Spectral Graph Drawing: A Survey

Elissa Ross

Department of Mathematics Simon Fraser University, Burnaby, BC, Canada elissa@cecm.sfu.ca

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Abstract

We give an overview of graph drawing techniques as discussed by Godsil/Royle, Koren and Pisanski/Shawe-Taylor. These techniques employ the eigenvectors of the Laplacian matrix to create an *n*-dimensional representation of an undirected graph.

Keywords: Spectral graph drawing, Laplacian, Algebraic graph theory.

1 Introduction

In this paper, we will discuss methods of graph drawing that employ the eigenvectors of the Laplacian matrix to generate a representation of a graph. This representation can be generalized to n dimensions, but we are usually interested in drawing in either 2 or 3 dimensions. A basic technique will be outlined in detail, and then two further results due to Pisanski/Shawe-Taylor and Koren respectively will be discussed. These results give insight into the relations between the structure of the eigenspaces of the Laplacian matrix with the resulting embedding of that graph.

2 Definitions and Background Results

2.1 Matrices associated with graphs

Let X be a graph on n vertices, with vertex set V(X) and edge set E(X). Assume that X has no loops or multiple edges. We may also assume that X is connected. The **adjacency matrix**, A(X) of a directed graph X is the $n \times n$ matrix where the uv-entry of A(X) is equal to the number of arcs from u to v. For an undirected graph X, the adjacency matrix is just the symmetric $n \times n$ matrix, where

$$A_{uv} = \begin{cases} 0 & \text{when } u = v \text{ or } u \text{ is not adjacent to } v \\ 1 & \text{when } u \text{ is adjacent to } v \end{cases}$$

The **characteristic polynomial** of A is $\phi(A, x) = det(xI - A)$. The zeros of this polynomial are the **eigenvalues** of the matrix and the **spectrum** is the list of its eigenvalues together with their multiplicities. Two graphs are **cospectral** if they have the same characteristic polynomial and spectrum. The spectrum of a graph is an invariant of the isomorphism class, although the spectrum does not determine its isomorphism class. For instance, the valencies of the vertices are not determined by the spectrum, nor is whether or not the graph is planar.

The **incidence matrix**, D(X) of an graph X is the 01-matrix with rows indexed by the vertices of X, columns indexed by the edges of X, such that the uf-entry of D(X),

$$D(X)_{uf} = \begin{cases} 1 & \text{iff the vertex } u \text{ is in the edge } f \\ 0 & \text{otherwise} \end{cases}$$

The incidence matrix $D(X^{\sigma})$ of an oriented graph X^{σ} is the $\{0, \pm 1\}$ -matrix with indices as above such that

$$D(X^{\sigma})_{uf} = \begin{cases} 1 & \text{if the vertex } u \text{ is the head of the edge } f \\ -1 & \text{if the vertex } u \text{ is the tail of the edge } f \\ 0 & \text{otherwise} \end{cases}$$

The **Laplacian** matrix, $Q(X^{\sigma})$ is the matrix $Q(X) = DD^{T}$. Note that the Laplacian matrix does not depend on the orientation, σ .

The Laplacian can also be defined alternatively. Let Δ be the $n \times n$ matrix (where n = |V(X)|) with nonzero diagonal entries:

$$\Delta_{vv} = \sum_{u:(u,v)\in E(X)} A_{uv}$$

where A is the adjacency matrix of X. Then the Laplacian is defined by $Q(X) = \Delta - A$. So the entries of the Laplacian are given by,

$$Q(X)_{uv} = \begin{cases} \deg(\mathbf{u}) & u = v \\ -A_{uv} & u \neq v \end{cases}$$

Some properties of the Laplacian:

- Q is a real, symmetric matrix \Rightarrow its n eigenvalues are real, and \mathbb{R}^n has an orthogonal basis consisting of eigenvectors of Q
- $Q = DD^T \Rightarrow$ it is positive semidefinite and its eigenvalues are nonnegative
- $j = (1, 1, ..., 1)^T \in \mathbb{R}^n$ is an eigenvector of Q with eigenvalue 0.
- ullet The multiplicity of the zero eigenvalue is equal to the number of connected components of X.

Denote the eigenvalues of Q by $\lambda_1(Q), \ldots, \lambda_n(Q)$. Assume that

$$\lambda_1 \le \lambda_2 \le \dots \le \lambda_n$$

Note that $\lambda_1(Q) = 0$ for any graph. For connected graphs, $\lambda_2(Q)$ is the smallest non-zero eigenvalue.

If X is a regular graph, then the eigenvalues of the Laplacian are related to those of the adjacency matrix:

Lemma 1 Let X be a regular graph with valency k. If the adjacency matrix A(X) has eigenvalues $\theta_1, \ldots, \theta_n$, then the Laplacian Q(X) has eigenvalues $k - \theta_1, \ldots, k - \theta_n$.

Proof. X is k-regular $\Rightarrow Q = \Delta - A$, where $\Delta = kI$. $\Rightarrow Q = kI - A$.

 \Rightarrow every eigenvector of A with eigenvalue θ is also an eigenvector of Q with eigenvalue $k-\theta$.

2.2 Representations of a graph

A representation ρ of a graph X in \mathbb{R}^m is a map

$$\rho: V(X) \mapsto \mathbb{R}^m$$

We can think of the vectors $\rho(u)$, where $u \in V(X)$, as row vectors, and we can represent ρ by the $|V(X)| \times m$ matrix R, with the images of the vertices under ρ as its rows.

A representation ρ is called **balanced** if

$$\sum_{u \in V(X)} \rho(u) = 0$$

In other words, ρ is balanced if and only if $j^T R = 0$, where j = (1, 1, ..., 1). A balanced representation has its centre of gravity at the origin. For the

remainder of this paper, we will assume that a representation is balanced, and that the columns of R are linearly independent. If a representation is not in this condition, it can be translated or shifted into a lower dimensional embedding. Representations in 2 or 3 dimensions are what we are principally concerned with in this paper, and could be called drawings.

2.3 Energy of a representation

Suppose we have a weight function, $w : E(X) \mapsto \mathbb{R}^+$. Let ||x|| denote the Euclidean length of a vector, x. Define the **energy** $\mathcal{E}(P)$ of the representation ρ to be

$$\mathcal{E}(\rho) = \sum_{uv \in E(X)} w_{uv} \|\rho(u) - \rho(v)\|^2$$

In other words, we define energy as the squared norm of weighted distances between nodes.

Let W be the diagonal matrix with rows and columns indexed by the edges of X and with the diagonal entry corresponding to the edge uv equal to the value of w on that edge. Then we have

Lemma 2 Let ρ be a representation of the edge-weighted graph given by the $|V(X)| \times m$ matrix R. If D is an oriented incidence matrix for X, then $\mathcal{E}(\rho) = tr(R^T D W D^T R)$

Proof. Consider D^TR . It has rows indexed by the edges of X. The uv-row of $D^TR = \pm (\rho(u) - \rho(v))$. Consequently, the diagonal entries of $(D^TR)(D^TR)^T = D^TRR^TD$ have the form $\|\rho(u) - \rho(v)\|^2$. Then $\mathcal{E}(\rho) = tr(WD^TRR^TD) = tr(R^TDWD^TR)$, as required.

Note that $R^T DWD^T R$ is a $m \times m$ symmetric matrix, so it has real eigenvalues. Recall that the sum of the eigenvalues is the trace of the matrix, so the energy of the representation is given by the sum of the eigenvalues of $R^T DWD^T R$.

We can think of $Q = DWD^T$ as a weighted Laplacian.

$$Q_{uv} = \begin{cases} -w_{uv} & u \neq v \\ \sum_{u \sim v} w_{uv} & u = v \end{cases}$$

Our lemma becomes:

$$\mathcal{E}(\rho) = tr(R^T Q R)$$

The matrix R of representation ρ is called an **orthogonal** representation if the columns of R are orthogonal to each other, and each column has norm 1. In this situation, R satisfies $R^T R = I_m$.

Lemma 3 Let M be a real symmetric $n \times n$ matrix. If R is an $n \times m$ matrix such that $R^T R = I_m$, then $tr(R^T M R)$ is less than or equal to the sum of the m largest eigenvalues of M. Equality holds if and only if the column space of R is spanned by eigenvectors belonging to these eigenvalues.

3 Spectral Graph Drawing

3.1 The basic graph drawing problem

The basic method of graph drawing using the spectrum of the Laplacian matrix is outlined by Godsil in [1]. Recall that we have defined the energy of a representation to be the weighted sum of squared distances between nodes. We can formulate the most simple graph drawing problem as an attempt to find a representation $\rho: |V(X)| \mapsto \mathbb{R}^m$ that minimizes this energy.

Theorem 4 Let X be a graph on n vertices with weighted Laplacian Q. Assume that the eigenvalues of Q are $\lambda_1 \leq \ldots \leq \lambda_n$, and that $\lambda_2 > 0$. Then the minimum energy of a balanced orthogonal representation of X in \mathbb{R}^m is

$$\sum_{i=2}^{m+1} \lambda_i$$

Proof. By Lemma 2 we have that $\mathcal{E}(\rho) = tr(R^T Q R)$. Take the columns of R to be vectors x_1, \ldots, x_l , where $Qx_i = \lambda_i x_i$. By Lemma 3, the energy of an orthogonal representation in \mathbb{R}^{ℓ} is bounded below by the sum of the ℓ smallest eigenvalues of Q. Now since $\lambda_2 > 0 \Rightarrow x_1 = \mathbf{j} = (1, 1, \ldots, 1)^T$. Deleting x_1 yields a balanced, orthogonal representation in $\mathbb{R}^{\ell-1}$ with the same energy (since x_1 corresponds to $\lambda_1 = 0$).

Conversely, we can reverse this process to obtain an orthogonal representation in $\mathbb{R}^{\ell-1}$ such that the two representations have the same energy. Thus, the minimum energy of a balanced orthogonal representation of X in \mathbb{R}^m equals the minimum energy of an orthogonal representation in \mathbb{R}^{m+1} , and this minimum is

$$\lambda_2 + \cdots + \lambda_{m+1}$$

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This result implies an automatic graph drawing technique, assuming that representations with lower energies correspond to visually pleasing and comprehendible drawings of the graph. According to Theorem 4, we need only compute an orthonormal basis of eigenvectors x_1, \ldots, x_r , for the Laplacian Q. We then let the columns of our representation matrix, R be the first m non-zero eigenvectors of Q: x_2, \ldots, x_{m+1} . In practice, these drawings may or may not be aesthetically appealing. See figure 1 in the Appendix.

3.2 Pisanski

Pisanski and Shawe-Taylor develop this basic problem more thoroughly in [3]. They pose the graph drawing problem as a optimization problem.

Problem 1: Find a mapping $\rho: V(X) \mapsto \mathbb{R}^m$, which **minimizes** the following energy function:

$$\mathcal{E}(\rho) = \sum_{(u,v)\in E(X)} A_{uv} \|\rho(u) - \rho(v)\|^2 - \beta \sum_{(u,v)\notin E(X)} \|\rho(u) - \rho(v)\|^2$$

subject to the constraints:

$$\|\rho_i\| = 1, \rho_i \perp j, \text{ for } i = 1, \dots, k$$

 $\rho_i \perp \rho_j, \text{ for } 1 \leq i < j \leq k$

where β is a positive constant which determines the strength of the repulsive forces between non-adjacent vertices. Note that these constraints are equivalent to the previous requirement that the representation ρ be balanced and orthogonal.

Theorem 5 Let X be a connected graph on n vertices. The graph drawing problem stated above is solved by considering the weighted graph with adjacency matrix B, where

$$B_{uv} = \begin{cases} (A_{uv} + \beta) & if (u, v) \in E(G) \\ 0 & otherwise \end{cases}$$

Take the eigenvectors x_1, x_2, \ldots, x_n with corresponding eigenvalues $0 = \lambda_1 < \lambda_2 \leq \cdots \leq \lambda_n$ of the Laplacian matrix, $Q(B) = \Delta - B$. Then the optimal representation ρ is given by $\rho_i = x_{i+1}$, for $i = 1, \ldots, m$ and the minimal value of $\mathcal{E}(\rho)$ is

$$\sum_{\ell=2}^{m+1} \lambda_{\ell} - \beta nk$$

If $\lambda_{m+1} < \lambda_{m+2}$, then the optimal embedding is unique up to orthogonal transformations in \mathbb{R}^m .

Corollary 6 When the graph X is not weighted $(A_{uv} \in \{0,1\})$, the optimal representation does not depend on β .

This is the situation discussed by Godsil in [1]. The proof of Theorem 5 is a variation of the proof of Theorem 4, and will not be presented here.

This solution to the graph drawing problem requires that the output has a normalized variance along the coordinate axes, and that projections on to these axes are orthogonal. This means that all drawings generated by this method will be somewhat spherical, and will exhibit symmetry in variance along any axes. As a result, this technique breaks down for highly asymmetric or eccentric graphs.

In addition, Pisanski notes that the algorithm of Theorem 5 does not necessarily produce optimal results. For instance, when presented with a planar graph without crossings, it will not necessarily render the graph without intersections. See figure 2 in the Appendix.

According to Pisanski and Shawe-Taylor, one problem with the previous statement of the graph drawing problem is that we can specify attractive forces between vertices, but not repulsive ones between non-adjacent vertices. They remedy this by an alternative statement of the problem:

Problem 2: Find a mapping $\rho: V(X) \mapsto \mathbb{R}^m$, such that the following energy function:

$$\mathcal{E}(\boldsymbol{\rho}) = \sum_{(u,v) \in E(X)} A_{uv} |\rho(u)_i - \rho(v)_i|^2 - \beta \sum_{(u,v) \notin E(X)} |\rho(u)_i - \rho(v)_i|^2 = 1$$

for i = 1, ..., m, while maximizing the sum of the norms

$$\sum_{i=1}^{m} \|\boldsymbol{\rho}_i\|^2 = \sum_{u \in E(X)} \|\rho(u)\|^2$$

subject to the constraints:

$$\boldsymbol{\rho}_i \perp \boldsymbol{j}$$
, for $i = 1, \dots, k$

$$\rho_i \perp \rho_j$$
, for $1 \le i < j \le k$

where β is a positive constant which determines the strength of the repulsive forces between non-adjacent vertices.

This model allows the images of the vertices under ρ to have different norms, but specifies that a one unit of "wire" is available in each dimension. Changing the amount of wire available has a scaling effect on the drawing, so we can replace the number 1 by any constant. This alternative statement of the

problem allows for more control over the shape of the graph, and overcomes (to some extent) the spherical tendencies of the former definition. The solution to this problem is a variation on Theorem 5.

Pisanski and Shawe-Taylor also discuss the solution to a problem in which the graph edges are allowed to have negative weights. This solution is only a slight variation on Theorem 5. This type of problem may occur naturally in the rendering of chemical molecules, where certain bonds have different repelling strengths. The authors note that at times it is better not to use the eigenvectors that minimize the energy, and that alternative selection of eigenvectors may be favorable.

3.3 Koren

Koren states the the spectral graph drawing method has several advantages. He says that it provides us with an exact solution to the layout problem, while most other techniques result in an NP-hard problem that can only be approximated. In addition, he notes that spectral graph drawing is superior in terms of computation speed.

Koren states the problem in a slightly different way, by formulating a 1D layout (to be generalized to n-dimensions). Recall that by Lemma 2

$$\mathcal{E}(\rho) = tr(R^T Q R)$$

In one dimension, this is just

$$\mathcal{E}(x) = x^T Q x = \sum_{uv \in E(X)} w_{uv} (x(u) - x(v))^2$$

where x is the desired layout. The minimization problem can be described as:

$$\min_{x} x^{T}Qx$$
 given: $x^{T}x = 1$ in the subspace: $x^{T}\mathbf{j} = 0$

This is simply an alternative statement of our original problem, and Koren finds that the optimal solution to this problem is the smallest nonzero eigenvector of Q. He then generalizes the problem to n-dimensions, and his findings concur with Theorem 4.

3.3.1 The degree-normalized method

The main result of [2] is the introduction of the method of graph drawing by degree-normalized eigenvectors. This method weights nodes by their degrees: mass of node i = deg(i). Koren makes the following definition: given a degrees matrix Δ , the Laplacian Q, then a vector \mathbf{u} and a scalar μ are called **generalized eigen-pairs** of (Q, Δ) if $L\mathbf{u} = \mu\Delta \mathbf{u}$. By convention, let the generalized eigenvalues be $0 = \mu_1 < \mu_2 \le \cdots \le \mu_n$. To uniquely define $\mathbf{u}_1, \ldots, \mathbf{u}_n$, force $\mathbf{u}_i^T \Delta \mathbf{u}_i = 1, i = 1, \ldots, n$. Koren terms these vectors the **degree normalized eigenvectors**. He describes the following degree-weighted minimization problem:

$$\min_{x} x^{T} Q x$$

given:
$$x^T \Delta x = 1$$

in the subspace:
$$x^T \Delta j = 0$$

where Δ is the degrees matrix, and j = (1, ..., 1). Koren finds that the solution to this 1D optimization problem is $x = u_2$, the second smallest generalized eigenvector of (Q, Δ) . The resulting minimal energy is the corresponding generalized eigenvalue λ_2 . Again, Koren generalizes this result to n-dimensions, by defining the i-th coordinate of the representation to be u_{i+1} .

Koren rewrites the previous minimization statement as:

$$\min_{x} \frac{x^{T}Qx}{x^{T}\Delta x}$$

in the subspace:
$$x^T \Delta \mathbf{j} = 0$$

He notes that the numerator "wants" to put nodes of high degree at the center of the drawing, while the denominator attempts to enlarge the scatter of these same nodes. Koren asserts that the combination of these facts makes the drawing more balanced.

This method does not have any clear advantage over standard methods when the graph is regular or close to regular. However, when there is a large variation in node degree, the degree weighted method is superior. See Figure 3 in the Appendix.

3.3.2 Aesthetic connections

An interesting aspect of this method of spectral graph drawing is that it can be linked clearly to an aesthetic motivation. Let i be a node. Differentiating \mathcal{E} with respect to x(i) yields

$$\frac{\partial \mathcal{E}}{\partial x(i)} = 2 \sum_{j \sim i} w_{ij}(x(i) - x(j))$$

Setting this to zero and solving,

$$x(i) = \frac{\sum_{j \sim i} w_{ij} x(j)}{deg(i)}$$

This means that if we allow only node i to vary, the location of i that minimizes the energy is the weighted centroid of vertices adjacent to i.

Koren shows that this induces an optimization process that iteratively places each vertex and the weighted centroid of its neighboring vertices. He provides an algorithm for this purpose, that, when initialized with a vector satisfying $x^T \Delta j = 0$, converges in the direction of either u_2 or u_n . This means that starting with an aesthetic criteria - that each node should be placed at the centroid of its neighbors - yields the same solution as the energy minimization process.

In summary, Koren introduces the idea of drawing with degree normalized eigenvectors. He also links the Laplacian spectrum directly with an aesthetic analysis of a graph drawing. He does this by asserting that spectral methods place each vertex at the centroid of its neighbors, and that there is a well defined characterization of this fact.

4 Discussion and Conclusion

In conclusion, we have seen a variety of spectral graph drawing methods. At its most basic level, this method takes the m smallest non-zero eigenvectors of the Laplacian matrix of a graph X as the representations of each vertex of the graph in the embedding.

Pisanski and Shawe-Taylor attempt a refinement of this procedure to reduce the "spherical" tendencies of graphs produced using this method. The also consider a technique that would allow the adjacency matrix to have negative weights, thereby admitting both attractive and repulsive forces between vertices.

Koren also presents a refinement on the basic technique, and attempts to

characterize the aesthetic qualities of a rendering as a function of the Laplacian eigenspaces. He asserts that spectral methods place each node at the centroid of their neighbors, and gives some definition to how this actually occurs. In addition, he introduces the concept of drawing by degree-normalized eigenvectors, which shows a marked advantage over the standard method when the graph has a large variation in vertex degree.

One of the reasons that the spectral graph drawing method has not been entirely popular is that it is difficult to characterize the aesthetic aspects of the graphs from the Laplacian. It is clearly a promising technique due to its rapid computation times. Both papers focus on characterizing when the spectral approach is likely to perform well. However, it would be good if we could develop techniques to remedy the situations in which they will not produce good results. For instance, it would be nice if we could ensure that a planar graph would have no crossings in the rendering. In addition, the method would be more robust if we could draw non-symmetric graph without degeneration. Lastly, we know that at times it is better not to use the eigenvectors that minimize the energy, but rather use a selection of other eigenvectors. It would be useful to develop this idea to determine specifically when this is the case.

5 An Implementation of the Graph Drawing Procedure in Maple

This is an implementation of the basic method of graph drawing as outlined by Godsil in [1] that employs the eigenvectors of the Laplacian to generate an embedding of the graph in \mathbb{R}^3 .

5.1 The procedure

GraphDraw will draw a three dimensional plot of the graph. The parameters are A, the adjacency matrix of the graph, and a, b, c specify the choice of eigenvectors to be used for the embedding. In general, $1 < a, b, c \le n$. The use of (a, b, c) = (2, 3, 4) should generate an optimal embedding, but other choices of eigenvectors can also be effective.

```
> GraphDraw := proc(A, a, b, c) local deg, Deg, Q, v, e, n,i,j,
L, K, k, M, plotseq;
> n:=Dimension(A); n:=n[1];
> j:= Vector(1..n, 1);
> deg:= MatrixVectorMultiply(A,j);
> Deg:= Matrix(1..n,1..n,deg,shape=diagonal);
> Q:=Deg-A;
> K:=Evectorize(Q);
> M:= GramSchmidt([K[a], K[b], K[c]]);
> M:=convert(M, Matrix);
> L:=NULL;
> for i from 1 to n do for j to i do
> if A[i,j] <> 0 then
           [[M[i,1],M[i,2],M[i,3]],[M[j,1],M[j,2],M[j,3]]];
> L:=L,
> fi;
> od od;
> L:=[L]; #print(L);
> plotseq:=display(seq(pointplot3d(p, ambientlight=[0.9,0.9,0.9],
thickness=2,connect=true), p=L));
> display([%],axes=none, scaling=constrained, insequence=true,
orientation=[-90,0]);
   end proc;
```

Evectorize will prepare the Eigenvectors of the Laplacian

```
> Evectorize := proc(Q) local E, K, G, n,D,F;
> D:=Eigenvectors(Q, output='list');
> D:=sort(D,(t1,t2) -> evalb(convert(op(1,t1),float) <= convert(op(1,t2),float)))
> D:=convert(D,float);
> E:=(map(es -> op(3,es),D));
> F:=(map(es -> op(1,es),D)); print(F);
> G:= map(es -> op(2, es),D); print(G);
> n:=nops(E);
> K:= seq(E[i][], i=1..n);
> return(K);
> end proc:
```

5.2 The results



Figure 1: The cube drawn with (a, b, c) = (2, 3, 4)



Figure 2: the cube drawn with (a,b,c)=(2,3,8)



Figure 3: the dodecahedron drawn with (a,b,c)=(2,3,4)



Figure 4: the dodecahedron drawn with (a,b,c)=(2,5,11)



Figure 5: the octohedron drawn with (a,b,c)=(2,3,4)

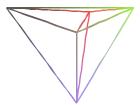


Figure 6: the complete graph on 8 vertices, C_n drawn with (a, b, c) = (2, 3, 4)

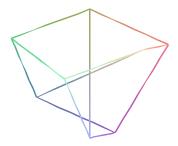


Figure 7: the Petersen graph drawn with (a,b,c)=(2,3,4)

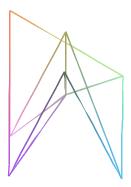


Figure 8: the Petersen graph drawn with (a,b,c)=(3,4,7)



Figure 9: the Petersen graph drawn with (a,b,c)=(7,8,9)

5.3 Remarks

Clearly, there problems with this procedure, and possibly with the implementation. Although it performs fairly well on the cube and the octohedron, it does not provide complete information for the Petersen graph, and fails entirely for the complete graphs.

References

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Appendix: Figures

Figure 10: Two examples of graphs drawn in \mathbb{R}^2 using the basic technique. The results are clearly variable. (from [1])

Figure 11: Two examples of graphs drawn using the variation of Pisanski and Shawe-Taylor. The first example illustrates that this technique does not guarantee planar results, even if the graph is planar. The buckminsterfullerene is a 2D projection of an embedding in \mathbb{R}^3 , and was drawn using the second, third and fourth eigenvectors. (from [3])

Figure 12: The visualization of 300 odors measured by an electronic nose. The traditional method (left) places most of the results at the same location, while the degree-normalized method (right) is more readable. (from [2])

Figure 13: These are good examples of the positive results of the spectral method. (from [2])