Chapter 2

Spectral Graph Drawing

2.1 Graph Drawing and Energy Minimization

Let $G = (V, E)$ be some undirected graph. It is often desirable to draw a graph, usually in the plane but possibly in 3D, and it turns out that the graph Laplacian can be used to design surprisingly good methods.

Say $|V| = m$. The idea is to assign a point $\rho(v_i)$ in $\mathbb{R}^n$ to the vertex $v_i \in V$, for every $v_i \in V$, and to draw a line segment between the points $\rho(v_i)$ and $\rho(v_j)$ iff there is an edge $\{v_i, v_j\}$.

Thus, a *graph drawing* is a function $\rho\colon V \to \mathbb{R}^n$.

We define the *matrix of a graph drawing ρ (in $\mathbb{R}^n$)* as a $m \times n$ matrix R whose ith row consists of the row vector $\rho(v_i)$ corresponding to the point representing v_i in $\mathbb{R}^n$.

Typically, we want $n < m$; in fact n should be much smaller than m.

A representation is *balanced* iff the sum of the entries of every column is zero, that is,

$$\mathbf{1}^\top R = 0.$$

If a representation is not balanced, it can be made balanced by a suitable translation.

We may also assume that the columns of R are linearly independent, since any basis of the column space also determines the drawing. Thus, from now on, we may assume that $n \leq m$.

Remark: A graph drawing $\rho\colon V \to \mathbb{R}^n$ is not required to be injective, which may result in degenerate drawings where distinct vertices are drawn as the same point.

For this reason, we prefer not to use the terminology *graph embedding*, which is often used in the literature. This is because in differential geometry, an embedding always refers to an injective map.

The term *graph immersion* would be more appropriate.

As explained in Godsil and Royle [7], we can imagine building a physical model of G by connecting adjacent vertices (in $\mathbb{R}^n$) by identical springs.

Then, it is natural to consider a *representation to be better if it requires the springs to be less extended*.

We can formalize this by defining the *energy* of a drawing R by

$$\mathcal{E}(R) = \sum_{\{v_i, v_j\} \in E} \|\rho(v_i) - \rho(v_j)\|^2,$$

where $\rho(v_i)$ is the ith row of R and $\|\rho(v_i) - \rho(v_j)\|^2$ is the square of the Euclidean length of the line segment joining $\rho(v_i)$ and $\rho(v_j)$.

Then, "good drawings" are drawings that minimize the energy function $\mathcal{E}$.

Of course, the trivial representation corresponding to the zero matrix is optimum, so we need to impose extra constraints to rule out the trivial solution.

We can consider the more general situation where the springs are not necessarily identical. This can be modeled by a symmetric weight (or stiffness) matrix $W = (w_{ij})$, with $w_{ij} \geq 0$.

Then our energy function becomes

$$\mathcal{E}(R) = \sum_{\{v_i, v_j\} \in E} w_{ij} \left\| \rho(v_i) - \rho(v_j) \right\|^2 .$$

It turns out that this function can be expressed in terms of the Laplacian $L = D - W$.

Proposition 2.1. *Let $G = (V, W)$ be a weighted graph, with $|V| = m$ and W an $m \times m$ symmetric matrix, and let R be the matrix of a graph drawing ρ of G in $\mathbb{R}^n$ (a $m \times n$ matrix). If $L = D - W$ is the unnormalized Laplacian matrix associated with W, then*

$$\mathcal{E}(R) = \mathrm{tr}(R^\top L R).$$

Since the matrix $R^\top LR$ is symmetric, it has real eigenvalues. Actually, since L is positive semidefinite, so is $R^\top LR$.

Then, the trace of $R^\top LR$ is equal to the sum of its positive eigenvalues, and this is the energy $\mathcal{E}(R)$ of the graph drawing.

If R is the matrix of a graph drawing in $\mathbb{R}^n$, then for any invertible matrix M, the map that assigns $\rho(v_i)M$ to v_i is another graph drawing of G, and these two drawings convey the same amount of information.

From this point of view, a graph drawing is determined by the column space of R. Therefore, it is reasonable to assume that the columns of R are pairwise orthogonal and that they have unit length.

Such a matrix satisfies the equation $R^\top R = I$, and the corresponding drawing is called an *orthogonal drawing*. This condition also rules out trivial drawings.

The following result tells us how to find minimum energy graph drawings, provided the graph is connected.

Theorem 2.2. *Let $G = (V, W)$ be a weigted graph with $|V| = m$. If $L = D - W$ is the (unnormalized) Laplacian of G, and if the eigenvalues of L are $0 = \lambda_1 < \lambda_2 \leq \lambda_3 \leq \ldots \leq \lambda_m$, then the minimal energy of any balanced orthogonal graph drawing of G in $\mathbb{R}^n$ is equal to $\lambda_2 + \cdots + \lambda_{n+1}$ (in particular, this implies that $n < m$). The $m \times n$ matrix R consisting of any unit eigenvectors $u_2, \ldots, u_{n+1}$ associated with $\lambda_2 \leq \ldots \leq \lambda_{n+1}$ yields a balanced orthogonal graph drawing of minimal energy; it satisfies the condition $R^\top R = I$.*

Observe that for any orthogonal $n \times n$ matrix Q, since

$$\mathrm{tr}(R^\top L R) = \mathrm{tr}(Q^\top R^\top L R Q),$$

the matrix RQ also yields a minimum orthogonal graph drawing.

Since $\mathbf{1}$ spans the nullspace of L, using u_1 (which belongs to $\mathrm{Ker}\, L$) as one of the vectors in R would have the effect that all points representing vertices of G would have the same first coordinate.

This would mean that the drawing lives in a hyperplane in $\mathbb{R}^n$, which is undesirable, especially when $n = 2$, where all vertices would be collinear. This is why we omit the first eigenvector u_1.

In summary, if $\lambda_2 > 0$, an automatic method for drawing a graph in $\mathbb{R}^2$ is this:

1. Compute the two smallest nonzero eigenvalues $\lambda_2 \leq \lambda_3$ of the graph Laplacian L (it is possible that $\lambda_3 = \lambda_2$ if λ_2 is a multiple eigenvalue);

2. Compute two unit eigenvectors u_2, u_3 associated with λ_2 and λ_3, and let $R = [u_2\, u_3]$ be the $m \times 2$ matrix having u_2 and u_3 as columns.

3. Place vertex v_i at the point whose coordinates is the ith row of R, that is, (R_{i1}, R_{i2}).

This method generally gives pleasing results, but beware that there is no guarantee that distinct nodes are assigned distinct images, because R can have identical rows.

2.2 Examples of Graph Drawings

We now give a number of examples using `Matlab`. Some of these are borrowed or adapted from Spielman [14].

Example 1. Consider the graph with four nodes whose adjacency matrix is

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

We use the following program to compute u_2 and u_3:

```
A = [0 1 1 0; 1 0 0 1; 1 0 0 1; 0 1 1 0];
D = diag(sum(A));
L = D - A;
[v, e] = eigs(L);
gplot(A, v(:,[3 2]))
hold on;
gplot(A, v(:,[3 2]),'o')
```

The graph of Example 1 is shown in Figure 2.1. It turns out that $\lambda_2 = \lambda_3 = 2$ is a double eigenvalue.

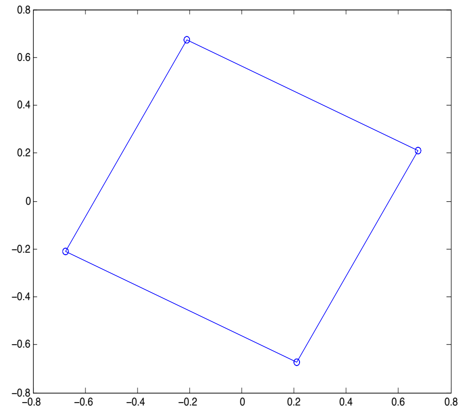

Figure 2.1: Drawing of the graph from Example 1.

Example 2. Consider the graph G_2 shown in Figure 1.2 given by the adjacency matrix

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

We use the following program to compute u_2 and u_3:

```
A = [0 1 1 0 0; 1 0 1 1 1; 1 1 0 1 0;
     0 1 1 0 1; 0 1 0 1 0];
D = diag(sum(A));
L = D - A;
[v, e] = eig(L);
gplot(A, v(:, [2 3]))
hold on
gplot(A, v(:, [2 3]),'o')
```

Note that node v_2 is assigned to the point $(0, 0)$, so the difference between this drawing and the drawing in Figure 1.2 is that the drawing of Figure 2.2 is not convex.

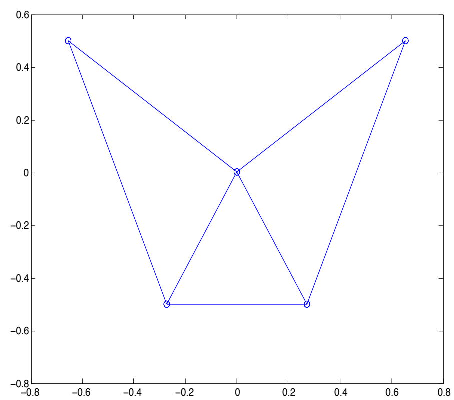

Figure 2.2: Drawing of the graph from Example 2.

Example 3. Consider the ring graph defined by the adjacency matrix A given in the `Matlab` program shown below:

```
A = diag(ones(1, 11),1);
A = A + A';
A(1, 12) = 1; A(12, 1) = 1;
D = diag(sum(A));
L = D - A;
[v, e] = eig(L);
gplot(A, v(:, [2 3]))
hold on
gplot(A, v(:, [2 3]),'o')
```

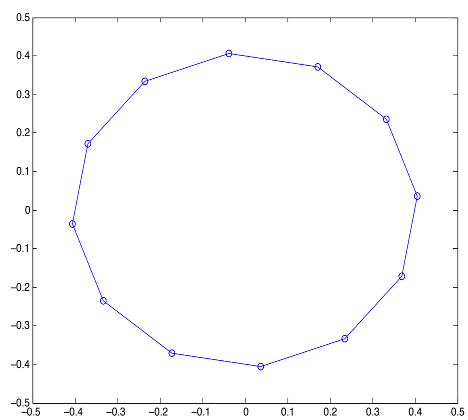

Figure 2.3: Drawing of the graph from Example 3.

Again $\lambda_2 = 0.2679$ is a double eigenvalue (and so are the next pairs of eigenvalues, except the last, $\lambda_{12} = 4$).

Example 4. In this example adpated from Spielman, we generate 20 randomly chosen points in the unit square, compute their Delaunay triangulation, then the adjacency matrix of the corresponding graph, and finally draw the graph using the second and third eigenvalues of the Laplacian.

```
A = zeros(20,20);
xy = rand(20, 2);
trigs = delaunay(xy(:,1), xy(:,2));
elemtrig = ones(3) - eye(3);
for i = 1:length(trigs),
 A(trigs(i,:),trigs(i,:)) = elemtrig;
end
A = double(A >0);
gplot(A,xy)
D = diag(sum(A));
L = D - A;
[v, e] = eigs(L, 3, 'sm');
figure(2)
gplot(A, v(:, [2 1]))
hold on
gplot(A, v(:, [2 1]),'o')
```

The Delaunay triangulation of the set of 20 points and the drawing of the corresponding graph are shown in Figure 2.4.

The graph drawing on the right looks nicer than the graph on the left but is is no longer planar.

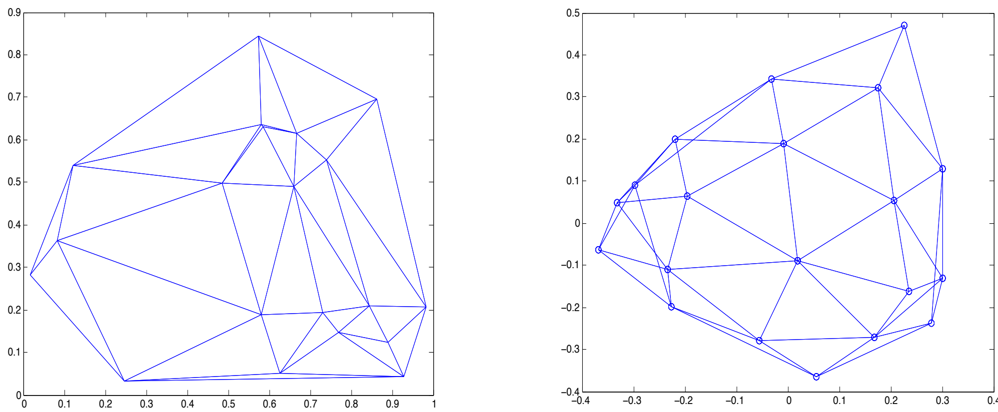

Figure 2.4: Delaunay triangulation (left) and drawing of the graph from Example 4 (right).

Example 5. Our last example, also borrowed from Spielman [14], corresponds to the skeleton of the "Buckyball," a geodesic dome invented by the architect Richard Buckminster Fuller (1895–1983).

The Montréal Biosphère is an example of a geodesic dome designed by Buckminster Fuller.

```
A = full(bucky);
D = diag(sum(A));
L = D - A;
[v, e] = eig(L);
gplot(A, v(:, [2 3]))
hold on;
gplot(A,v(:, [2 3]), 'o')
```

Figure 2.5 shows a graph drawing of the Buckyball. This picture seems a bit squashed for two reasons. First, it is really a 3-dimensional graph; second, $\lambda_2 = 0.2434$ is a triple eigenvalue. (Actually, the Laplacian of L has many multiple eigenvalues.) What we should really do is to plot this graph in $\mathbb{R}^3$ using three orthonormal eigenvectors associated with λ_2.

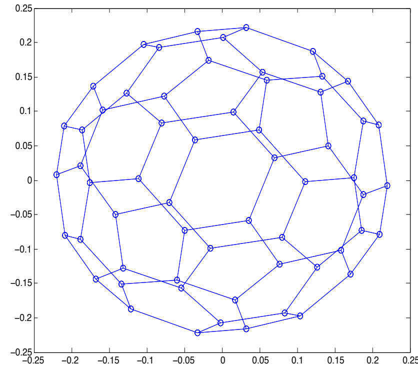

Figure 2.5: Drawing of the graph of the Buckyball.

A 3D picture of the graph of the Buckyball is produced by the following `Matlab` program, and its image is shown in Figure 2.6. It looks better!

```
[x, y] = gplot(A, v(:, [2 3]));
[x, z] = gplot(A, v(:, [2 4]));
plot3(x,y,z)
```

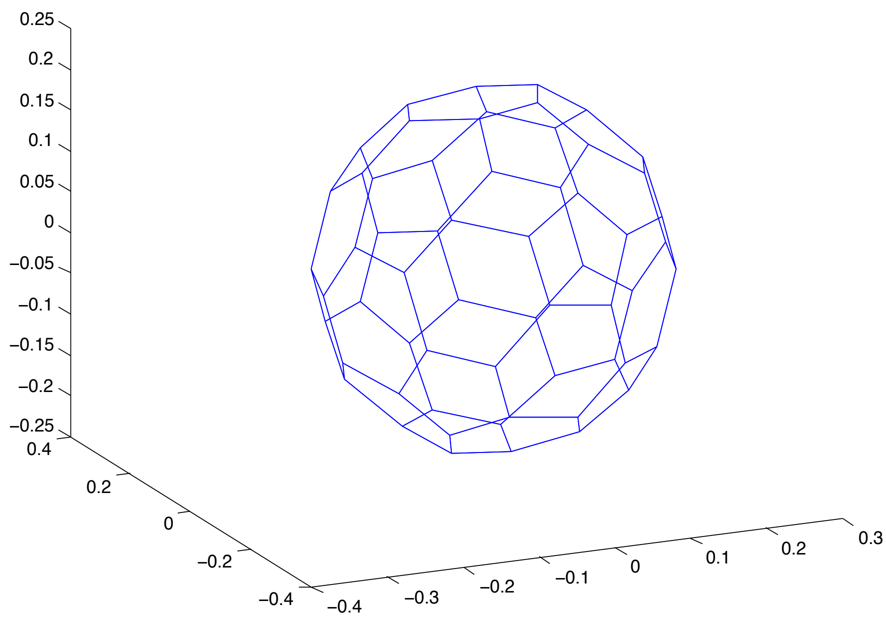

Figure 2.6: Drawing of the graph of the Buckyball in $\mathbb{R}^3$.