_m}p_{y_my'} - p_{xy'}p_{y'y_m}}{p_{xy_m}} \end{pmatrix}\right]. \end{aligned} \quad \text{(A.18)}$$

We conclude this Appendix with the following Lemma.

Lemma A.1. *Let $G = (V, w, \mu)$ be a weighted graph. Then we have for any $x \in V$,*

$$\frac{\mathbf{v}_0(x)^\top A_\infty(x) \mathbf{v}_0(x)}{\mathbf{v}_0(x)^\top \mathbf{v}_0(x)} = \frac{1}{2}\left(\frac{d_x}{\mu_x} + 3\frac{\mu_x}{d_x} p_{xx}^{(2)} - \frac{\mu_x}{d_x} \sum_{z\in S_2(x)} p_{xz}^{(2)}\right) =: \mathcal{K}_\infty^0(x).$$

Proof. By (A.13), we obtain

$$\mathbf{v}_0(x)^\top A_\infty(x) \mathbf{v}_0(x) = \sum_{i,j} \sqrt{p_{xy_i} p_{xy_j}} A_\infty(x)_{y_iy_j} = 2\sum_{i,j} Q(x)_{y_iy_j}.$$

We will continue the calculation by applying (A.17). We observe the following facts:

$$\sum_{i,j} \Delta_{S_1''}(x)_{y_iy_j} = 0 \text{ and } \sum_i \sum_{y'\in S_1(x)} (p_{xy_i} p_{y_iy'} - p_{xy'} p_{y'y_i}) = 0.$$

Furthermore, we derive from (A.1) that $\sum_{i,j}\left(\left(\Delta(x)\Delta(x)^\top\right)_{\hat{1}}\right)_{y_iy_j} = \left(\frac{d_x}{\mu_x}\right)^2$. Therefore, applying (A.17) yields that

$$\begin{aligned} 2\sum_{i,j} Q(x)_{y_iy_j} =& \frac{1}{2}\left(\frac{d_x}{\mu_x}\right)^2 + \frac{1}{2}\sum_i \left(3p_{xy_i}p^-(y_i) - p_{xy_i}p^+(y_i)\right) \\ =& \frac{1}{2}\left(\frac{d_x}{\mu_x}\right)^2 + \frac{1}{2}\left(3p_{xx}^{(2)} - \sum_{z\in S_2(x)} p_{xz}^{(2)}\right). \end{aligned}$$

Recalling that $\mathbf{v}_0(x)^\top\mathbf{v}_0(x) = \frac{d_x}{\mu_x}$, we finish the proof of this lemma. □

Acknowledgement

Supanat Kamtue is supported by the Thai Institute for Promotion of Teaching Science and Technology. Shiping Liu is supported by the National Key Research and Development Project SQ2020YFA070080 and the National Natural Science Foundation of China (No. 12031017).

References

[1] D. Bakry, L'hypercontractivité et son utilisation en théorie des semigroupes, In: Lectures on Probability Theory, Lecture Notes in Math. 1581, P. Bernard (Eds.), Springer, Berlin, Heidelberg, 1994, pp. 1–114.

[2] D. Bakry and M. Émery, Diffusions hypercontractives, In: Séminaire de probabilités, XIX, 1983/84, Lecture Notes in Math. 1123, J. Azéma and M. Yor (Eds.), Springer, Berlin, 1985, pp. 177–206.

[3] D. Bakry, I. Gentil and M. Ledoux, Analysis and geometry of Markov diffusion operators, Grundlehren der Mathematischen Wissenschaften 348, Springer, 2014.

[4] F. Bauer, P. Horn, Y. Lin, G. Lippner, D. Mangoubi, S.-T. Yau, Li-Yau inequality on graphs, J. Differential Geom. 99 (2015), no. 3, pp. 359–405.

[5] S. Boyd and L. Vandenberghe, Convex Optimization, First edition. Cambridge University Press, 2004.

[6] D. Carlson, What are Schur Complements, Anyway? Linear Algebra Appl. 74 (1986), 257–275.

[7] F. R. K. Chung, Y. Lin, S.-T. Yau, Harnack inequalities for graphs with non-negative Ricci curvature, J. Math. Anal. Appl. 415 (2014), 25–32.

[8] D. Cushing, R. Kangaslampi, V. Lipiäinen, S. Liu and G. W. Stagg, The Graph Curvature Calculator and the curvatures of cubic graphs, Exp. Math. (2019), 1–13, doi.org/10.1080/10586458.2019.1660740.

[9] D. Cushing, S. Kamtue, R. Kangaslampi, S. Liu and N. Peyerimhoff, Curvatures, graph products and Ricci flatness, J. Graph Theory 96 (2021), no. 4, 522–553.

[10] D. Cushing, S. Kamtue, N. Peyerimhoff and L. Watson May, Quartic graphs which are Bakry-Émery curvature sharp, Discrete Math. 343 (2020), no. 3, 111767.

[11] D. Cushing, S. Liu, F. Münch and N. Peyerimhoff, Curvature calculations for antitrees, in: Analysis and geometry on graphs and manifolds, London Mathematical Society Lecture Notes Series, 461, M. Keller, D. Lenz, and R. Wojciechowski (Eds.), Cambridge University Press, 2020, pp. 21–54.

[12] D. Cushing, S. Liu and N. Peyerimhoff, Bakry-Émery curvature functions on graphs, Canad. J. Math. 72 (2020), no. 1, 89–143.

[13] D. Dier, M. Kassmann and R. Zacher, Discrete versions of the Li-Yau gradent estimate, arXiv: 1701:04807.

[14] K. D. Elworthy, Manifolds and graphs with mostly positive curvatures, in Stochastic analysis and applications (Lisbon, 1989), Progr. Probab., 26, A. B. Cruzeiro and J. C. Zambrini (Eds.), Birkhäuser, 1991, pp. 96–110.

[15] M. Fathi and Y. Shu, Curvature and transport inequalities for Markov chains in discrete spaces, Bernoulli 24 (2018), no. 1, 672–698.

[16] J. Gallier, The Schur complement and symmetric positive semidefinte (and definite) matrices, August 24, 2019. https://www.cis.upenn.edu/ jean/schur-comp.pdf

[17] C. Gong and Y. Lin, Equivalent properties for CD inequalities on graphs with unbounded Laplacians, Chinese Ann. Math. Ser. B. 38 (2017), 1059–1070.

[18] C. Gong, Y. Lin, Shuang Liu and S.-T. Yau, Li-Yau inequality for unbounded Laplacian on graphs, Adv. Math. 357 (2019), 106822.

[19] P. Horn, Y. Lin, Shuang Liu and S.-T. Yau, Volume doubling, Poincaré inequality and Gaussian heat kernel estimate for nonnegative curvature graphs, J. Reine Angew. Math. 757 (2019), 89–130.

[20] B. Hua, Liouville theorem for bounded harmonic functions on manifolds and graphs satisfying non-negative curvature dimension condition, Calc. Var. Partial Differential Equations 58 (2019), no. 2, Article 42.

[21] B. Hua and Y. Lin, Stochastic completeness for graphs with curvature dimension conditions, Adv. Math. 306 (2017), 279–302.

[22] B. Hua and Y. Lin, Graphs with large girth and nonnegative curvature dimension condition, Comm. Anal. Geom. 27 (2019), no. 3, 619–638.

[23] B. Hua and F. Münch, Ricci curvature on birth-death processes, arXiv: 1712.01494.

[24] B. Hua, F. Münch, and R. K. Wojciechowski, Coverings and the heat equation on graphs: stochastic incompleteness, the Feller property, and uniform transience, Trans. Amer. Math. Soc. 372 (2019), no. 7, 5123–5151.

[25] J. Jost, Riemannian geometry and geometric analysis, Seventh edition. Universitext, Springer, 2017.

[26] J. Jost and S. Liu, Ollivier's Ricci curvature, local clustering and curvature-dimension inequalities on graphs, Discrete Comput. Geom. 51 (2014), no. 2, 300–322.

[27] M. Keller and F. Münch, Gradient estimates, Bakry-Emery Ricci curvature and ellipticity for unbounded graph Laplacians, arXiv:1807.10181.

[28] M. Kempton, F. Münch, and S.-T. Yau, Relationships between cycle spaces, gain graphs, graph coverings, fundamental groups, path homology, and graph curvature, arXiv:1710.01264.

[29] B. Klartag, G. Kozma, P. Ralli, and P. Tetali, Discrete curvature and abelian groups, Canad. J. Math. 68 (2016), 655–674.

[30] S. G. Krantz and H. R. Parks, The implicit function theorem, History, theory, and applications, Modern Birkhäuser Classics, Reprint of the 2003 edition, Birkhäuser/Springer, New York, 2013.

[31] S. Lakzian and Z. Mcguirk, Global Poincaré inequality on graphs via conical curvature-dimension conditions, Anal. Geom. Metr. Spaces 6 (2018), no. 1, 32–47.

[32] Y. Lin and Shuang Liu, Equivalent properties of CD inequality on graph, Acta Math. Sin. Chinese Ser. 61 (2018), no. 3, 431–440.

[33] Y. Lin and S.-T. Yau, Ricci curvature and eigenvalue estimate on locally finite graphs, Math. Res. Lett. 17 (2010), no. 2, 343–356.

[34] S. Liu, F. Münch, and N. Peyerimhoff, Bakry-Emery curvature and diameter bounds on graphs, Calc. Var. Partial Differential Equations 57 (2018), no. 2, Article 67.

[35] S. Liu, F. Münch, and N. Peyerimhoff, Rigidity properties of the hypercube via Bakry-Émery curvature, arXiv:1705.06789.

[36] S. Liu, F. Münch, and N. Peyerimhoff, Curvature and higher order Buser inequalities for the graph connection Laplacian, SIAM J. Discrete Math. 33 (2019), no.1, 257–305.

[37] S. Liu, F. Münch, N. Peyerimhoff and C. Rose, Distance bounds for graphs with some negative Bakry-Émery curvature, Anal. Geom. Metr. Space 7 (2019), no. 1, 1–14.

[38] S. Liu and N. Peyerimhoff, Eigenvalue ratios of nonnegatively curved graphs, Comb. Probab. Comput. 27 (2018), no. 5, 829–850.

[39] Shuang Liu, Buser's inequality on infinite graphs, J. Math. Anal. Appl., 475 (2019), no. 2, 1416–1426.

[40] M. Marden, Geometry of polynomials, Second edition. Mathematical Surveys, No. 3, American Mathematical Society, Providence, R.I, 1966.

[41] J. M. Mazón, M. Solera, and J. Toledo, The heat flow on metric random walk spaces, J. Math. Anal. Appl. 483 (2020), no. 2, 123645.

[42] F. Münch, Remarks on curvature dimension conditions on graphs, Calc. Var. Partial Differential Equations 56 (2017), no. 1, Article 11.

[43] F. Münch, Li-Yau inequality on finite graphs via non-linear curvature dimension conditions, J. Math. Pures Appl. 120 (2018), pp. 130–164.

[44] F. Münch, Li-Yau inequality under $CD(0, n)$ on graphs, arXiv:1909:10242.

[45] F. Münch and C. Rose, Spectrally positive Bakry-Émery Ricci curvature on graphs, J. Math. Pures Appl. 143 (2020), 334–344.

[46] P. Petersen, Riemannian geometry, Third edition. Graduate Texts in Mathematics 171, Springer, 2016.

[47] J. Salez, Sparse expanders have negative curvature, arXiv:2101.08242.

[48] J. Salez, Cutoff for non-negatively curved Markov chains, arXiv:2102.05597.

[49] M. Schmuckenschläger, Curvature of nonlocal Markov generators, in Convex geometric analysis (Berkeley, CA, 1996), Math. Sci. Res. Inst. Publ., 34, K. Ball and V. Milman (Eds.), Cambridge University Press, 1999, pp. 189–197.

[50] V. Siconolfi, Coxeter groups, graphs and Ricci curvature, Proceedings of the 32nd Conference on Formal Power Series and Algebraic Combinatorics, Séminaire Lotharingien de Combinatoire **84B** (2020). Article #67, 12 pp.

[51] V. Siconolfi, Ricci curvature, graphs and eigenvalues, arXiv:2102.10134.

[52] A. Spener, F. Weber, and R. Zacher, Curvature-dimension inequalities for non-local operators in the discrete setting, Calc. Var. Partial Differential Equations 58 (2019), no. 5, Article 171.

[53] P. Topping, Lectures on the Ricci flow, London Mathematical Society Lecture Notes Series, 325, Cambridge University Press, 2006.

[54] C. Villani, Optimal Transport: old and new, Grundlehren der Mathematischen Wissenschaften, vol. 338, Springer-Verlag, Berlin, 2009.