Sensitivity Analysis of Perfect State Transfer in Quantum Spin Networks

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Abstract

For a weighted graph G with adjacency matrix A, let $U(t) = e^{itA}$. For indices s, r, the fidelity of transfer at time t is $p(t) = |u(t)_{s,r}|^2$, and there is perfect state transfer if $p(t_0) = 1$ for some t_0. Under the hypothesis of perfect state transfer, we provide closed form expressions for $\frac{d^k p}{dt^k}$ at t_0 for any $k \in \mathbb{N}$. Those expressions then yield an easily computed lower bound on $p(t_0 + h)$ for any h. We also produce expressions for the first two partial derivatives of p with respect to the weight of an edge in G, with the expression for the second derivative holding under the hypothesis of perfect state transfer. A parallel suite of results using the Laplacian matrix of G is also developed, and examples illustrating the results are included. The techniques rely on the spectral decomposition of the adjacency (respectively, Laplacian)

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matrix, and on perturbation theory for eigenvalues and eigenvectors of symmetric matrices.

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1 Introduction and preliminaries

Suppose that G is a weighted graph on n vertices – that is, a loop–free undirected graph on vertices labelled $1, \ldots, n$, with an accompanying weight function w mapping from the edge set to the positive real numbers. Associated with our weighted graph is its *adjacency matrix* A, the $n \times n$ matrix given by

$$a_{k,j} = \begin{cases} w(k,j), & \text{if } k \text{ is adjacent to } j \text{ and } w(k,j) \text{ is the edge weight,} \\ 0, & \text{if } k \text{ is not adjacent to } j \end{cases}$$

for $k, j = 1, \ldots, n$. Letting D be the diagonal matrix of row sums of A, we may also define the *Laplacian matrix* corresponding to the weighted graph G via $L = D - A$. Both the adjacency matrix and the Laplacian matrix are well–studied objects and in particular much is known about their spectral structure, see for example [4], [7] and [10].

The adjacency matrix and the Laplacian matrix for weighted graphs play a central role in the analysis of state transfer in quantum spin networks (equivalently, quantum walks on a graph). Here is the setting. For a weighted graph G with adjacency matrix A, set $U(t) = e^{itA}$, and suppose that we are given a pair of distinct vertices s, r of G. Our weighted graph corresponds to a network of spins; each vertex of the graph represents a spin, and two spins are coupled if and only if there is an edge between the corresponding vertices. Further, the strength of that coupling is determined by the corresponding entry in A. Under so–called XY dynamics, the adjacency matrix A serves as a time independent Hamiltonian. The *fidelity of transfer* (from s to r at time t) is then given by $p(t) = |u(t)_{s,r}|^2$, and can be interpreted as the probability that a single excitation travels from s to r after a free evolution of time t. (As an aside, we note that $\sum_{k=1}^{n} |u(t)_{s,k}|^2 = 1$, so that the probabilistic interpretation is appropriate here.) A slightly different setup leads to the Laplacian matrix. If we assume that the process evolves under so–called XX dynamics, then the Laplacian matrix L serves as the Hamiltonian; setting $U(t) = e^{itL}$, the fidelity of transfer is again $p(t) = |u(t)_{s,r}|^2$ (with an analogous probabilistic interpretation) under this alternate hypothesis on the dynamics.

In either setting, there is particular interest in the phenomenon of *perfect state transfer*: we say that there is perfect state transfer from s to r at time t_0 if the corresponding fidelity of transfer $p(t_0)$ is equal to 1. This notion, introduced in [6], has attracted considerable attention (as evidenced by the fact that [6] has received upwards of 800 citations to date) in part because perfect state transfer is proposed as a mechanism for the transfer of information in a quantum computer. A number of families of weighted graphs exhibiting perfect state transfer are known – see, for example [2], [3], [5], [9] and [16].

In this paper, we address the following question: given a weighted graph exhibiting perfect state transfer (where the Hamiltonian in question is either the adjacency matrix or the Laplacian matrix), how sensitive is the fidelity of transfer to changes in either the readout time t_0, or the weight of a particular edge? We are not the first to consider questions of this type. In [15], the author considers the class of centrosymmetric adjacency matrices – that is, the those adjacency matrices A such that $PAP = A$, where P is the back–diagonal permutation matrix. Specifically, for those centrosymmetric adjacency matrices exhibiting perfect state transfer, say from state s to state r, [15] discusses so–called timing errors and manufacturing errors. The former are errors in the fidelity of transfer from s to r arising from small changes in the readout time, while the latter are errors in the fidelity of transfer from s to r arising from small changes in the weights of the edges. Not surprisingly, these lead to the consideration of the derivatives of the fidelity of transfer with respect to the readout time and the edge weights. Also related is the work in [11] and [18], which investigate the effect on fidelity of transfer arising from changes in the edge weights in spin chains (where the underlying undirected graph is restricted to be a path). However, the approach of those articles has a probabilistic flavour, as the edge weights are considered to be subject to random perturbations. As will become evident, this is a different perspective than the one taken in the present paper.

Our approach in this paper is informed by that of [15]. But while that paper includes a general discussion of the derivatives in question (and unfortunately appears to contain an error in the expression for the second derivative with respect to time, evaluated at t_0), our aim in the present work is to establish precise formulas for derivatives of the fidelity of transfer with respect to the edge weights and the readout time. As in [11], [15] and [18], our primary focus is on the context of perfect state transfer. We emphasise that our results do not impose any extra assumptions on the weighted graphs under consideration, and cover the cases that the Hamiltonian is either a Laplacian matrix or an adjacency matrix. Specifically, this paper makes the following contributions:

i) we derive explicit expressions for derivatives (with respect to time, evaluated at t_0) of all orders of the fidelity of transfer when perfect state transfer holds (Theorems 2.2 and 2.4);

ii) we provide an estimate of the remainder in the corresponding Taylor series

for the fidelity of transfer (Corollary 2.10);
iii) when perfect state transfer holds for some t_0, we prove a lower bound on the fidelity of transfer at any time (Remark 2.11);
iv) we give an expression for the first partial derivative of the fidelity of transfer with respect to the weight of an edge, even in the absence of perfect state transfer (Theorem 3.3);
v) in the setting of perfect state transfer, we derive an expression for the second partial derivative of the fidelity of transfer with respect to the weight of an edge (Theorem 3.10).
Note that both iv) and v) require one to identify a special eigenbasis of the Hamiltonian matrix, and we provide algorithms for finding such an eigenbasis in subsections 3.1 and 3.2, depending on whether the Hamiltonian under consideration is a Laplacian matrix (the former subsection) or an adjacency matrix (the latter subsection). Throughout, the results are illustrated with examples.

As noted above, a number of families of weighted graphs with perfect state transfer are now known. It is hoped that the results in this paper will not only help to differentiate between such families of graphs by allowing one to identify those with desirable sensitivity properties, but also inform the construction of new families of graphs with perfect state transfer and insensitive fidelity of transfer.

Most of the notation we use in the paper is standard, but for clarity we now outline some of the less standard notation that is used in the sequel. For adjacent vertices k, l of a graph, we denote the edge between them by $k \sim l$. For a matrix M we use $M^\top$ and $M^\dagger$ to denote the transpose and Moore–Penrose inverse, respectively. If M is a square matrix, we use $\rho(M)$ to denote its spectral radius. Given a vector $v \in \mathbb{R}^n, diag(v)$ denotes the $n \times n$ diagonal matrix whose diagonal entries are the corresponding entries of v. We use 0_k and $\mathbf{1}_k$ to denote the zero vector and all–ones vector of order k, respectively, while for a complex number z, we denote its real and imaginary parts by $\mathfrak{Re}(z), \mathfrak{Im}(z)$, respectively. Throughout the paper, we assume basic knowledge of matrix theory and graph theory; the reader is referred to [13] and [8], respectively, for background.

2 Sensitivity with respect to readout time

In this section, we extend the work of [15] on timing errors. The following lemma will be useful in the development of some of the results below.

Lemma 2.1 *Let M be a symmetric matrix of order n, let $t_0 > 0$, and let $U = e^{it_0 M}$. Suppose that we have $M = V \Lambda V^\top$, where V is an orthogonal matrix and Λ is a diagonal matrix. If there are indices s, r such that $|u_{s,r}(t_0)| = 1$, then*

$$e_r^\top V e^{-it_0 \Lambda} = \overline{u_{s,r}(t_0)} e_s^\top V. \tag{1}$$

Proof. Evidently $u_{s,r}(t_0) = e_s^\top V e^{it_0 \Lambda} V^\top e_r$. Since $|u_{s,r}(t_0)| = 1$, we find that $1 = |e_s^\top V e^{it_0 \Lambda} V^\top e_r| = |(e^{-it_0 \Lambda} V^\top e_s)^* V^\top e_r| \le ||e^{-it_0 \Lambda} V^\top e_s|| \, ||V^\top e_r|| = 1$, so that equality holds in the Cauchy–Schwarz inequality. From the characterisation of the equality case in that inequality, we find that $e^{-it_0 \Lambda} V^\top e_s$ and $V^\top e_r$ are linearly dependent, so that for some $\delta \in \mathbb{C}$,

$$V^\top e_r = \delta e^{-it_0 \Lambda} V^\top e_s. \tag{2}$$

We find readily that $\delta = u_{s,r}(t_0)$, and now (1) now follows from (2). $\square$

As noted in section 1, [15] includes a discussion (in the context of perfect state transfer) of the second derivative of the fidelity of transfer with respect to the readout time. The next result provides expressions for the derivatives of all orders in terms of diagonal entries of powers of M.

Theorem 2.2 *Let M be a symmetric matrix of order n, and for each $t \geq 0$, let $U(t) = e^{itM}$. Fix a pair of indices s, r, and for each $t \geq 0$, let $p(t) = |u_{s,r}(t)|^2$. Suppose that for some $t_0 > 0$, we have $p(t_0) = 1$. For each $j \in \mathbb{N}$, let $w(j) = e_s^\top M^j e_s$, and set $w(0) \equiv 1$. Then for each $k \in \mathbb{N}$,*

$$\left.\frac{d^k p}{dt^k}\right|_{t_0} = \begin{cases} (-1)^{(k \mod 4)/2} \sum_{j=0}^{k} (-1)^j \binom{k}{j} w(j) w(k-j), & \text{if } k \text{ is even} \\ 0, & \text{if } k \text{ is odd.} \end{cases} \tag{3}$$

Proof. Write M as $M = V \Lambda V^\top$, where V is an orthogonal matrix and Λ is a diagonal matrix. Fix a $j \in \mathbb{N}$, and note that $\left.\frac{d^j u_{s,r}(t)}{dt^j}\right|_{t_0} = (i)^j e_s^\top V \Lambda^j e^{it_0 \Lambda} V^\top e_r$. From Lemma 2.1, we have $e_s^\top V \Lambda^j e^{it_0 \Lambda} V^\top e_r = u_{s,r}(t_0) e_s^\top V \Lambda^j V^\top e_s$, so that $\left.\frac{d^j u_{s,r}(t)}{dt^j}\right|_{t_0} = (i)^j u_{s,r}(t_0) w(j)$. Setting $\mathfrak{Re}(u_{s,r}(t_0)) = \alpha, \mathfrak{Im}(u_{s,r}(t_0)) = \beta$, it now follows that

$$\left.\frac{d^j u_{s,r}(t)}{dt^j}\right|_{t_0} = \begin{cases} (\alpha + i\beta) w(j), & \text{if } j \equiv 0 \mod 4, \\ (-\beta + i\alpha) w(j), & \text{if } j \equiv 1 \mod 4, \\ (-\alpha - i\beta) w(j), & \text{if } j \equiv 2 \mod 4, \\ (\beta - i\alpha) w(j), & \text{if } j \equiv 3 \mod 4. \end{cases} \tag{4}$$

Set $x(t) = \mathfrak{Re}(u_{s,r}(t))$ and $y(t) = \mathfrak{Im}(u_{s,r}(t))$ (so that in particular $x(t_0) = \alpha, y(t_0) = \beta$), and note that $p(t) = x(t)^2 + y(t)^2$. It now follows that for each $k \in \mathbb{N}$,

$$\left.\frac{d^k p}{dt^k}\right|_{t_0} = \sum_{j=0}^{k} \binom{k}{j} \left(\left.\frac{d^j x}{dt^j}\right|_{t_0} \left.\frac{d^{k-j} x}{dt^{k-j}}\right|_{t_0} + \left.\frac{d^j y}{dt^j}\right|_{t_0} \left.\frac{d^{k-j} y}{dt^{k-j}}\right|_{t_0} \right).$$

Suppose first that k is odd. Considering the cases arising from (4), we find that $\left.\frac{d^j x}{dt^j}\right|_{t_0} \left.\frac{d^{k-j} x}{dt^{k-j}}\right|_{t_0} + \left.\frac{d^j y}{dt^j}\right|_{t_0} \left.\frac{d^{k-j} y}{dt^{k-j}}\right|_{t_0}$ is either $\alpha(-\beta) + \beta\alpha, \alpha\beta + \beta(-\alpha), (-\alpha)(-\beta) + (-\beta)\alpha$, or $(-\alpha)(-\beta) + \beta(-\alpha)$, all of which equal zero. It now follows immediately that $\left.\frac{d^k p}{dt^k}\right|_{t_0} = 0$ when k is odd.

Next we suppose that k is even with $k \equiv 2 \mod 4$. Then again referring to (4), we have

$$\begin{aligned} &\frac{d^j x}{dt^j}\Big|_{t_0} \frac{d^{k-j} x}{dt^{k-j}}\Big|_{t_0} + \frac{d^j y}{dt^j}\Big|_{t_0} \frac{d^{k-j} y}{dt^{k-j}}\Big|_{t_0} \\ = w(j)w(k-j) &\begin{cases} -\alpha^2 - \beta^2, & j \equiv 0 \mod 4, \\ \beta^2 + \alpha^2, & j \equiv 1 \mod 4, \\ -\alpha^2 - \beta^2, & j \equiv 2 \mod 4, \\ \beta^2 + \alpha^2, & j \equiv 3 \mod 4 \end{cases} \\ &= (-1)^{j-1} w(j)w(k-j). \end{aligned}$$

A similar argument shows that if $k \equiv 0 \mod 4$, then $\frac{d^j x}{dt^j}\Big|_{t_0} \frac{d^{k-j} x}{dt^{k-j}}\Big|_{t_0} + \frac{d^j y}{dt^j}\Big|_{t_0} \frac{d^{k-j} y}{dt^{k-j}}\Big|_{t_0}$ $= (-1)^j w(j)w(k-j)$. This establishes (3) when k is even. $\square$

Remark 2.3 Suppose that M is the adjacency matrix of an *unweighted graph* – that is, a graph in which each of the edges has weight 1. Again using the notation of Theorem 2.2, we see that $w(2)$ is the degree of vertex s, say d. In particular, $\frac{d^2 p}{dt^2}\Big|_{t_0} = -2d$ in that case. Similarly, if M is the Laplacian matrix of an unweighted graph, then $w(1) = d, w(2) = d^2 + d$, and we find that $\frac{d^2 p}{dt^2}\Big|_{t_0} = -(d^2 + d - 2d^2 + d^2 + d) = -2d$. Thus, in both cases we find that $\frac{d^2 p}{dt^2}\Big|_{t_0}$ is correlated with the degree of vertex s.

Next, we provide alternate expressions for the derivatives in Theorem 2.2 in terms of the spectral information associated with the matrix in question. As noted above, [15] discusses the second derivative of the fidelity of transfer, and does so by using the eigendecomposition of the Hamiltonian. Thus, (5) offers an extension of the discussion in [15].

Theorem 2.4 *Let M be a symmetric matrix of order n, and for each $t \geq 0$, and let $U(t) = e^{itM}$. Fix a pair of indices s, r, and for each $t \geq 0$, let*

$p(t) = |u_{s,r}(t)|^2$. Suppose that for some $t_0 > 0$, we have $p(t_0) = 1$. Denote the distinct eigenvalues of M by $\lambda_1, \ldots, \lambda_q$, and for each $l = 1, \ldots, q$, let a_l denote the (s, s) entry in the orthogonal idempotent eigenprojection matrix associated with λ_l. Then for each even $k \in \mathbb{N}$, we have

$$\left.\frac{d^k p}{dt^k}\right|_{t_0} = (-1)^{(k \mod 4)/2} \sum_{1 \le l < m \le q} 2a_l a_m (\lambda_l - \lambda_m)^k. \tag{5}$$

Proof. For each $l = 1, \ldots, q$, let P_l denote the orthogonal idempotent eigenprojection matrix associated with λ_l. For each $j \in \mathbb{N}$ we have $M^j = \sum_{l=1}^q \lambda_l^j P_l$, from which we find that

$$w(j) = \sum_{l=1}^{q} a_l \lambda_l^j \tag{6}$$

for any such j.

Let k be a positive even integer, and consider the expression

$$\sum_{j=0}^{k} (-1)^j \binom{k}{j} w(j) w(k-j).$$

From (6), we find that

$$\sum_{j=0}^{k} (-1)^j \binom{k}{j} w(j) w(k-j) = \sum_{j=0}^{k} (-1)^j \binom{k}{j} \left(\sum_{l=1}^{q} a_l \lambda_l^j \right) \left(\sum_{m=1}^{q} a_m \lambda_m^{k-j} \right).$$

Expanding the right hand side and simplifying now yields the following:

$$\sum_{j=0}^{k}(-1)^j\binom{k}{j}w(j)w(k-j) = \sum_{j=0}^{k}(-1)^j\binom{k}{j}\left(\sum_{l=1}^{q}a_l\lambda_l^j\right) =$$

$$\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left\{\sum_{l=1}^{q}a_l^2\lambda_l^k + \sum_{1\le l<m\le q}a_la_m(\lambda_l^j\lambda_m^{k-j}+\lambda_l^{k-j}\lambda_m^j)\right\} =$$

$$\left(\sum_{l=1}^{q}a_l^2\lambda_l^k\right)\sum_{j=0}^{k}(-1)^j\binom{k}{j} + \sum_{j=0}^{k}(-1)^j\binom{k}{j}\sum_{1\le l<m\le q}a_la_m(\lambda_l^j\lambda_m^{k-j}+\lambda_l^{k-j}\lambda_m^j) =$$

$$\sum_{1\le l<m\le q}a_la_m\sum_{j=0}^{k}(-1)^j\binom{k}{j}(\lambda_l^j\lambda_m^{k-j}+\lambda_l^{k-j}\lambda_m^j) =$$

$$\sum_{1\le l<m\le q}2a_la_m(\lambda_l-\lambda_m)^k.$$

The expression $\left.\frac{d^kp}{dt^k}\right|_{t_0}$ in (5) now follows immediately. □

We have the following consequence of Theorem 2.4.

Corollary 2.5 *Suppose that the hypothesis and notation of Theorem 2.4 holds. Then* $\left.\frac{d^kp}{dt^k}\right|_{t_0} < 0$ *when* $k \equiv 2 \mod 4$ *and* $\left.\frac{d^kp}{dt^k}\right|_{t_0} > 0$ *when* $k \equiv 0 \mod 4$*.*

Proof. Since each a_l is a diagonal entry of a (non–zero) idempotent matrix, we find that $a_l > 0, l = 1, \dots, q$. Further, since we have perfect state transfer from s to r, M is not the identity matrix, so that $q \ge 2$. Hence for any even $k \in \mathbb{N}, \sum_{1\le l<m\le q}2a_la_m(\lambda_l-\lambda_m)^k > 0$. The conclusion now follows. □

Example 2.6 Consider the matrix A given by

$$A = \begin{bmatrix} 0 & \sqrt{5} & 0 & 0 & 0 & 0 \\ \sqrt{5} & 0 & \sqrt{8} & 0 & 0 & 0 \\ 0 & \sqrt{8} & 0 & \sqrt{9} & 0 & 0 \\ 0 & 0 & \sqrt{9} & 0 & \sqrt{8} & 0 \\ 0 & 0 & 0 & \sqrt{8} & 0 & \sqrt{5} \\ 0 & 0 & 0 & 0 & \sqrt{5} & 0 \end{bmatrix}.$$

Let $U(t) = e^{itA}$ for each $t \geq 0$, and let $p(t) = |u_{1,6}(t)|^2$, again for $t \geq 0$. As is observed in [9], we have $p(\frac{\pi}{2}) = 1$. The eigenvalues of A are known to be given by $\lambda_l = 7 - 2l, l = 1, \ldots, 6$, and we have the following list of corresponding eigenvectors:

$$v_1 = \frac{1}{\sqrt{32}} \begin{bmatrix} 1 \\ \sqrt{5} \\ \sqrt{10} \\ \sqrt{10} \\ \sqrt{5} \\ 1 \end{bmatrix}, v_2 = \sqrt{\frac{5}{32}} \begin{bmatrix} 1 \\ \frac{3}{\sqrt{5}} \\ \sqrt{\frac{2}{5}} \\ -\sqrt{\frac{2}{5}} \\ -\frac{3}{\sqrt{5}} \\ -1 \end{bmatrix}, v_3 = \frac{\sqrt{5}}{4} \begin{bmatrix} 1 \\ \frac{1}{\sqrt{5}} \\ -\sqrt{\frac{2}{5}} \\ -\sqrt{\frac{2}{5}} \\ \frac{1}{\sqrt{5}} \\ 1 \end{bmatrix},$$

$$v_4 = \frac{\sqrt{5}}{4} \begin{bmatrix} 1 \\ -\frac{1}{\sqrt{5}} \\ -\sqrt{\frac{2}{5}} \\ \sqrt{\frac{2}{5}} \\ \frac{1}{\sqrt{5}} \\ -1 \end{bmatrix}, v_5 = \sqrt{\frac{5}{32}} \begin{bmatrix} 1 \\ -\frac{3}{\sqrt{5}} \\ \sqrt{\frac{2}{5}} \\ \sqrt{\frac{2}{5}} \\ -\frac{3}{\sqrt{5}} \\ 1 \end{bmatrix}, v_6 = \frac{1}{\sqrt{32}} \begin{bmatrix} 1 \\ -\sqrt{5} \\ \sqrt{10} \\ -\sqrt{10} \\ \sqrt{5} \\ -1 \end{bmatrix}.$$

It now follows that, in the notation of Theorem 2.4, $a_1 = \frac{1}{32}, a_2 = \frac{5}{32}, a_3 = \frac{5}{16}, a_4 = \frac{5}{16}, a_5 = \frac{5}{32}$ and $a_6 = \frac{1}{32}$. Substituting the expressions for λ_l and

$a_l, l = 1, \ldots, 6$ into (5) and simplifying, we find that for each even $k \in \mathbb{N}$,

$$\left.\frac{d^k p}{dt^k}\right|_{\frac{\pi}{2}} = 2(-1)^{(k \mod 4)/2}\left[\left(\frac{105}{512}\right)2^k + \left(\frac{15}{128}\right)4^k + \left(\frac{45}{1024}\right)6^k + \left(\frac{5}{512}\right)8^k + \left(\frac{1}{1024}\right)10^k\right].$$

Example 2.7 Consider the graph on n vertices given by $G = K_n - e$, where e denotes the edge between vertices 1 and 2, and suppose that $n \equiv 0 \mod 4$. Let L denote the Laplacian matrix for G. As is shown in [16], the $(1, 2)$ entry of $e^{i\frac{\pi}{2}L}$ has modulus one, so that there is perfect state transfer from vertex 1 to vertex 2 at time $\frac{\pi}{2}$. The eigenvalues of L are known to be $\lambda_1 = n$ (with multiplicity $n - 2$), $\lambda_2 = n - 2$ (simple), and $\lambda_3 = 0$ (also simple), with the following as the respective orthogonal idempotent eigenprojection matrices:

$$P_1 = \left[\begin{array}{c|c} \frac{n-2}{2n}J_2 & -\frac{1}{n}J_{2,n-2} \\ \hline -\frac{1}{n}J_{n-2,2} & I - \frac{1}{n}J_{n-2} \end{array}\right], P_2 = \frac{1}{2}(e_1 - e_2)(e_1 - e_2)^\top, P_3 = \frac{1}{n}J.$$

In the notation of Theorem 2.4, we then have $a_1 = \frac{n-2}{2n}, a_2 = \frac{1}{2}, a_3 = \frac{1}{n}$. Substituting into (5), it now follows that for each even $k \in \mathbb{N}$, we have

$$\left.\frac{d^k p}{dt^k}\right|_{\frac{\pi}{2}} = (-1)^{(k \mod 4)/2}\left[\frac{n-2}{2n}2^k + \frac{n-2}{n^2}n^k + \frac{1}{n}(n-2)^k\right].$$

Example 2.8 Suppose that $d \in \mathbb{N}$, and consider the d–*cube*, that is, the graph on 2^d vertices whose adjacency matrix A_d can be generated via the following iteration:

$$A_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, A_{k+1} = \left[\begin{array}{c|c} A_k & I \\ \hline I & A_k \end{array}\right], k = 0, \ldots, d-1.$$

It is shown in [9] that with this labelling of the vertices, the d–cube exhibits perfect state transfer from vertex 1 to vertex 2^d at time $\frac{\pi}{2}$. Next, we consider the 'standard' Hadamard matrix of order 2^d generated by the following iteration:

$$H_1 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, H_{k+1} = \left[\begin{array}{c|c} H_k & H_k \\ \hline H_k & -H_k \end{array}\right], k = 0, \ldots, d-1.$$

It is readily shown that the columns of $\frac{1}{\sqrt{2^d}} H_d$ form an orthonormal basis of eigenvectors for the adjacency matrix A_d. We note further that the eigenvalues of A_d are given by $d - 2j, j = 0, \ldots, d$, with respective multiplicities $\binom{d}{j}$.

Let $p(t)$ denote the fidelity of transfer from vertex 1 to vertex 2^d at time t. From the fact that A_d is diagonalised by $\frac{1}{\sqrt{2^d}} H_d$, it follows that for each $j = 0, \ldots, d$, the diagonal entries of the eigenprojection matrix for the eigenvalue $n - 2j$ are all equal to $\frac{\binom{d}{j}}{2^d}$. From (5), we thus find that for each even k,

$$\begin{aligned} \left.\frac{d^k p}{dt^k}\right|_{\frac{\pi}{2}} &= (-1)^{(k \mod 4)/2} \sum_{j=0}^{d} \sum_{l=0}^{d} \frac{\binom{d}{j}}{2^d} \frac{\binom{d}{l}}{2^d} (n - 2j - n + 2l)^k \\ &= \frac{(-1)^{(k \mod 4)/2}}{2^{2d-k}} \sum_{j=0}^{d} \sum_{l=0}^{d} (l-j)^k \binom{d}{j} \binom{d}{l}. \end{aligned} \tag{7}$$

When $k = 2$, it is not difficult to show that $\left.\frac{d^2 p}{dt^2}\right|_{\frac{\pi}{2}} = -2d$, in agreement with Remark 2.3, while substituting $k = 4$ into (7) and simplifying, we find that $\left.\frac{d^4 p}{dt^4}\right|_{\frac{\pi}{2}} = 4d(3d-1)$.

Next we provide an upper bound on the sizes of the derivatives (of all orders, and taken with respect to the readout time) of the fidelity of transfer.

Theorem 2.9 *Let M be a symmetric matrix of order n, and for each $t \geq 0$, and let $U(t) = e^{itM}$. Fix a pair of indices s, r, and for each $t \geq 0$, let $p(t) =$*

$|u_{s,r}(t)|^2$. *Then for any $k \in \mathbb{N}$ and any $t \geq 0$ we have*

$$\Big|\frac{d^k p}{dt^k}\Big| \leq 2^{k+1}\rho(M)^k.$$

Proof. For each $t \geq 0$ let $x(t) = \mathfrak{Re}(u_{s,r}(t)), y(t) = \mathfrak{Im}(u_{s,r}(t))$, and note that $p(t) = x^2(t) + y^2(t)$. We find that for any $k \in \mathbb{N}$,

$$\frac{d^k p}{dt^k} = \sum_{j=0}^{k} \binom{k}{j} \left[\frac{d^j x}{dt^j}\frac{d^{k-j}x}{dt^{k-j}} + \frac{d^j y}{dt^j}\frac{d^{k-j}y}{dt^{k-j}}\right].$$

We claim that for each $m \in \mathbb{N}$ and any $t \geq 0, |\frac{d^m x}{dt^m}|, |\frac{d^m y}{dt^m}| \leq \rho(M)^m$. In order to establish the claim, we begin by writing $M = V\Lambda V^\top$, where $\Lambda = diag\left(\left[\begin{array}{c} \lambda_1 \ldots \lambda_n \end{array}\right]\right)$ is a diagonal matrix of eigenvalues and V is an orthogonal matrix of corresponding eigenvectors. It now follows that $x(t) + iy(t) = u_{s,r}(t) = e_s^\top V e^{it\Lambda} V^\top e_r$, so that for each $m \in \mathbb{N}, \frac{d^m x}{dt^m} + i\frac{d^m y}{dt^m} = \frac{d^m u_{s,r}}{dt^m} = (i)^k e_s^\top V \Lambda^m e^{it\Lambda} V^\top e_r$. Observe that $|\frac{d^m u_{s,r}}{dt^m}| = |\sum_{j=1}^n \lambda_j^m v_{s,j} e^{it\lambda_j} v_{r,j}| \leq \sum_{j=1}^n \rho(M)^m |v_{s,j}||v_{r,j}| \leq \rho(M)^m$, the last inequality following from the Cauchy–Schwarz inequality and the fact that V is an orthogonal matrix. Since $|\frac{d^m x}{dt^m}|, |\frac{d^m y}{dt^m}| \leq |\frac{d^m u_{s,r}}{dt^m}|$, the claim now follows.

Applying our claim, along with the triangle inequality now yields

$$\Big|\frac{d^k p}{dt^k}\Big| \leq$$
$$\sum_{j=0}^{k} \binom{k}{j} \left(\Big|\frac{d^j x}{dt^j}\Big|\Big|\frac{d^{k-j}x}{dt^{k-j}}\Big| + \Big|\frac{d^j y}{dt^j}\Big|\Big|\frac{d^{k-j}y}{dt^{k-j}}\Big|\right) \leq$$
$$2\rho(M)^k \sum_{j=0}^{k} \binom{k}{j} = 2^{k+1}\rho(M)^k,$$

as desired. □

The following is immediate.

Corollary 2.10 *Suppose that M and p are as in Theorem 2.9, and that $p(t_0) = 1$ for some $t_0 > 0$. Denote the distinct eigenvalues of M by $\lambda_1, \ldots, \lambda_q$, and for each $k = 1, \ldots, q$, let a_k be the (s, s) entry of the orthogonal idempotent eigenprojection matrix corresponding to λ_k. For each $j \in \mathbb{N}$, let $w(j) = e_s^\top M^j e_s$, and set $w(0) = 1$. Let $l \in \mathbb{N}$, and $h \in \mathbb{R}$. Then*

$$p(t_0 + h) = 1 + \sum_{j=1}^{l} (-1)^{(2j \mod 4)/2} \frac{h^{2j}}{(2j)!} \left[\sum_{m=0}^{2j} (-1)^m \binom{2j}{m} w(m) w(2j - m) \right] + \frac{h^{2l+2}}{(2l+2)!} R_{2l+2}$$

$$= 1 + \sum_{j=1}^{l} (-1)^{(2j \mod 4)/2} \frac{h^{2j}}{(2j)!} \sum_{1 \le k < m \le q} 2 a_k a_m (\lambda_k - \lambda_m)^{2j} + \frac{h^{2l+2}}{(2l+2)!} R_{2l+2},$$

where $|R_{2l+2}| \le 2^{2l+3} \rho(M)^{2l+2}$.

Remark 2.11 In this remark, we maintain the hypotheses of Theorem 2.4, and suppose that M, p, t_0 and the a_ls are as in that theorem. For our symmetric matrix M, the *spread* of M, $\mathfrak{s}(M)$, is the difference between its largest and smallest eigenvalues. Since each of the a_ls is a diagonal entry of a symmetric idempotent matrix, we find readily that in fact each a_l must be positive. Further, since $\sum_{1 \le l < m \le q} 2 a_l a_m = 1 - \sum_{l=1}^{q} a_l^2 < 1$, it follows from (5) that for each even $k \in \mathbb{N}$, $\left| \frac{d^k p}{dt^k} \Big|_{t_0} \right| < (\mathfrak{s}(M))^k$.

We now apply the spread–based upper bound on the derivatives of the fidelity of transfer. From Taylor's theorem, for any h, we have $p(t_0 + h) = 1 + \sum_{j=1}^{\infty} \frac{h^{2j}}{(2j)!} \frac{d^{2j} p}{dt^{2j}} \Big|_{t_0}$. Further, from Corollary 2.5, $\frac{d^{2j} p}{dt^{2j}} \Big|_{t_0}$ is positive or negative according as j is even or odd, respectively. It now follows that

$$p(t_0 + h) \ge 1 - \sum_{l=0}^{\infty} \frac{h^{4l+2}}{(4l+2)!} \frac{d^{4l+2} p}{dt^{4l+2}} \Big|_{t_0} \ge 1 - \sum_{l=0}^{\infty} \frac{(\mathfrak{s}(M) h)^{4l+2}}{(4l+2)!} = 1 - \frac{1}{2} \left[\frac{e^{\mathfrak{s}(M) h} + e^{-\mathfrak{s}(M) h}}{2} - \cos(\mathfrak{s}(M) h) \right]. \tag{8}$$

Thus (8) quantifies the notion that if h is small relative to $\frac{1}{\mathfrak{s}(M)}$, then $p(t_0+h)$ is necessarily close to 1.

We note that a result in [17] provides an easily computed upper bound for the spread of any symmetric matrix. Specifically, for our symmetric matrix M of order n, we have $\mathfrak{s}(M) \le \sqrt{2\text{trace}(M^\top M) - \frac{2}{n}(\text{trace}(M))^2}$. For a connected unweighted undirected graph on n vertices, it is well–known that the spread of the corresponding Laplacian matrix is bounded above by n; in [14] it is conjectured that the maximum possible spread of the adjacency matrix of such a graph is equal to $\sqrt{\lfloor \frac{4}{3}(n^2 - n + 1) \rfloor}$.

3 Sensitivity with respect to edge weights

While the derivatives of the fidelity of transfer with respect to the readout time (under the hypothesis of perfect state transfer) are established fairly readily, the corresponding partial derivatives with respect to the edge weights require a rather more technical development. As we have seen above, the fidelity of transfer depends on the eigenvalues and eigenvectors of the Hamiltonian, and evidently perturbing an edge weight will affect both the eigenvalues and the corresponding eigenvectors. Consequently, in order to compute derivatives of the fidelity of transfer, it is first necessary to identify an eigenbasis of the Hamiltonian that is analytic in the edge weight being perturbed. As noted in section 1, our Hamiltonian may take the form of the Laplacian matrix of a weighted graph, or of the adjacency matrix of a weighted graph. We treat those two cases separately below in our discussion of how to find a differentiable eigenbasis. We note that the Laplacian case is slightly simpler to address, as in that case, perturbing an edge weight leads to a perturbing matrix of rank 1, while the adjacency case leads to a perturbing matrix of rank 2.

3.1 Differentiable eigenbasis with respect to an edge weight: Laplacian case

Let L be the Laplacian matrix of a weighted graph, select a pair of vertices k, l, and set E equal to $(e_k - e_l)(e_k - e_l)^\top$. According to [1], there is an $\epsilon > 0$ such that for each $h \in (-\epsilon, \epsilon)$, the matrix $L + hE$ can be diagonalised as $L + hE = V(h)\Lambda(h)V(h)^\top$, where both $V(h)$ and $\Lambda(h)$ are analytic in h, $V(h)$ is orthogonal, and $\Lambda(h) = diag\left(\left[\begin{array}{c} \lambda_1(h) \dots \lambda_n(h) \end{array}\right]\right)$ is diagonal. Suppose that we have such an eigenbasis in hand and consider the j–th eigen–equation $(L + hE)V(h)e_j = \lambda_j(h)V(h)e_j$. Differentiating both sides with respect to h and evaluating at $h = 0$ yields $EV(0)e_j + L\frac{dV}{dh}\Big|_{h=0} e_j = \frac{d\lambda_j}{dh}\Big|_{h=0} V(0)e_j + \lambda_j(0)\frac{dV}{dh}\Big|_{h=0} e_j$. It now follows readily that

$$\frac{d\lambda_j}{dh}\Big|_{h=0} = e_j^\top V(0)^\top EV(0)e_j.$$

Thus, once we have the differentiable eigenbasis in hand, the derivatives of the corresponding eigenvalues are easily computed.

Our goal thus is to determine $V(0)$ and $\frac{dV}{dh}\Big|_{h=0}$; to do so we follow Algorithm 1 of [1], which sets out a general method for finding a differentiable eigenbasis, as well as its derivative, at $h = 0$. Suppose that L has eigenvalue λ of multiplicity r. Let $x_1, \dots, x_r$ be an orthonormal basis for the λ–eigenspace of L. If it happens that $Ex_j = 0$ for $j = 1, \dots, r$, then in fact each x_j is a λ–eigenvector of $L + hE$ for all h in a neighbourhood of 0. The corresponding columns of $V(h)$ can be taken to be $x_1, \dots, x_r$, and evidently they have derivative 0 on that neighbourhood of 0.

Suppose now that $Ex_j \neq 0$ for some j, and without loss of generality we take $j = 1$. If $r \geq 2$, set $\delta_j = (e_k - e_l)^\top x_j, j = 1, \dots, r$, and let $\hat{x}_1 = \frac{1}{\sqrt{\sum_{j=1}^r \delta_j^2}} \sum_{j=1}^r \delta_j x_j$. Observe that the λ–eigenspace of L can be decomposed as a direct sum of $Span\{\hat{x_1}\}$ and $S \equiv Span\{\delta_1 x_j - \delta_j x_1 | j = 2, \dots, r\}$. Evidently S is a subspace of the null space of E, and each vector in S is orthogonal to $\hat{x}_1$. Selecting an orthonormal basis $\hat{x}_j, j = 2, \ldots, r$ of S, it now follows that there is a differentiable eigenbasis $V(h)$ of $L + hE$ such that the columns of $V(0)$ corresponding to the eigenvalue λ can be taken to be $\hat{x}_j, j = 1, \ldots, r$. Suppose that the m–th column of $V(h)$ corresponds to the eigenvalue λ, say with $V(0)e_m = \hat{x}_p$ for some $p \geq 2$. It is straightforward to determine then that $\frac{dV}{dh}\Big|_{h=0} e_m = 0$. On the other hand, if $V(0)e_m = \hat{x}_1$, then as above we have $EV(0)e_m + L\frac{dV}{dh}\Big|_{h=0} e_m = \frac{d\lambda}{dh}\Big|_{h=0} V(0)e_m + \lambda(0)\frac{dV}{dh}\Big|_{h=0} e_m$. From this we find readily that $(\lambda I - L)^\dagger(\lambda I - L)\frac{dV}{dh}\Big|_{h=0} e_m = (\lambda I - L)^\dagger EV(0)e_m$. Recalling that $(\lambda I - L)^\dagger(\lambda I - L) = I - \sum_{j=1}^r \hat{x}_j\hat{x}_j^\top$, we find from the orthonormality of the columns of $V(h)$ that $(\lambda I - L)^\dagger(\lambda I - L)\frac{dV}{dh}\Big|_{h=0} e_m = \frac{dV}{dh}\Big|_{h=0} e_m$. We thus deduce that in this case,

$$\frac{dV}{dh}\Big|_{h=0} e_m = (\lambda I - L)^\dagger EV(0)e_m.$$

We observe here that the eigenvalue and eigenvector matrices $\Lambda(h)$ and $V(h)$, and hence the associated eigenvalue and eigenvector derivatives, depend on the choice of the indices k, l (equivalently, on the edge $k \sim l$ whose weight is perturbed). In order to emphasise that dependence in the sequel, we will use the notation $\frac{\partial \Lambda}{\partial_{k,l}}$ and $\frac{\partial V}{\partial_{k,l}}$ to denote the diagonal matrix of derivatives with respect to the weight of edge $k \sim l$, and the matrix whose columns are the derivatives (again with respect to the weight of edge $k \sim l$) of the associated eigenvectors, respectively.

Example 3.1 Here we revisit Example 2.7 and illustrate the formulas above concerning the differentiable eigenbases associated with the various pairs of indices k, l. Recall that the Laplacian matrix for $K_n \setminus e$ has 0 and $n - 2$ as simple eigenvalues, and n as an eigenvalue of multiplicity $n - 2$.
Case 1, $(k, l) = (1, 2)$: Here we have $E = (e_1 - e_2)(e_1 - e_2)^\top$. In this instance,

our $V(0)$ can be taken as follows

$$V(0)e_1 = \frac{1}{\sqrt{n}}\mathbf{1}_n \text{ (an eigenvector for the eigenvalue 0)},$$

$$V(0)e_2 = \frac{1}{\sqrt{2}}(e_1 - e_2) \text{ (an eigenvector for the eigenvalue } n-2\text{)},$$

$$V(0)e_3 = \frac{1}{\sqrt{2n(n-2)}}\left[\begin{array}{c} -(n-2)\mathbf{1}_2 \\ \hline 2\mathbf{1}_{n-2} \end{array}\right] \text{ (one eigenvector for the eigenvalue } n\text{)},$$

$$V(0)e_{k+3} = \frac{1}{\sqrt{k(k+1)}}\left[\begin{array}{c} 0_2 \\ \hline \mathbf{1}_k \\ \hline -k \\ \hline 0_{n-k-3} \end{array}\right], k = 1, \dots, n-3$$

(the remaining eigenvectors for the eigenvalue n).

Note that for each $j \neq 2, EV(0)e_j = 0$, while $((n-2)I - L)^\dagger EV(0)e_2 = \sqrt{2}((n-2)I - L)^\dagger(e_1 - e_2) = 0$. It now follows that $\frac{\partial V}{\partial_{1,2}}$ is the zero matrix. We also find that $\frac{\partial \Lambda}{\partial_{1,2}} = diag\left(\begin{bmatrix} 0 & 2 & 0 & \dots & 0 \end{bmatrix}\right)$.

Case 2, $(k, l) = (1, 3)$: Here we take $E = (e_1 - e_3)(e_1 - e_3)^\top$, and our $V(0)$ can be taken as follows

$$V(0)e_1 = \frac{1}{\sqrt{n}}\mathbf{1}_n \text{ (for the eigenvalue 0)},$$

$$V(0)e_2 = \frac{1}{\sqrt{2}}(e_1 - e_2) \text{ (for the eigenvalue } n-2\text{)},$$

$$V(0)e_3 = \frac{1}{\sqrt{6}}(e_1 + e_2 - 2e_3) \text{ (for the eigenvalue } n\text{)},$$

$$V(0)e_{k+3} = \frac{1}{\sqrt{(k+2)(k+3)}}\left[\begin{array}{c} \mathbf{1}_2 \\ \hline \mathbf{1}_k \\ \hline -(k+2) \\ \hline 0_{n-k-3} \end{array}\right], k = 1, \dots, n-3$$

(for the eigenvalue n).

Observe that $EV(0)e_j = 0$ for $j \neq 2, 3$. Using the orthogonal idempotent decomposition for L from Example 2.7, it follows that (using the notation of that example) $(-L)^\dagger = -\frac{1}{n}P_1 - \frac{1}{n-2}P_2$, $((n-2)I-L)^\dagger = -\frac{1}{2}P_1 + \frac{1}{n-2}P_3$, $(nI-L)^\dagger = \frac{1}{2}P_2 + \frac{1}{n}P_3$. We thus find that

$$\frac{\partial V}{\partial_{1,3}} e_2 = -\frac{1}{2\sqrt{2}}\left(\frac{1}{2}e_1 + \frac{1}{2}e_2 - e_3\right), \text{ and } \frac{\partial V}{\partial_{1,3}} e_3 = \frac{3}{4\sqrt{6}}(e_1 - e_2), \text{ while}$$

$$\frac{\partial V}{\partial_{1,3}} e_j = 0, j \neq 2, 3.$$

Finally, we observe that $\frac{\partial \Lambda}{\partial_{1,3}} = diag\left(\begin{bmatrix} 0 & \frac{1}{2} & \frac{3}{2} & 0 & \ldots & 0 \end{bmatrix}\right)$.

Case 3, $(k,l) = (3,4)$: Here we take $E = (e_3 - e_4)(e_3 - e_4)^\top$, and our $V(0)$ can be taken as follows

$$V(0)e_1 = \frac{1}{\sqrt{n}}\mathbf{1}_n \text{ (for the eigenvalue 0)},$$
$$V(0)e_2 = \frac{1}{\sqrt{2}}(e_1 - e_2) \text{ (for the eigenvalue } n-2),$$
$$V(0)e_3 = \frac{1}{\sqrt{2}}(e_3 - e_4) \text{ (for the eigenvalue } n),$$
$$V(0)e_4 = \frac{1}{\sqrt{2n(n-2)}}\left[\begin{array}{c} -(n-2)\mathbf{1}_2 \\ \hline 2\mathbf{1}_{n-2} \end{array}\right] \text{ (for the eigenvalue } n),$$
$$V(0)e_{k+3} = \frac{1}{\sqrt{k(k+1)}}\left[\begin{array}{c} 0_2 \\ \hline \mathbf{1}_k \\ \hline -k \\ \hline 0_{n-k-3} \end{array}\right], k = 2, \ldots, n-3 \text{ (for the eigenvalue } n).$$

Observe that $EV(0)e_j = 0$ for $j \neq 3$; using our expression for $(nI - L)^\dagger$ above, we also find that $(nI-L)^\dagger V(0)e_3 = 0$. Hence $\frac{\partial V}{\partial_{3,4}}$ is the zero matrix. Finally, we note that $\frac{\partial \Lambda}{\partial_{3,4}} = diag\left(\begin{bmatrix} 0 & 0 & 2 & 0 & \ldots & 0 \end{bmatrix}\right)$.

3.2 Differentiable eigenbasis with respect to an edge weight: adjacency case

Suppose that we have a weighted graph on n vertices with adjacency matrix A. Select a pair of vertices k, l, and set E equal to $e_k e_l^\top + e_l e_k^\top$. As in subsection 3.1, there is an $\epsilon > 0$ such that for each $h \in (-\epsilon, \epsilon)$, the matrix $A + hE$ can be diagonalised as $A + hE = V(h)\Lambda(h)V(h)^\top$, where both $V(h)$ and $\Lambda(h)$ are analytic in h, $V(h)$ is orthogonal, and $\Lambda(h) = diag\left(\left[\begin{array}{c} \lambda_1(h) \ldots \lambda_n(h) \end{array}\right]\right)$ is diagonal. Again we find that

$$\left.\frac{d\lambda_j}{dh}\right|_{h=0} = e_j^\top V(0)^\top E V(0) e_j, j = 1, \ldots, n.$$

It remains now to compute $V(0)$ and $\left.\frac{dV}{dh}\right|_{h=0}$, and we do so by implementing Algorithm 1 of [1]. Fix an eigenvalue λ of A of multiplicity r, and let $x_1, \ldots, x_r$ denote an orthonormal eigenbasis of the λ–eigenbasis of A. Observe that since E has rank two, the subspace spanned by $Ex_j, j = 1, \ldots, r$ has dimension zero, one or two.

In the dimension zero case we find that each x_j is a λ–eigenvector of $A + hE$, from which it follows that the corresponding columns of $V(h)$ can be taken to be $x_1, \ldots, x_r$, and that the derivative (at $h = 0$) of each such column is 0.

In the dimension one case, we assume without loss of generality that $Ex_1 \neq 0$. For each $j = 1, \ldots, r$, let $\delta_j = \frac{x_1^\top E^\top E x_j}{x_1^\top E^\top E x_1}$. If $r \geq 2$, then necessarily for each $j = 2, \ldots, r, Ex_j$ is a scalar multiple of Ex_1, from which we find that $E(x_j - \delta_j x_1) = 0, j = 2, \ldots, r$. Set $\hat{x}_1 = \frac{1}{\sqrt{\sum_{j=1}^r \delta_j^2}} \sum_{j=1}^r \delta_j x_j$, and observe that the λ–eigenspace of A decomposes as a direct sum of $Span\{\hat{x_1}\}$ and $S \equiv Span\{\delta_1 x_j - \delta_j x_1 | j = 2, \ldots, r\}$. Select an orthonormal basis $\hat{x_j}, j = 2, \ldots, r$ of S. We then find that there is a differentiable eigenbasis $V(h)$ of $A + hE$ such that the columns of $V(0)$ corresponding to the eigenvalue λ can be taken to be $\hat{x_j}, j = 1, \ldots, r$. Again reasoning as in subsection 3.1, we see that if

$V(0)e_m = x_j$ for some $j = 2, \ldots, r$, then $\frac{dV}{dh}\Big|_{h=0} e_m = 0$, while if $V(0)e_m = x_1$, then $\frac{dV}{dh}\Big|_{h=0} e_m = (\lambda I - A)^\dagger E x_1$.

Next we suppose that the subspace spanned by $Ex_j, j = 1, \ldots, r$ has dimension two; without loss of generality, the vectors Ex_1, Ex_2 form a basis for that space. If $r \geq 3$, then for each $j = 1, \ldots, r$, define the scalars α_j, β_j via

$$\begin{bmatrix} \alpha_j \\ \beta_j \end{bmatrix} = \left(\begin{bmatrix} e_k^\top \\ e_l^\top \end{bmatrix} \begin{bmatrix} x_1 & x_2 \end{bmatrix} \right)^{-1} \begin{bmatrix} e_k^\top \\ e_l^\top \end{bmatrix} x_j.$$

We observe in passing that $\alpha_1 = 1, \beta_1 = 0, \alpha_2 = 0, \beta_2 = 1$. It now follows that for each $j = 3, \ldots, r, x_j - \alpha_j x_1 - \beta_j x_2$ is a null vector of E. We can decompose the λ–eigenspace of A as the direct sum of $S_1 = Span\{\sum_{j=1}^r \alpha_j x_j, \sum_{j=1}^r \beta_j x_j\}$ and $S_2 = Span\{x_j - \alpha_j x_1 - \beta_j x_2 | j = 3, \ldots, r\}$. Let $\tilde{x}_1, \tilde{x}_2$ be an orthonormal basis of S_1, and let $\hat{x}_j, j = 3, \ldots, r$ be an orthonormal basis of S_2.

Consider the 2×2 matrix

$$B = \begin{bmatrix} \tilde{x}_1^\top \\ \tilde{x}_2^\top \end{bmatrix} E \begin{bmatrix} \tilde{x}_1 & \tilde{x}_2 \end{bmatrix}.$$

A straightforward computation shows that $det(B) = -(e_l^\top \tilde{x}_1 e_k^\top \tilde{x}_2 - e_k^\top \tilde{x}_1 e_1^\top \tilde{x}_2)^2$ < 0, the strict inequality following from the fact that $E\tilde{x}_1$ and $E\tilde{x}_2$ are linearly independent. Evidently B has distinct eigenvalues, one of which is positive, the other negative. Let

$$U = \begin{bmatrix} \sigma_1 & \tau_1 \\ \sigma_2 & \tau_2 \end{bmatrix}$$

be an orthogonal matrix that diagonalises B (i.e. $U^\top BU$ is diagonal). Setting $\hat{x}_1 = \sigma_1 \tilde{x}_1 + \sigma_2 \tilde{x}_2$ and $\hat{x}_2 = \tau_1 \tilde{x}_1 + \tau_2 \tilde{x}_2$, it follows from Algorithm 1 of [1] that there is a differentiable eigenbasis $V(h)$ of $A + hE$ such that the columns of $V(0)$ corresponding to the eigenvalue λ can be taken to be $\hat{x}_j, j = 1, \ldots, r$. Further, if $V(0)e_m = x_j$ for some $j = 3, \ldots, r$, then $\frac{dV}{dh}\Big|_{h=0} e_m = 0$.

Finally, again referring to [1], if p, q are indices such that $V(0)\left[\begin{array}{cc} e_p & e_q \end{array}\right] = \left[\begin{array}{cc} \hat{x}_1 & \hat{x}_2 \end{array}\right]$, then

$$\left.\frac{dV}{dh}\right|_{h=0}\left[\begin{array}{cc} e_p & e_q \end{array}\right] = \left[\begin{array}{cc} (\lambda I - A)^{\dagger} E\hat{x}_1 & (\lambda I - A)^{\dagger} E\hat{x}_2 \end{array}\right] + \frac{\hat{x}_1^{\top} E(\lambda I - A)^{\dagger} E\hat{x}_2}{\hat{x}_2^{\top} E\hat{x}_2 - \hat{x}_1^{\top} E\hat{x}_1}\left[\begin{array}{cc} -\hat{x}_2 & \hat{x}_1 \end{array}\right]. \quad (9)$$

(We note in passing that $\left[\begin{array}{c} \hat{x}_1^{\top} \\ \hat{x}_2^{\top} \end{array}\right] E \left[\begin{array}{cc} \hat{x}_1 & \hat{x}_2 \end{array}\right]$ is a diagonal matrix whose diagonal entries are the eigenvalues of B. It now follows readily that either $\hat{x}_2^{\top} E\hat{x}_2 > 0 > \hat{x}_1^{\top} E\hat{x}_1$ or either $\hat{x}_2^{\top} E\hat{x}_2 < 0 < \hat{x}_1^{\top} E\hat{x}_1$. In either case, the denominator of the rational expression appearing in (9) is not zero.)

In keeping with the comment made in subsection 3.1, in the context of the adjacency matrix of a weighted graph, we will use the notation $\frac{\partial \Lambda}{\partial_{k,l}}$ and $\frac{\partial V}{\partial_{k,l}}$, to denote the diagonal matrix of derivatives with respect to the weight of edge $k \sim l$, and the matrix whose columns are the derivatives (again with respect to the weight of edge $k \sim l$) of the associated eigenvectors, respectively.

Remark 3.2 As we will see below, the second term on the right hand side of (9) is a bit of a nuisance, in the sense that it is not so readily analysed (see Remark 3.6, for example). Nevertheless, there are circumstances in which this nuisance term does not appear, and in this remark we outline one such setting.

Suppose that $d \in \mathbb{N}$, and consider the d–cube, which is described in Example 2.8. Recall that the corresponding adjacency matrix A_d is diagonalised by $\frac{1}{\sqrt{2^d}} H_d$, where H_d is the 'standard' Hadamard matrix of order 2^d. Fix a pair of distinct indices k, l and let $E = e_k e_l^{\top} + e_l e_k^{\top}$. Since H_d is a Hadamard matrix, it follows that for the vectors $H_d e_k$ and $H_d e_l$, there are 2^{d-1} positions in which the entries in both vectors are equal, and 2^{d-1} positions in which the entries in both vectors have opposite sign. It now follows that for any diagonal matrix $D, (e_k+e_l)^\top H_d D H_d^\top (e_k-e_l) = 0$, from which we deduce that for any eigenvalue λ of A_d, we have $(e_k+e_l)^\top(\lambda I - A_d)^\dagger(e_k-e_l) = 0$.

Fix an eigenvalue λ of A_d, suppose that $x_1,\ldots,x_p$ are the columns of $\frac{1}{\sqrt{2^d}}H_d$ that span the corresponding eigenspace, and assume that $Span\{Ex_j|j = 1,\ldots,p\}$ has dimension two. Scaling the x_js by -1 if necessary and re-ordering them (also if necessary), we find that there is an index m between 1 and $p-1$ such that $\begin{bmatrix} e_k^\top \\ e_l^\top \end{bmatrix} x_j = \frac{1}{\sqrt{2^d}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}, j = 1,\ldots,m$, and $\begin{bmatrix} e_k^\top \\ e_l^\top \end{bmatrix} x_j = \frac{1}{\sqrt{2^d}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}, j = m+1,\ldots,p$. Implementing the construction above, it now follows that $\hat{x}_1 = \frac{1}{\sqrt{m}}\sum_{j=1}^m x_j$ and $\hat{x}_2 = \frac{1}{\sqrt{p-m}}\sum_{j=m+1}^p x_j$, while $E\hat{x}_j = 0, j = 3,\ldots,p$. As a result, we have $E\hat{x}_1 = \sqrt{\frac{m}{2^d}}(e_k+e_l)$ and $E\hat{x}_2 = -\sqrt{\frac{p-m}{2^d}}(e_k - e_l)$. Hence we have $\hat{x}_1^\top E(\lambda I - A_d)^\dagger E\hat{x}_2 = -\frac{\sqrt{m(p-m)}}{2^d}(e_k + e_l)^\top(\lambda I - A_d)^\dagger(e_k-e_l) = 0$, thus yielding the desired simplification of (9) for the d–cube.

3.3 First derivative with respect to an edge weight

Subsections 3.1 and 3.2 allow us to find an eigenbasis that is suitable for discussing the perturbation of an edge weight. With such an eigenbasis in hand, we turn to our next result. In order to simplify the notation in the sequel, we suppress the explicit dependence on $h = 0$ – i.e. we use $V, \Lambda, \frac{\partial V}{\partial_{k,l}}$ and $\frac{\partial \Lambda}{\partial_{k,l}}$ in place of $V(0), \Lambda(0), \left.\frac{\partial V}{\partial_{k,l}}\right|_{h=0}$ and $\left.\frac{\partial \Lambda}{\partial_{k,l}}\right|_{h=0}$, respectively.

Theorem 3.3 *Let M be a symmetric matrix of order n, and for each $t \geq 0$, and let $U(t) = e^{itM}$. Fix a pair of indices s, r, and for each $t \geq 0$, let $p(t) = |u_{s,r}(t)|^2$. Fix a $t_0 > 0$ and denote $u_{s,r}(t_0)$ by $a + ib$.*

Suppose that k and l are distinct indices between 1 and n. We consider the following two scenarios:

i) M is the Laplacian matrix of a weighted graph and $V \equiv V(0), \Lambda \equiv \Lambda(0)$

are orthogonal and diagonal, respectively, and are constructed as in subsection 3.1;

ii) M is the adjacency matrix of a weighted graph and $V \equiv V(0), \Lambda \equiv \Lambda(0)$ are orthogonal and diagonal, respectively, and are constructed as in subsection 3.2.

In either scenario, we have the following, where $\frac{\partial V}{\partial_{k,l}}$, and $\frac{\partial \Lambda}{\partial_{k,l}}$ are computed as described in either subsection 3.1 or 3.2, as appropriate:

$$\frac{\partial u_{s,r}(t_0)}{\partial_{k,l}} = e_s^\top \frac{\partial V}{\partial_{k,l}} \left(\cos(t_0\Lambda) + i\sin(t_0\Lambda)\right) V^\top e_r + e_s^\top V \left(\cos(t_0\Lambda) + i\sin(t_0\Lambda)\right) \frac{\partial V^\top}{\partial_{k,l}} e_r + it_0 e_s^\top V \frac{\partial \Lambda}{\partial_{k,l}} \left(\cos(t_0\Lambda) + i\sin(t_0\Lambda)\right) V^\top e_r; \quad (10)$$

and

$$\frac{\partial p(t_0)}{\partial_{k,l}} = 2\left[e_s^\top \frac{\partial V}{\partial_{k,l}} \left(a\cos(t_0\Lambda) + b\sin(t_0\Lambda)\right) V^\top e_r + e_s^\top V \left(a\cos(t_0\Lambda) + b\sin(t_0\Lambda)\right) \frac{\partial V^\top}{\partial_{k,l}} e_r\right] + 2t_0 \left[e_s^\top V \frac{\partial \Lambda}{\partial_{k,l}} \left(b\cos(t_0\Lambda) - a\sin(t_0\Lambda)\right) V^\top e_r\right]. \quad (11)$$

Proof. We have $U(t_0) = Ve^{it_0\Lambda}V^\top$; differentiating that equation with respect to the weight of the edge between vertices k and l and then evaluating at the weight of $k \sim l$ yields

$$\frac{\partial U(t_0)}{\partial_{k,l}} = \frac{\partial V}{\partial_{k,l}} e^{it_0\Lambda} V^\top + Ve^{it_0\Lambda} \frac{\partial V^\top}{\partial_{k,l}} + it_0 V \frac{\partial \Lambda}{\partial_{k,l}} e^{it_0\Lambda} V^\top.$$

Hence

$$\frac{\partial u_{s,r}(t_0)}{\partial_{k,l}} = e_s^\top \frac{\partial V}{\partial_{k,l}} e^{it_0\Lambda} V^\top e_r + e_s^\top V e^{it_0\Lambda} \frac{\partial V^\top}{\partial_{k,l}} e_r + it_0 e_s^\top V \frac{\partial \Lambda}{\partial_{k,l}} e^{it_0\Lambda} V^\top e_r,$$

from which (10) follows readily.

Setting $x(t) = \mathfrak{Re}(u_{s,r}(t))$ and $y(t) = \mathfrak{Im}(u_{s,r}(t))$, we have $p(t) = x^2(t) + y^2(t)$. Thus,

$$\frac{\partial p(t_0)}{\partial_{k,l}} = 2\left[x(t_0)\frac{\partial x(t_0)}{\partial_{k,l}} + y(t_0)\frac{\partial y(t_0)}{\partial_{k,l}}\right].$$

By hypothesis, $x(t_0) = a$ and $y(t_0) = b$, while (10) yields

$$\frac{\partial x(t_0)}{\partial_{k,l}} = e_s^\top \frac{\partial V}{\partial_{k,l}} \cos(t_0\Lambda)V^\top e_r + e_s^\top V \cos(t_0\Lambda)\frac{\partial V^\top}{\partial_{k,l}} e_r - t_0 e_s^\top V \frac{\partial \Lambda}{\partial_{k,l}} \sin(t_0\Lambda)V^\top e_r$$

and

$$\frac{\partial y(t_0)}{\partial_{k,l}} = e_s^\top \frac{\partial V}{\partial_{k,l}} \sin(t_0\Lambda)V^\top e_r + e_s^\top V \sin(t_0\Lambda)\frac{\partial V^\top}{\partial_{k,l}} e_r + t_0 e_s^\top V \frac{\partial \Lambda}{\partial_{k,l}} \cos(t_0\Lambda)V^\top e_r.$$

Substituting those expressions now yields (11). □

The following is immediate from (11) upon application of the Cauchy–Schwarz inequality, as well as the fact that for the diagonal matrices $a\cos(t_0\Lambda) + b\sin(t_0\Lambda)$ and $b\cos(t_0\Lambda) - a\sin(t_0\Lambda)$, all diagonal elements have absolute value bounded above by 1.

Corollary 3.4 *With the notation as in Theorem 3.3, we have*

$$\left|\frac{\partial p(t_0)}{\partial_{k,l}}\right| \le 2\left[\sqrt{e_s^\top \frac{\partial V}{\partial_{k,l}}\frac{\partial V^\top}{\partial_{k,l}} e_s} + \sqrt{e_r^\top \frac{\partial V}{\partial_{k,l}}\frac{\partial V^\top}{\partial_{k,l}} e_r} + t_0\sqrt{e_s^\top V\left(\frac{\partial \Lambda}{\partial_{k,l}}\right)^2 V^\top e_s}\right].$$

In our next two remarks, we maintain the notation of Theorem 3.3.

Remark 3.5 Suppose that M is the Laplacian matrix of a weighted graph, and denote the distinct eigenvalues of M by $\lambda_j, j = 1, \ldots, m$. Recall from subsection 3.1 that $\frac{\partial \lambda_j}{\partial_{k,l}} = e_j^\top V(e_k - e_l)(e_k - e_l)^\top V^\top e_j$. We now find readily that $|\frac{\partial \lambda_j}{\partial_{k,l}}| \le 2$; hence we find that $\sqrt{e_s^\top V\left(\frac{\partial \Lambda}{\partial_{k,l}}\right)^2 V^\top e_s} \le 2$.

From the construction of the special eigenbasis matrix V, we find that $e_s^\top \frac{\partial V}{\partial_{k,l}}$ has at most m nonzero entries (i.e. one for each distinct eigenvalue), and that each such entry has the form $e_s^\top(\lambda_j I - M)^\dagger(e_k - e_l)(e_k - e_l)^\top V e_{\tilde{j}}$ for some suitable index $\tilde{j}$. From the Cauchy–Schwarz inequality it follows that for any such $\tilde{j}$, $\left(e_s^\top(\lambda_j - M)^\dagger(e_k - e_l)(e_k - e_l)^\top V e_{\tilde{j}}\right)^2 \le 4\left(\rho((\lambda_j I - M)^\dagger)\right)^2$. Consequently, we find that

$$e_s^\top \frac{\partial V}{\partial_{k,l}} \frac{\partial V^\top}{\partial_{k,l}} e_s \le 4 \sum_{j=1}^m \frac{1}{\min_{p \ne j}(\lambda_j - \lambda_p)^2}.$$

A similar argument applies to $e_r^\top \frac{\partial V}{\partial_{k,l}} \frac{\partial V^\top}{\partial_{k,l}} e_r$, and so we find from Corollary 3.4 that

$$\left|\frac{\partial p(t_0)}{\partial_{k,l}}\right| \le 4t_0 + 8\sqrt{\sum_{j=1}^m \frac{1}{\min_{p \ne j}(\lambda_j - \lambda_p)^2}}.$$

Remark 3.6 Suppose that M is the adjacency matrix of a weighted graph, and let $\lambda_j, j = 1, \dots, m$ denote the distinct eigenvalues of M. From subsection 3.2, we find that $\frac{\partial \lambda_j}{\partial_{k,l}} = e_j^\top V(e_k e_l^\top + e_l e_k^\top) V^\top e_j$, so that $\left|\frac{\partial \lambda_j}{\partial_{k,l}}\right| \le 1$. Hence $\sqrt{e_s^\top V \left(\frac{\partial \Lambda}{\partial_{k,l}}\right)^2 V^\top e_s} \le 1$.

Next we consider the entries of $e_s^\top \frac{\partial V}{\partial_{k,l}}$. From the discussion in subsection 3.2, we find that the nonzero entries of $e_s^\top \frac{\partial V}{\partial_{k,l}}$ come in two types: i) entries of the form $e_s^\top(\lambda_j I - M)^\dagger(e_k e_l^\top + e_l e_k^\top) V e_{\tilde{j}}$ for some suitable index $\tilde{j}$ (arising from the dimension one case in subsection 3.2); and ii) pairs of entries of the form

$$\left[\begin{array}{cc} e_s^\top(\lambda_j I - M)^\dagger(e_k e_l^\top + e_l e_k^\top) V e_{\tilde{j}_1} & e_s^\top(\lambda_j I - M)^\dagger(e_k e_l^\top + e_l e_k^\top) V e_{\tilde{j}_2} \end{array}\right] +$$
$$\frac{(V e_{\tilde{j}_1})^\top(e_k e_l^\top + e_l e_k^\top)(\lambda_j I - M)^\dagger(e_k e_l^\top + e_l e_k^\top) V e_{\tilde{j}_2}}{V e_{\tilde{j}_2}^\top(e_k e_l^\top + e_l e_k^\top) V e_{\tilde{j}_2} - (V e_{\tilde{j}_1})^\top(e_k e_l^\top + e_l e_k^\top) V e_{\tilde{j}_1}} \left[\begin{array}{cc} -e_s^\top V e_{\tilde{j}_2} & e_s^\top V e_{\tilde{j}_1} \end{array}\right]$$

for suitable indices $\tilde{j}_1, \tilde{j}_2$ (arising from the dimension two case, see (9)). Evidently the entries in case i) are bounded above by $\rho((\lambda_j I - M)^\dagger)$ in absolute value.

Next we consider case ii), and we let

$$\delta = \max\left\{\left|\frac{\sqrt{(Ve_{\tilde{j}_1})^\top(e_ke_k^\top + e_le_l^\top)Ve_{\tilde{j}_1}(Ve_{\tilde{j}_2})^\top(e_ke_k^\top + e_le_l^\top)Ve_{\tilde{j}_2}}}{(Ve_{\tilde{j}_2})^\top(e_ke_l^\top + e_le_k^\top)Ve_{\tilde{j}_2} - (Ve_{\tilde{j}_1})^\top(e_ke_l^\top + e_le_k^\top)Ve_{\tilde{j}_1}}\right|\right\},$$

where the maximum is taken over all pairs of indices $\tilde{j}_1, \tilde{j}_2$ such that $Ve_{\tilde{j}_1}, Ve_{\tilde{j}_2}$ are pairs of eigenvectors corresponding to the same eigenvalue, as constructed in subsection 3.2. It follows that any nonzero entry of $e_s^\top \frac{\partial V}{\partial_{k,l}}$ is case ii) is bounded above by $(1+\delta)\rho((\lambda_j I - M)^\dagger)$ in absolute value.

In either case i) or case ii), we find that there are at most $2m$ nonzero entries in $e_s^\top \frac{\partial V}{\partial_{k,l}}$ (i.e., either 1 or 2 such nonzero entries for each of the m distinct eigenvalues of M). We thus deduce that

$$e_s^\top \frac{\partial V}{\partial_{k,l}} \frac{\partial V^\top}{\partial_{k,l}} e_s \le 2(1+\delta)^2 \sum_{j=1}^m \frac{1}{\min_{p\neq j}(\lambda_j - \lambda_p)^2}.$$

A similar inequality holds for $e_r^\top \frac{\partial V}{\partial_{k,l}} \frac{\partial V^\top}{\partial_{k,l}} e_r$. Assembling the observations above, we thus find that

$$\left|\frac{\partial p(t_0)}{\partial_{k,l}}\right| \le 2t_0 + 4(1+\delta)\sqrt{\sum_{j=1}^m \frac{1}{\min_{p\neq j}(\lambda_j - \lambda_p)^2}}.$$

Remark 3.7 Referring to Remarks 3.5 and 3.6 we see that in both cases, the upper bounds on $\left|\frac{\partial p(t_0)}{\partial_{k,l}}\right|$ depend in part on the separation between distinct eigenvalues of M. Specifically, if the distinct eigenvalues are not well separated, then the upper bound is large. Notice that in the context of perfect state transfer, there is a tradeoff between Theorem 2.4 and Remarks 3.5 and 3.6. From (5), we might hope that the eigenvalues are close together so that the derivatives of the fidelity of transfer with respect to the readout time are not too large; however, if the eigenvalues are close together, it may be the case that the derivatives of fidelity of transfer with respect to edge weights are large.

Example 3.8 Here we consider the adjacency matrix of the unweighted path on 3 vertices, namely $A = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$. Fix the time $t_0 = \frac{\pi}{\sqrt{8}}$, let $U(t) = e^{itA}$, and let $p(t) = |u_{1,3}(t)|^2$. Set $k = 1, l = 2$; we wish to find $\frac{\partial u_{1,3}(t_0)}{\partial_{1,2}}$ and $\frac{\partial p(t_0)}{\partial_{1,2}}$.

First, note that we may diagonalise A as $A = V\Lambda V^\top$, where

$$\Lambda = diag\left(\begin{bmatrix} \sqrt{2} & 0 & -\sqrt{2} \end{bmatrix}\right) \text{ and } V = \begin{bmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \end{bmatrix}.$$

It is now readily determined that $u(1,3) = -\frac{1}{2}$.

Since A has distinct eigenvalues, the method of subsection 3.2 to compute derivatives of the eigenvectors is significantly streamlined. Using the approach of subsection 3.2, we find that

$$\frac{\partial V}{\partial_{1,3}} = \begin{bmatrix} \frac{1}{4} & -\frac{1}{\sqrt{8}} & \frac{1}{4} \\ 0 & 0 & 0 \\ -\frac{1}{4} & -\frac{1}{\sqrt{8}} & -\frac{1}{4} \end{bmatrix}.$$

Making the appropriate substitutions into (10) and (11), we find that $\frac{\partial u_{1,3}(t_0)}{\partial_{1,2}} = -\frac{\pi}{8}$ while $\frac{\partial p(t_0)}{\partial_{1,2}} = \frac{\pi}{8}$.

Remark 3.9 Here we consider the conclusions of Theorem 3.3 in the context of perfect state transfer. Maintaining the notation of that theorem, suppose that there is perfect state transfer from vertex s to vertex r at time t_0. Applying Lemma 2.1, it follows that $e^{it_0\Lambda}V^\top e_r = (a+ib)V^\top e_s$. Hence we find that $e_s^\top \frac{\partial V}{\partial_{k,l}} e^{it_0\Lambda}V^\top e_r = e_s^\top \frac{\partial V}{\partial_{k,l}} V^\top e_s = 0$, and a similar argument shows that $e_s^\top V e^{it_0\Lambda} \frac{\partial V^\top}{\partial_{k,l}} e_r = 0$. Referring to (10), we find that $\frac{\partial u_{s,r}(t_0)}{\partial_{k,l}} = it_0 e_s^\top V \frac{\partial \Lambda}{\partial_{k,l}} \left(\cos(t_0\Lambda) + i\sin(t_0\Lambda)\right) V^\top e_r = i(a+ib)t_0 e_s^\top V \frac{\partial \Lambda}{\partial_{k,l}} V^\top e_s$.

From this simpler expression for $\frac{\partial u_{s,r}(t_0)}{\partial_{k,l}}$, we find that

$$\frac{\partial p(t_0)}{\partial_{k,l}} = 2t_0 \left(e_s^\top V \frac{\partial \Lambda}{\partial_{k,l}} V^\top e_s\right)(-ab + ab) = 0.$$

This last conclusion is of course not a surprise: since $p(t_0) = 1$, we have a local maximum for p (considered as a function of the weight of the edge between vertices k and l), and hence the corresponding partial derivative *must* be zero.

3.4 Second derivative with respect to an edge weight, under perfect state transfer

Suppose that we are given a Hamiltonian, and we want to consider the effect of perturbing an edge weight on the fidelity of transfer. The results of [1] show how to compute derivatives of all orders of the eigenvalues, as well as derivatives of all orders of an appropriate analytic eigenbasis. Thus, in principle, one can compute the derivative of any desired order of the fidelity of transfer; however, it should be noted that the expressions that arise in such a computation become increasingly involved as the order of the derivative increases. Our next result tackles the second derivative of the fidelity of transfer with respect to an edge weight, under the hypothesis of perfect state transfer.

Theorem 3.10 *Let M be a symmetric matrix of order n, and for each $t \geq 0$, let $U(t) = e^{itM}$. Fix a pair of indices s, r, and for each $t \geq 0$, let $p(t) = |u_{s,r}(t)|^2$. Suppose that for some $t_0 > 0$, $p(t_0) = 1$ and denote $u_{s,r}(t_0)$ by $\alpha + i\beta$.*

Suppose that k and l are distinct indices between 1 and n. We consider the following two scenarios:
i) M is the Laplacian matrix of a weighted graph and $V \equiv V(0), \Lambda \equiv \Lambda(0)$ are orthogonal and diagonal, respectively, and are constructed as in subsection 3.1;
ii) M is the adjacency matrix of a weighted graph and $V \equiv V(0), \Lambda \equiv \Lambda(0)$

are orthogonal and diagonal, respectively, and are constructed as in subsection 3.2.

In either scenario, we have the following, where $\frac{\partial V}{\partial_{k,l}}$, and $\frac{\partial \Lambda}{\partial_{k,l}}$ are computed as described in either subsection 3.1 or 3.2, as appropriate:

$$\frac{\partial^2 p(t_0)}{\partial_{k,l}^2} = -2t_0^2 \left[e_s^\top V \left(\frac{\partial \Lambda}{\partial_{k,l}} \right)^2 V^\top e_s - \left(e_s^\top V \frac{\partial \Lambda}{\partial_{k,l}} V^\top e_s \right)^2 \right]$$
$$-2 \left[e_s^\top \frac{\partial V}{\partial_{k,l}} \frac{\partial V^\top}{\partial_{k,l}} e_s + e_r^\top \frac{\partial V}{\partial_{k,l}} \frac{\partial V^\top}{\partial_{k,l}} e_r - 2e_s^\top \frac{\partial V}{\partial_{k,l}} \left(\alpha \cos(t_0 \Lambda) + \beta \sin(t_0 \Lambda) \right) \frac{\partial V^\top}{\partial_{k,l}} e_r \right] \tag{12}$$

Proof. Set $x(t) = \mathfrak{Re}(u_{s,r}(t))$ and $y(t) = \mathfrak{Im}(u_{s,r}(t))$, so that $p(t) = x(t)^2 + y(t)^2$. Evidently

$$\frac{\partial^2 p(t_0)}{\partial_{k,l}^2} = 2 \left[x(t_0) \frac{\partial^2 x(t_0)}{\partial_{k,l}^2} + y(t_0) \frac{\partial^2 y(t_0)}{\partial_{k,l}^2} + \left(\frac{\partial x(t_0)}{\partial_{k,l}} \right)^2 + \left(\frac{\partial y(t_0)}{\partial_{k,l}} \right)^2 \right].$$

Observe that $x(t_0) = \alpha, y(t_0) = \beta$, and from (10),

$$\left(\frac{\partial x(t_0)}{\partial_{k,l}} \right)^2 + \left(\frac{\partial y(t_0)}{\partial_{k,l}} \right)^2 = t_0^2 \left(e_s^\top V \frac{\partial \Lambda}{\partial_{k,l}} V^\top e_s \right)^2.$$

Thus, it remains only to find $\alpha \frac{\partial^2 x(t_0)}{\partial_{k,l}^2} + \beta \frac{\partial^2 y(t_0)}{\partial_{k,l}^2}$.

Differentiating (10) with respect to the weight of the edge between vertices k and l and then evaluating at the weight of $k \sim l$ yields

$$\frac{\partial^2 u_{s,r}(t_0)}{\partial_{k,l}^2} = e_s^\top \frac{\partial^2 V}{\partial_{k,l}^2} e^{it_0\Lambda} V^\top e_r + e_s^\top V e^{it_0\Lambda} \frac{\partial^2 V^\top}{\partial_{k,l}^2} e_r + 2e_s^\top \frac{\partial V}{\partial_{k,l}} e^{it_0\Lambda} \frac{\partial V^\top}{\partial_{k,l}} e_r +$$
$$2it_0 \left[e_s^\top \frac{\partial V}{\partial_{k,l}} \frac{\partial \Lambda}{\partial_{k,l}} e^{it_0\Lambda} V^\top e_r + e_s^\top V \frac{\partial \Lambda}{\partial_{k,l}} e^{it_0\Lambda} \frac{\partial V^\top}{\partial_{k,l}} e_r \right] +$$
$$it_0 e_s^\top V \frac{\partial^2 \Lambda}{\partial_{k,l}^2} e^{it_0\Lambda} V^\top e_r - t_0^2 e_s^\top V \left(\frac{\partial \Lambda}{\partial_{k,l}} \right)^2 e^{it_0\Lambda} V^\top e_r. \tag{13}$$

Next we observe that $e^{it_0\Lambda}V^\top e_r = (\alpha+i\beta)V^\top e_s$, $e_s^\top \frac{\partial^2 V}{\partial^2_{k,l}} V^\top e_s = -e_s^\top \frac{\partial V}{\partial_{k,l}} \frac{\partial V^\top}{\partial_{k,l}} e_s$, and $e_r^\top \frac{\partial^2 V}{\partial^2_{k,l}} V^\top e_r = -e_r^\top \frac{\partial V}{\partial_{k,l}} \frac{\partial V^\top}{\partial_{k,l}} e_r$, the last two equalities following from the fact that $V^\top e_s$ and $V^\top e_r$ are constrained to have norm 1. Using those observations in conjunction with (13), and simplifying, it now follows that

$$\alpha \frac{\partial^2 x(t_0)}{\partial^2_{k,l}} + \beta \frac{\partial^2 y(t_0)}{\partial^2_{k,l}} =$$

$$-\left[e_s^\top \frac{\partial V}{\partial_{k,l}} \frac{\partial V^\top}{\partial_{k,l}} e_s + e_r^\top \frac{\partial V}{\partial_{k,l}} \frac{\partial V^\top}{\partial_{k,l}} e_r + t_0^2 e_s^\top V \left(\frac{\partial \Lambda}{\partial_{k,l}} \right)^2 V^\top e_s \right]$$

$$+2\alpha e_s^\top \frac{\partial V}{\partial_{k,l}} \cos(t_o \Lambda) \frac{\partial V^\top}{\partial_{k,l}} e_r +$$

$$2\beta e_s^\top \frac{\partial V}{\partial_{k,l}} \sin(t_o \Lambda) \frac{\partial V^\top}{\partial_{k,l}} e_r.$$

Assembling the various component pieces and simplifying now yields (12). □

Our next example illustrates the effect of an edge weight perturbation in the case of periodic perfect state transfer.

Example 3.11 Here we consider the matrix B given by

$$B = \begin{bmatrix} 0 & \sqrt{5} & 0 & 0 & 0 & 0 \\ \sqrt{5} & 0 & \sqrt{8} & 0 & 0 & 0 \\ 0 & \sqrt{8} & 0 & 2.95 & 0 & 0 \\ 0 & 0 & 2.95 & 0 & \sqrt{8} & 0 \\ 0 & 0 & 0 & \sqrt{8} & 0 & \sqrt{5} \\ 0 & 0 & 0 & 0 & \sqrt{5} & 0 \end{bmatrix},$$

which can be thought of as a perturbation of the matrix A in Example 2.6 (where the weight of the edge $3 \sim 4$ has been changed from 3 to 2.95). Note that for the matrix A, there is perfect state transfer from vertex 1 to vertex 6 at any time of the form $(j - \frac{1}{2})\pi, j \in \mathbb{N}$. Thus, for $U(t) = e^{itA}$ and $p(t) = |u_{1,6}(t)|^2$, we have $p((j - \frac{1}{2})\pi) = 1$ for $j \in \mathbb{N}$.

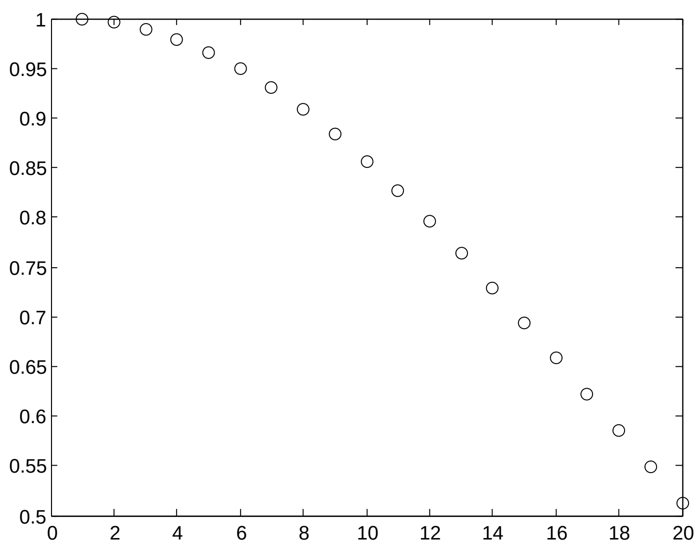

Figure 1: $\tilde{p}((j-\frac{1}{2})\pi)$ in Example 3.11 for $j=1,\ldots,20$

Next, we set $\tilde{U}(t) = e^{itB}$ and $\tilde{p}(t) = |\tilde{u}_{1,6}(t)|^2$. Referring to (12), we see that $\frac{\partial^2 p(t)}{\partial^2_{3,4}}|_{t=(j-\frac{1}{2})\pi}$ is nonincreasing in j, and consequently we expect the values of $\tilde{p}((j-\frac{1}{2})\pi)$ to drift away from 1 as j increases. Figure 1 illustrates that phenomenon for values of j between 1 and 20.

Next, we show how, even in the context of an unweighted graph admitting perfect state transfer, different edges can yield varying second order derivatives of the fidelity of transfer.

Example 3.12 Once again, we consider the graph $K_n \setminus e$ of Examples 2.7 and 3.1. Recall that if $n \equiv 0 \mod 4$, and e is the edge between vertices 1 and 2, then letting L be the Laplacian matrix and $U(t) = e^{itL}$, we have $p(\frac{\pi}{2}) = 1$, where $p(t) = |u(t)_{1,2}|^2, t > 0$. It is readily determined that in fact $u(\frac{\pi}{2})_{1,2} = 1 \equiv \alpha + i\beta$. Our goal in the present example is to compute $\frac{\partial^2 p(\frac{\pi}{2})}{\partial^2_{k,l}}$ for the pairs $(k,l) \in \{(1,2),(1,3),(3,4)\}$.

Case 1, $(k,l) = (1,2)$: From Example 3.1 we find that the desired orthogonal eigenmatrix V can be taken to be given as follows

$$Ve_1 = \frac{1}{\sqrt{n}}\mathbf{1}_n, Ve_2 = \frac{1}{\sqrt{2}}(e_1 - e_2), Ve_3 = \frac{1}{\sqrt{2n(n-2)}}\left[\begin{array}{c} -(n-2)\mathbf{1}_2 \\ \hline 2\mathbf{1}_{n-2} \end{array}\right],$$

$$Ve_{k+3} = \frac{1}{\sqrt{k(k+1)}}\left[\begin{array}{c} 0_2 \\ \hline \mathbf{1}_k \\ \hline -k \\ \hline 0_{n-k-3} \end{array}\right], k = 1, \ldots, n-3.$$

Again referring to Example 3.1, we have $\frac{\partial \Lambda}{\partial_{1,2}} = diag(2e_2)$, and $E = (e_1 - e_2)(e_1 - e_2)^\top$. We now find that $EV = \sqrt{2}(e_1 - e_2)e_2^\top$, from which it follows that $\frac{\partial V}{\partial_{1,2}} = 0$. (We note in passing that the matrices $-L^\dagger, ((n-2)I - L)^\dagger$, and $(nI - L)^\dagger$ are readily computed from the orthogonal idempotent decomposition of L given in Example 2.7.) Substituting into (12) now yields $\frac{\partial^2 p(\frac{\pi}{2})}{\partial^2_{1,2}} = -\frac{\pi^2}{2}$.

Case 2, $(k,l) = (1,3)$: In this case, our orthogonal eigenmatrix V can be taken to be as follows

$$Ve_1 = \frac{1}{\sqrt{n}}\mathbf{1}_n, Ve_2 = \frac{1}{\sqrt{2}}(e_1 - e_2), Ve_3 = \frac{1}{\sqrt{6}}(e_1 + e_2 - 2e_3),$$

$$Ve_{k+3} = \frac{1}{\sqrt{(k+2)(k+3)}} \left[\begin{array}{c} \mathbf{1}_2 \\ \hline \mathbf{1}_k \\ \hline -(k+2) \\ \hline 0_{n-k-3} \end{array}\right], k = 1, \dots, n-3.$$

From Example 3.1, we have $\frac{\partial \Lambda}{\partial_{1,3}} = diag(\begin{bmatrix} 0 & \frac{1}{2} & \frac{3}{2} & 0 & \dots & 0 \end{bmatrix})$, and $E = (e_1 - e_3)(e_1 - e_3)^\top$. We now find that the second column of EV is $\frac{1}{\sqrt{2}}(e_1 - e_3)$, the third column of EV is $\frac{3}{\sqrt{6}}(e_1 - e_3)$, and all remaining columns of EV are zero. It follows that the second and third columns of $\frac{\partial V}{\partial_{1,3}}$ are given by $-\frac{1}{4\sqrt{2}}(e_1 + e_2 - 2e_3)$ and $\frac{3}{4\sqrt{6}}(e_1 - e_2)$, respectively, while all remaining columns of $\frac{\partial V}{\partial_{1,3}}$ are zero.

Substituting these various expressions into (12), now yields that $\frac{\partial^2 p(\frac{\pi}{2})}{\partial^2_{1,3}} = -\frac{\pi^2}{8} - 1$. It is straightforward to see that for each $j = 3, \dots, n$, we also have $\frac{\partial^2 p(\frac{\pi}{2})}{\partial^2_{1,j}} = -\frac{\pi^2}{8} - 1$.

Case 3, $(k,l) = (3,4)$: The orthogonal eigenmatrix V in question can be taken as follows

$$Ve_1 = \frac{1}{\sqrt{n}}\mathbf{1}_n, Ve_2 = \frac{1}{\sqrt{2}}(e_1 - e_2), Ve_3 = \frac{1}{\sqrt{2}}(e_3 - e_4),$$

$$Ve_4 = \frac{1}{\sqrt{2n(n-2)}} \left[\begin{array}{c} -(n-2)\mathbf{1}_2 \\ \hline 2\mathbf{1}_{n-2} \end{array}\right], Ve_{k+3} = \frac{1}{\sqrt{k(k+1)}} \left[\begin{array}{c} 0_2 \\ \hline \mathbf{1}_k \\ \hline -k \\ \hline 0_{n-k-3} \end{array}\right],$$
$$k = 2, \dots, n-3.$$

We have $E = (e_3 - e_4)(e_3 - e_4)^\top$, and $\frac{\partial \Lambda}{\partial_{3,4}} = diag(2e_3)$. Hence $EV = \sqrt{2}(e_3 - e_4)e_3^\top$, and it now follows that $\frac{\partial V}{\partial_{3,4}} = 0$.

Substitution into (12), shows that $\frac{\partial^2 p(\frac{\pi}{2})}{\partial^2_{3,4}} = 0$. It is straightforward to see that for $k, l = 3, \ldots, n$ with $k \neq l$, $\frac{\partial^2 p(\frac{\pi}{2})}{\partial^2_{k,l}} = 0$.

Thus we see that even though our weighting of $K_n \setminus e$ assigns every edge the same weight, the edges themselves have different influences on the fidelity of transfer at readout time $\frac{\pi}{2}$.

Our next two remarks analyse (12) in further detail.

Remark 3.13 Here we consider signs of the expressions appearing in (12). From the Cauchy–Schwarz inequality, we find that

$$\left(e_s^\top V \frac{\partial \Lambda}{\partial_{k,l}} V^\top e_s\right)^2 \leq$$
$$e_s^\top V \frac{\partial \Lambda}{\partial_{k,l}} (\frac{\partial \Lambda^\top}{\partial_{k,l}}) V^\top e_s e_s^\top V V^\top e_s =$$
$$e_s^\top V (\frac{\partial \Lambda}{\partial_{k,l}})^\top V^\top e_s.$$

We thus find that the coefficient of t_0^2 in (12) is nonpositive.

Let $b^\top = e_s^\top \frac{\partial V}{\partial_{k,l}}$ and $c^\top = e_s^\top \frac{\partial V}{\partial_{k,l}}$, and choose ω so that $\cos\omega = \alpha, \sin\omega = \beta$, so that $\alpha\cos(t_0\Lambda) + \beta\sin(t_0\Lambda) = \cos(t_0\Lambda + \omega I)$. We then have

$$e_s^\top \frac{\partial V}{\partial_{k,l}} \frac{\partial V^\top}{\partial_{k,l}} e_s + e_r^\top \frac{\partial V}{\partial_{k,l}} \frac{\partial V^\top}{\partial_{k,l}} e_r - 2e_s^\top \frac{\partial V}{\partial_{k,l}} \left(\alpha\cos(t_0\Lambda) + \beta\sin(t_0\Lambda)\right) \frac{\partial V^\top}{\partial_{k,l}} e_r =$$
$$b^\top b + c^\top c - 2b^\top \cos(t_0\Lambda + \omega I)c \geq b^\top b + c^\top c - 2\sqrt{b^\top b c^\top (\cos(t_0\Lambda + \omega I))^2 c} \geq$$
$$(\sqrt{b^\top b} - \sqrt{c^\top c})^2.$$

Consequently the constant term in (12) (i.e. the term not multiplying t_0^2) is also nonpositive.

Remark 3.14 Suppose that M is the Laplacian matrix of a weighted graph, and suppose that the hypothesis (and notation) of Theorem 3.10 hold. It is straightforward to see from (12) that

$$\left|\frac{\partial^2 p(t_0)}{\partial^2_{k,l}}\Big|_{t_0}\right| \le 2t_0^2 e_s^\top V \left(\frac{\partial \Lambda}{\partial_{k,l}}\right)^2 V^\top e_s + 2\left(\sqrt{e_s^\top \frac{\partial V}{\partial_{k,l}}\frac{\partial V^\top}{\partial_{k,l}} e_s} + \sqrt{e_r^\top \frac{\partial V}{\partial_{k,l}}\frac{\partial V^\top}{\partial_{k,l}} e_r}\right)^2.$$

As in Remark 3.5 we find that $e_s^\top V \left(\frac{\partial \Lambda}{\partial_{k,l}}\right)^2 \le \rho((e_k - e_l)(e_k - e_l)^\top)^2 = 4.$ Also, denoting the distinct eigenvalues of M by $\lambda_1, \ldots, \lambda_m$, we find, again from Remark 3.5, that

$$e_s^\top \frac{\partial V}{\partial_{k,l}}\frac{\partial V^\top}{\partial_{k,l}} e_s \le 4\sum_{j=1}^m \frac{1}{\min_{p\ne j}(\lambda_j - \lambda_p)^2}.$$

We thus deduce that

$$\left|\frac{\partial^2 p(t_0)}{\partial^2_{k,l}}\Big|_{t_0}\right| \le 8t_0^2 + 32\sum_{j=1}^m \frac{1}{\min_{p\ne j}(\lambda_j - \lambda_p)^2}.$$

Remark 3.15 Suppose that M is the adjacency matrix of a weighted graph, and that the hypothesis (and notation) of Theorem 3.10 hold. Parallelling 3.5, we want to provide an upper bound on $\left|\frac{\partial^2 p(t_0)}{\partial^2_{k,l}}\Big|_{t_0}\right|$. As in Remark 3.5 we find that $e_s^\top V \left(\frac{\partial \Lambda}{\partial_{k,l}}\right)^2 V^\top e_s \le (\rho(e_k e_l^\top + e_l e_k^\top)^\top)^2 = 1$. From Remark 3.6, we find that

$$e_s^\top \frac{\partial V}{\partial_{k,l}}\frac{\partial V^\top}{\partial_{k,l}} e_s \le 2(1+\delta)^2\sum_{j=1}^m \frac{1}{\min_{p\ne j}(\lambda_j - \lambda_p)^2},$$

where $\lambda_1, \ldots, \lambda_m$ are the distinct eigenvalues of M, and δ is as defined in Remark 3.6. From the observations above, we thus find that

$$\left|\frac{\partial^2 p(t_0)}{\partial^2_{k,l}}\Big|_{t_0}\right| \le 2t_0^2 + 16(1+\delta)^2\sum_{j=1}^m \frac{1}{\min_{p\ne j}(\lambda_j - \lambda_p)^2}.$$

We close the paper by considering a couple of examples of graphs for which there is not perfect state transfer, but instead, a variant known as pretty good state transfer: a weighted graph exhibits *pretty good state transfer* between vertices s and r if, for any $\epsilon > 0$, there is a time t such that the fidelity of transfer from s to r at time t exceeds $1 - \epsilon$. The main result of [12] is that for an unweighted path on n vertices, when the adjacency matrix is used as the Hamiltonian, there is pretty good state transfer from one end point of the path to the other if and only if $n + 1$ is prime, twice a prime, or a power of two. Some of the techniques developed in this section allow us to compute the first two derivatives of the fidelity of transfer even in the absence of perfect state transfer, as the following two examples illustrate.

Example 3.16 Consider the unweighted path on six vertices, whose adjacency matrix A can be written as

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}.$$

From [12], there is pretty good state transfer between vertices 1 and 6. In particular, a computation on MATLAB® shows that for $\hat{t} \approx 356.5$ we have $p(\hat{t}) \approx 0.9995$. Using (11) to find $\frac{\partial p(\hat{t})}{\partial_{3,4}}$, we find from a MATLAB® computation that $\frac{\partial p(\hat{t})}{\partial_{3,4}} \approx 1.5576$. In view of the modest size of this derivative, one might imagine that the fidelity of state transfer from vertex 1 to vertex 6 at time $\hat{t}$ will not be especially sensitive to small changes in the weight of the edge between vertices 3 and 4.

To test that intuition, we next consider the effect of perturbing the weight of the edge between vertices 3 and 4. To that end, set

$$B_w = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & w & 0 & 0 \\ 0 & 0 & w & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix},$$

$U_w(t) = e^{itB_w}$ and $p_w(t) = |u_w(t)_{1,6}|^2$. Figure 2 plots $p(t)$ (equivalently, $p_1(t)$) and $p_w(t), t \in [355, 358]$ for the values $w = 0.999, 0.997, 0.995$. Not surprisingly, we see a decay from the value of $p(\hat{t})$ as w decreases through the values $0.999, 0.997, 0.995$, with the following computed values: $p_{0.999}(\hat{t}) \approx 0.9851, p_{0.997}(\hat{t}) \approx 0.8837$, and $p_{0.995}(\hat{t}) \approx 0.7076$. The modest size of $\frac{\partial p(\hat{t})}{\partial_{3,4}}$ does not account for much of the discrepancy between $p(\hat{t})$ and $p_{0.995}(\hat{t})$. Thus it may be instructive to consider $\frac{\partial^2 p(\hat{t})}{\partial^2_{3,4}}$.

Setting $x(t) = \mathfrak{Re}\left((e^{itA})_{1,6}\right)$ and $y(t) = \mathfrak{Im}\left((e^{itA})_{1,6}\right)$, we have

$$\frac{\partial^2 p(\hat{t})}{\partial^2_{3,4}} = 2\left[x(\hat{t})\frac{\partial^2 x(\hat{t})}{\partial^2_{3,4}} + y(\hat{t})\frac{\partial^2 y(\hat{t})}{\partial^2_{3,4}} + \left(\frac{\partial x(\hat{t})}{\partial_{3,4}}\right)^2 + \left(\frac{\partial y(\hat{t})}{\partial_{3,4}}\right)^2\right]. \tag{14}$$

Evidently we need the first and second order partial derivatives of x and y, and (10) supplies the necessary first order derivatives. Inspecting (13), we find that in order to find the desired second order partial derivatives, we need to compute the second partial derivatives (with respect to the weight of the edge between vertices 3 and 4) of the eigenvalues as well as the eigenvectors.

The derivation of the expressions for those second partial derivatives is facilitated by the fact that the eigenvalues of any tridiagonal matrix are all simple. Letting λ, v be an analytic (with respect to w) eigenvalue–eigenvector pair, and denoting $e_3 e_4^\top + e_4 e_3^\top$ by E, we find readily that

$$(\lambda I - B_1)\frac{\partial^2 v}{\partial^2_{3,4}}\Big|_{w=1} = 2\left(E - \frac{\partial \lambda}{\partial_{3,4}}\Big|_{w=1} I\right)\frac{\partial v}{\partial_{3,4}}\Big|_{w=1} - \frac{\partial \lambda^2}{\partial^2_{3,4}}\Big|_{w=1} v.$$

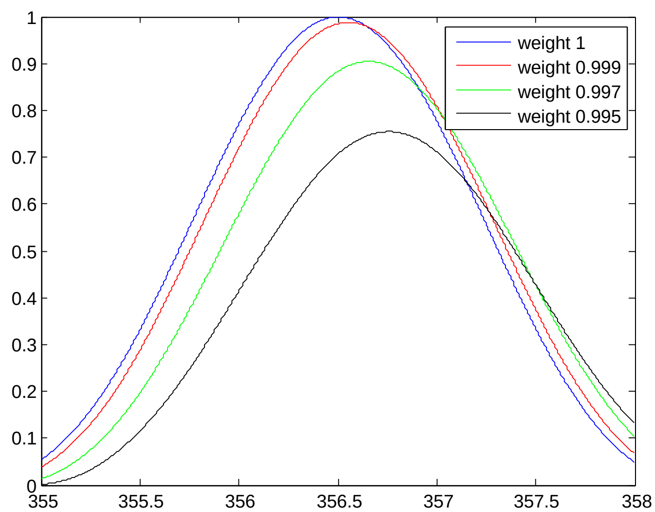

Figure 2: fidelities of transfer in Example 3.16 for $t \in [355, 358]$ with four weightings of the edge $3 \sim 4$

From the fact that $v^\top \frac{\partial v}{\partial_{3,4}}\Big|_{w=1} = 0$ (since we are taking $v^\top v = 1$) it now follows that $\frac{\partial \lambda^2}{\partial^2_{3,4}}\Big|_{w=1} = 2v^\top E \frac{\partial v}{\partial_{3,4}}\Big|_{w=1}$ and that

$$\frac{\partial^2 v}{\partial^2_{3,4}}\Big|_{w=1} = -\left(\frac{\partial v}{\partial_{3,4}}\Big|_{w=1}^\top \frac{\partial v}{\partial_{3,4}}\Big|_{w=1}\right) + (\lambda I - B_1)^\dagger 2 \left(E - \frac{\partial \lambda}{\partial_{3,4}}\Big|_{w=1} I\right) \frac{\partial v}{\partial_{3,4}}\Big|_{w=1}.$$

Computing the various first and second order partial derivatives in MATLAB®, and substituting them into (14) now yields that $\frac{\partial^2 p(\hat{t})}{\partial^2_{3,4}} \approx -25,920.5$. In particular, this example indicates that first partial derivatives may not be enough to explain the effect of even small perturbations in edge weights, and that higher order derivatives may also play a significant role.

Example 3.17 Here we consider the unweighted path on 15 vertices, with all edge weights equal to 1. Again we have pretty good state transfer from vertex 1 to vertex 15. Set $U(t) = e^{itA}$, where A is the corresponding adjacency matrix, and let $p(t) = |u_{1,15}(t)|^2$. For $\hat{t} = 33,535.1$, a MATLAB® computation yields $p(\hat{t}) \approx 0.9610$.

Suppose that vertex 1 is an end point of the path, and that vertex 2 is adjacent to it. We now consider the effect of perturbing the weight of the edge between vertices 1 and 2. Following the approach of Example 3.16 to compute the first two partial derivatives of the fidelity of transfer with respect to the weight of the edge between vertices 1 and 2, we find that $\frac{\partial p(\hat{t})}{\partial_{1,2}} \approx 393.9$ and $\frac{\partial^2 p(\hat{t})}{\partial^2_{1,2}} \approx -41,815,858.7$. This suggests that the fidelity of transfer at time $\hat{t}$ may be quite sensitive to the weight of the edge between vertices 1 and 2. That notion is reinforced by Figure 3.17, which plots the fidelity of transfer for $t \in [33534, 33536]$ for the cases that the edge weight for $1 \sim 2$ is taken as $1, 0.9999, 0.9995$, and 0.999, respectively. As further evidence of this sensitivity, we note that the approximate values of the fidelity of transfer at $\hat{t}$ for the $1 \sim 2$ edge weights $0.9999, 0.9995$, and 0.999, are $0.7357, 0.1266$ and 0.0595, respectively.

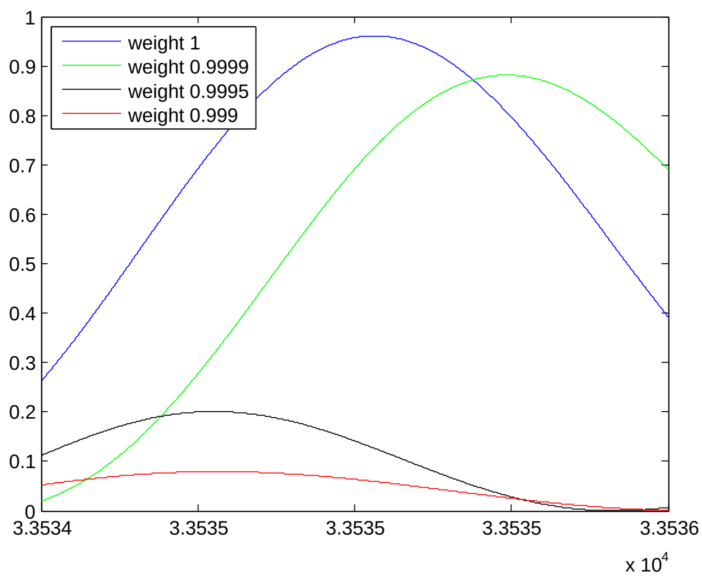

Figure 3: fidelities of transfer in Example 3.17 for $t \in [33534, 33536]$ with four weightings of the edge $1 \sim 2$

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