

Understanding Atmospheric Chemistry using Graph-Theory, Visualisation and Machine Learning.

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*Veritatem inquirenti, semel in vita de omnibus,
quantum fieri potest, esse dubitandum:*

*In order to seek truth, it is necessary once in the course of our life, to
doubt, as far as possible, of all things.*

- Descartes, Rene, *Principles of Philosophy*

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Chapter 1

Applying Visual Analytics to the Atmospheric Chemistry Network

“ I have a notion that when the mind is thinking, it is simply talking to itself, asking questions and answering them. ”

- Socrates, *The collected dialogues of Plato*

1.1 Introduction

?? viewed the importance of a carefully selected visualisation/metaphor in the representation of scientific data. One such category is that of relational data, where we have a set of items, joined by a chosen relationship. Historically this type of problem was solved using sociographs to present a set of items and the links between them.

This chapter begins by looking at the use of sociograms in chemistry (Subsection 1.1.2) and the different ways in which these can help convey information to the reader (Section 1.2, Section 1.4). These sections find the force-directed graph to be the most suited for representing the chemical reactions within a mechanism, and therefore this shall be applied to the network of reactions representing the chemistry within an urban environment - Beijing (Section 1.5).

1.1.1 Networks And Their Role In Visual Analytics

Networks are present everywhere - this ranges from interactions within social media to bank transactions, internet routing, genetics to epidemiology [Martin Grandjean, 2016; Staples et al., 2013; Needham and Hodler, 2019; Baronchelli et al., 2013; Sangers et al., 2019; Kohlbacher et al., 2014; Archambault et al., 2014; Schreiber et al., 2014]. The sociogram (or graph) structure can be applied to any set of items which contain one or more relationships between them. In visualisation, these ‘items’ are referred to as nodes/vertices, and their relationships as edges/links [Kerren et al., 2014] - terms that will be used interchangeably throughout this thesis.

1.1.2 Graphs In Chemistry

Node-link representations have been at the core of chemistry for many years. They have been used to show the bonds between atoms and are integral to the representation of molecules - both physically (with the aid of molecular model kits) or pictorially to show various structural properties (Figure 1.1). These graph-like analogies provide a pseudo-physical representation of the molecules and their reactions in a way that is intuitive to the user. Subsubsection 1.1.2.1 shows the use of a sociograph structure to represent reactions within the troposphere; however, this method of representation is not limited to atmospheric science - for example, Figure 1.3 depicts the biochemical metabolic pathways of the human body. This is an example of another complex chemical network that benefits from this method of representation.

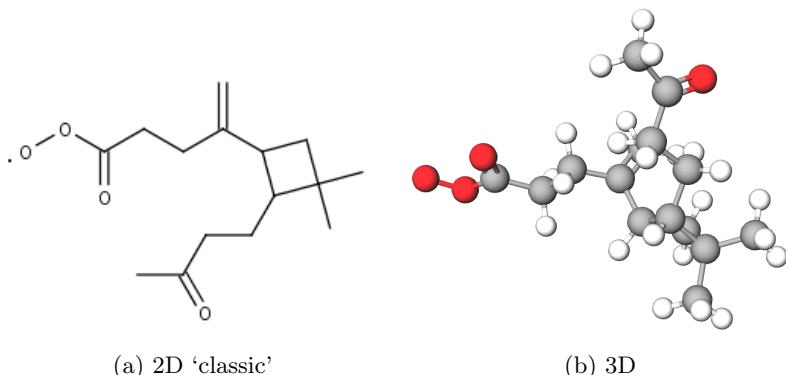


Figure 1.1: **The molecule $C_{141}CO_3$ shown in both 2D and 3D node-link structures.** This is a the result of a series of inorganic species reactions and a desociation from BCARY - the only sesqueterpine in the MCM. 3D visualisation by [Bergwerf, 2019].

1.1.2.1 Using Sociograms To Describe Reactions

A collection of reactions representing the chemistry of a region is called a mechanism. The Master Chemical Mechanism [?] provides a collection of equations describing the gas-phase chemistry which exists within the troposphere (??). In its use in policy, and the evaluation of Air Quality Models ([Dick Derwent, 2010]), it is often useful to understand the degradation process different VOCs undergo. In general, this can be achieved through a series of interconnected reactions in the form of a reaction cycle (Figure 1.2). This type of sociograph shows the directional nature of chemical reactions and the relationships between different species. This has many similarities to a conventional directed graph, except that species (nodes) are sometimes duplicated (for example OH, HO₂, O₂ in Figure 1.2) to aid in the clarity of the figure.

This provides an excellent example of how the flow-like nature of a sociogram aids in the understanding of a potentially complex chemical system of 171 organic species and 600 reactions. Evolutionary traits, including the genetic predisposition to interpret shapes faster than text ([Harari, 2015]) make the graph structure a much better method for representing such a system.

1.1.3 Modeling Chemistry As A Directed Graph.

Historically it is shown that the graph format has proven to be an efficient means of understanding the reactions within a mechanism. Traditionally these are constructed manually, with the designer making a series of choices on how best to place, and simplify the chemistry based on their application. As our understanding of chemistry improves and we have started to progress into automated and semi-automated mechanism construction. This makes the construction of mechanisms with tens of millions of species and billions of reaction possible ([Aumont et al., 2005]) and is the point where the manual design/simplification of reaction networks becomes infeasible.

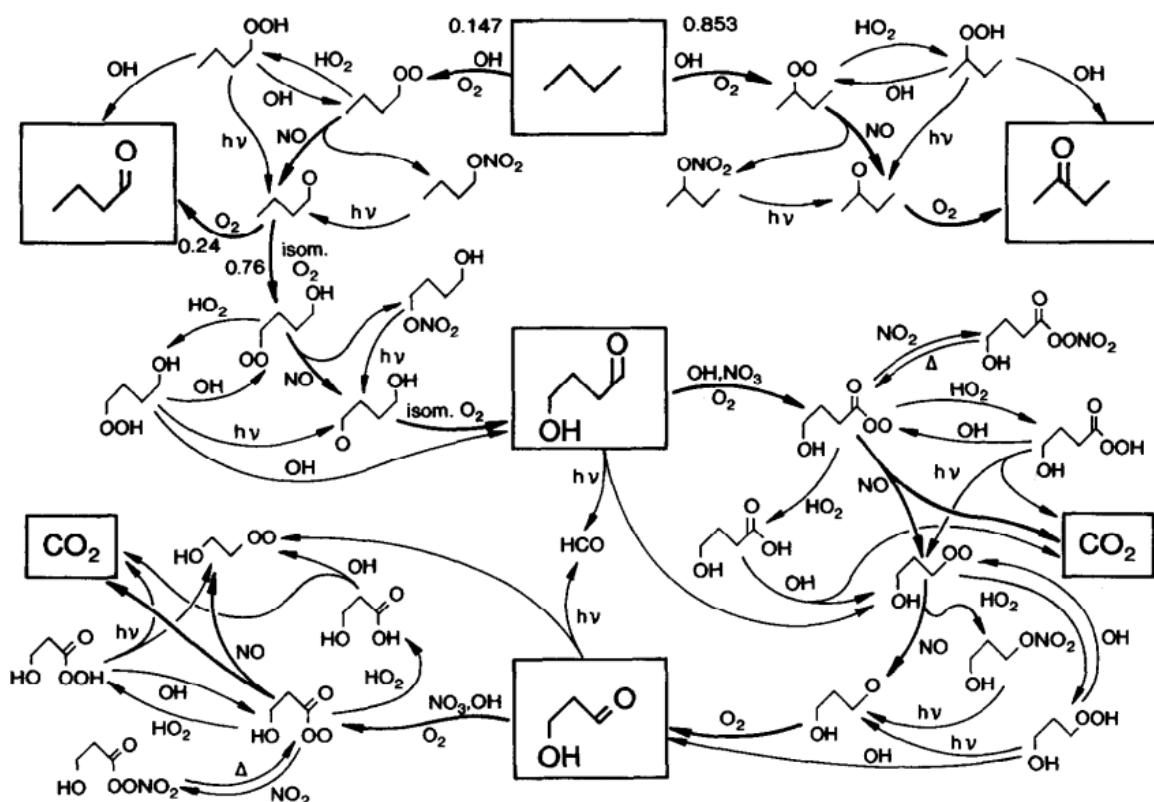


Figure 1.2: A systematic representation of the degregation of butane. Using this we are able to see the process C_4H_{10} undergoes before its ultimate demise as carbon monoxide and water. Source: [Jenkin et al., 1997]

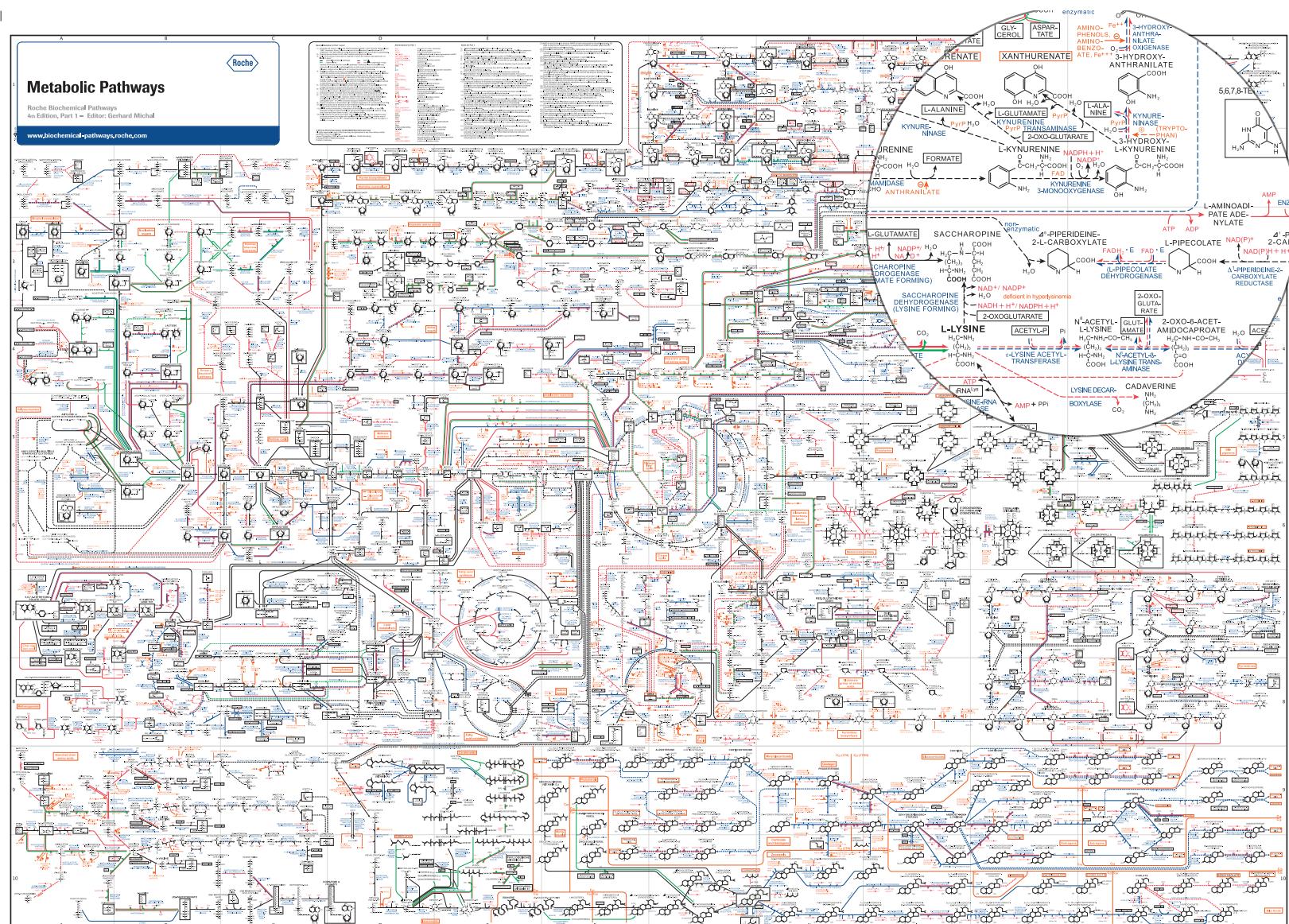


Figure 1.3: **The Roche Metabolic Pathways of the human body.** This example demonstrates the ability to manually represent the complex chemistry of the body using a graph structure. (Original A0 version is available at the source). Source: [Michal, 1965]

Today automatic graph layouts allow us to generate multivariate and complex graphs quickly [Muelder et al., 2014] -This means that, much like in the construction of a mechanism, we can rely on computer-aided design to generate a directed graph representation of the chemistry. Montañez [2016] states that "The beauty of a good information graphic is that it can tell a whole story in a single unit of visual content". This is particularly true for the use of directed graphs in chemistry where we can compare different mechanism subsets,(??) or model simulations (??).

However, several problems emerge from the complete automation of a task. Firstly real-world data very rarely reacts how it is expected to. Here networks of high edge density often obfuscate the graph data and produce what is only described as a ‘birds nest’, ‘hairball’ or ‘ball of yarn’ within the literature [Roberts et al., 2014]. Although such problems can be shown as moments of turbulence, they encourage a greater understanding of the graphic design process and can catalyze to merge unique ideas into an effective visualisation [Johnson, 2010] - much like the composite metaphors in ??.

Having established that a graph network ties in both modern and historical methods for representing relational data, we now look at how to present the graph, both in syntax (Section 1.2) and semantics (Section 1.4).

1.2 Graph Syntactics

Syntactic representation considers how best to distribute information on a page for maximum impact. This can be seen between the force-directed graph (top) and geographical location (bottom) layouts in Figure 1.4. Although the geographical layout gives a more accurate representation of the distances between unconnected nodes (airports), a force-directed graph provides greater insight into the relationships (flights) between each airport. This highlights the importance of choosing a suitable syntactic representation to highlight the features of interest. The remainder of this section discusses the syntactic choices required for the visualisation of a complex chemical mechanism.

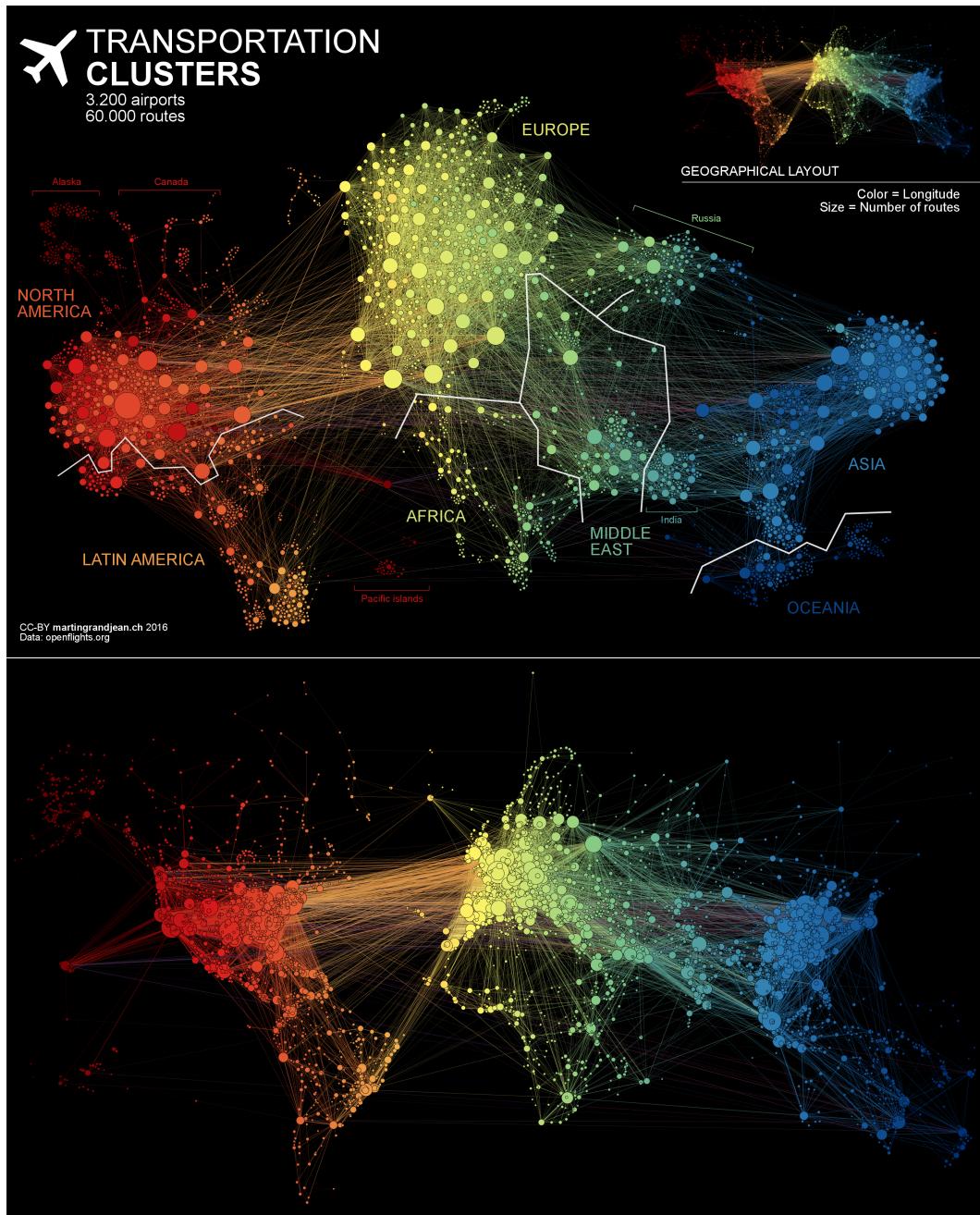


Figure 1.4: **Comparison of different representations of flight data by [Martin Grandjean, 2016].** The top figure shows the data represented by a force-directed graph layout (described below) and a Geo-layout showing each point at its location on the Earth.

1.2.1 Selecting The Correct Evaluation Criteria.

As chemical networks provide a wealth of information on the reactions within a system, this can prove challenging to user cognition and computational resources [Kerren et al., 2014]. In selecting the best possible graph layout, there are many metrics designed around the improving of visualisations aesthetics [Purchase, 2002]; however, these have often only been evaluated with a handful of criteria in mind. Such metrics can make it difficult to accurately quantify the changes in user-readability,

especially if they are not treated as originally intended [Pohl et al., 2009].

1.2.1.1 Edge Crossing

One of the greatest limitations to understanding a graph is the number of overlapping (crossing) edges [Purchase, 1997], especially since users often spend most of their time looking at the edges of a graph in order to understand it [Pohl et al., 2009].

There exist several types of graph layout algorithms which aim to reduce the number of overlapping edges in a graph. The two most common ones are force-directed and orthogonal. Orthogonal designs are those of straight edges at 90-degree angles, such as in architectural or circuit schematics (Figure 1.5). Force-directed graphs (Subsubsection 1.2.2.3) are a graph layout designed to simulate a physical system, where node positions are the result of the push and pull of the edges between them. In the task selecting nodes from a specific path, users were twice as more accurate using this layout than the orthogonal one [Pohl et al., 2009].

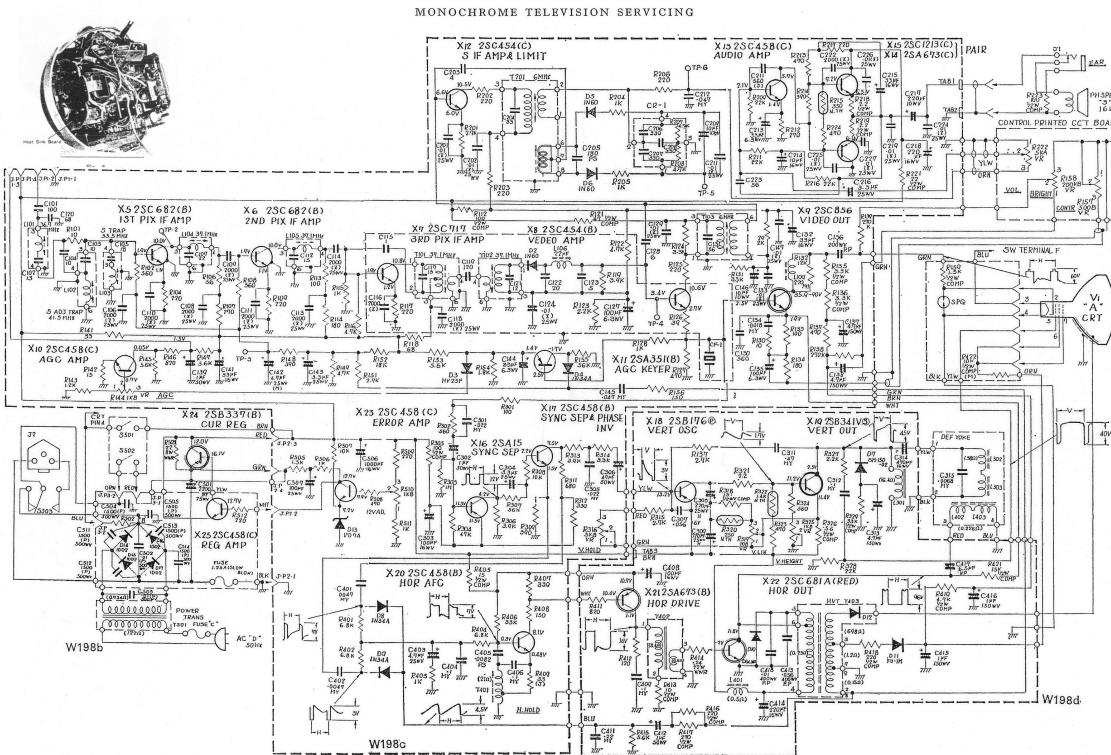


Figure 1.5: An orthogonal circuit schematic of the Model 3 240 portable cathode ray tube television. The circuit schematic of the television (top left) shows a much simpler representation of how different components within the television are connected. Source: [?]

1.2.1.2 Node Distribution And Overlap

The distribution of nodes across the page can both hinder or increase the readability of a graph - especially since larger nodes may obscure smaller ones at the same location. Purchase et al. [2003] found that graphs with an equal node distribution across space, at a medium edge length greatly improved graph readability - with node distribution and graph-symmetry ranking second in a study on user preference on graphs.

In addition to selecting the best graph layout, there exist several methods in which overlapping nodes may be removed - an issue that is sometimes difficult by the treating of nodes as ‘point masses’ within an algorithm [Dwyer et al., 2006c]. Dwyer et al. [2006b] explains that there are usually two methods for reducing the number of overlapping nodes in a graph; these are:

1. Create a layout design capable of taking node size (e.g. [Friedrich and Schreiber, 2004]) into consideration. These designs tend to be layout specific and not absolute in removing all overlap between nodes.
2. This requires a level of post-processing in the form of a ‘layout adjustment’. Here we reposition nodes after a chosen layout has finished computing. The drawback of this method is that information contained in the graph’s shape may be degraded. This can be done through the use of collision detection, or moving nodes to the centre of the vernouli cells [Lyons, 1992].

1.2.2 Automated Graph Drawing Layouts

In their design and evaluation, automatic graph drawing algorithms are created to minimise a specific criterion. This subsection will compare several graph layouts and make a verdict on which one is most suited for the representation of tropospheric chemistry. This task shall use the mechanism extracted in ?? to represent the VOC’s within the Beijing city - a real-world case study using the MCM.

To do this we begin by exploring hand-drawn / map inspired graph layouts (Subsubsection 1.2.2.1, Subsubsection 1.2.2.2) eventually ending at a number of automated force-directed graphs (Subsubsection 1.2.2.3).

1.2.2.1 Replication Of Hand-Drawing Methods

With the rise of computation, many traditional visualisations adapted for the computer-aided generation. Fields of architecture and circuit design adopted computational software to alleviate some of the difficulties presented by large or complex designs. Similar ideas such as the use of automatically generated transit maps can be used to link chronological or topological items such as ideas [Foo, 2019]. Figure 1.6 shows all the possible paths for the oxidation of methane to produce carbon dioxide

(and water), using the MemoryMap algorithm Foo [2019]. Although such methods can be useful in showing isolated pathways, they provide a convoluted representation of large interconnected systems and require some manual intervention.

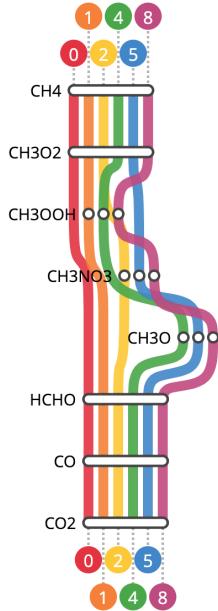


Figure 1.6: **A transit map showing all the possible routes from methane to carbon dioxide.** This was drawn using MemoryMap [Foo, 2019] and uses a version of the MCM methane subset, where carbon dioxide has been introduced.

1.2.2.2 Projection Based

One of the oldest fields of data visualisation fall in the realm of cartography. Here the shapes and distances between points on the surface of the earth (an oblate spheroid) are mathematically mapped onto a 1D plane for graphing purposes [Thomas, 1952]. Since the process of dimensionality reduction will produce inherent distortions within the final product, we end up with a range of map projections, with each striving to achieve a different aim (Figure 1.7). The Pierce Quincuncial, for example, is a conformal mapping technique mapping the surface of a sphere to a square with minimal deviation in scale and the ability to be tessellated in all directions. The Mercator, on the other hand, is a cylindrical projection which grew in popularity due to its unique ability to represent any course of constant bearing¹ as a linear segment within the shipping and navigation industry. Finally, the Waterman butterfly presents the globe as a truncated octahedron. This allows for the reconstruction of a three-dimensional world from a 2D plane (i.e. a printed sheet).

¹Also known as a ‘rhumb’, or ‘loxodrome’, and consists of an arc crossing all meridians of longitude at the same angle.

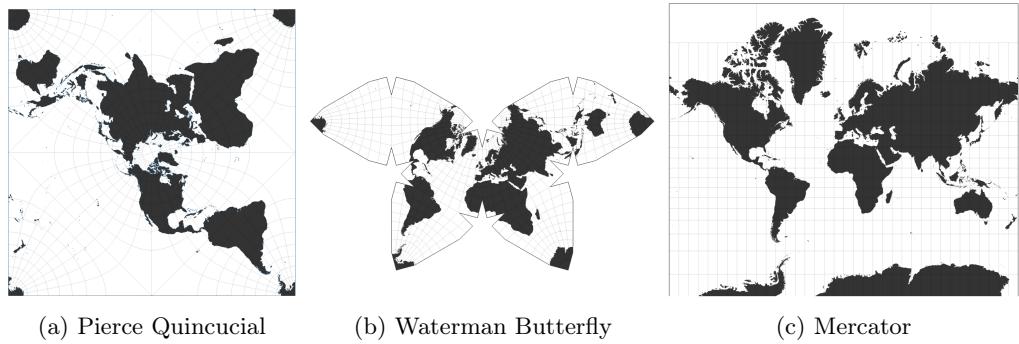


Figure 1.7: **A selection of map projections.** These have been created using DataDrivenDocuments [?] and show a range of methods for mapping the spheroid shape of the Earth onto a 2D plane.

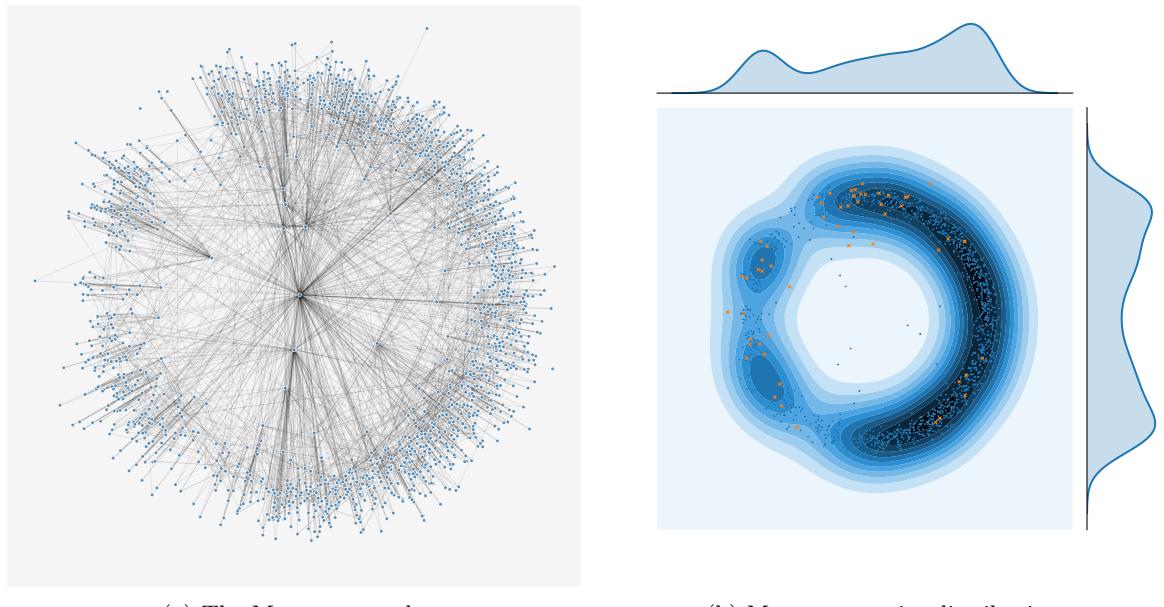


Figure 1.8: **The Mercator Projection.** (a) represents the output from the Mercator graph layout algorithm. (b) provides a kernel density analysis of the node distribution within this. Here (a) shows graph structure by revealing the density of connections between different nodes, while (b) reveals the density of nodes at a specific location.

More recently, the mathematics of mapping a large dimension onto a simpler one has been applied to the problem of graph representation. [García-Pérez et al., 2019] uses the latent hyperbolic geometry of the Mercator layout to provide a 2D embedding for complex real-world networks. This produces a polar representation (r and θ) of the system, where relationships of related species are of the same angle (θ), with nodes of a high degree are closer to the centre (low r value, where r is the radius from the centre). Using the chemical mechanism from the APHH Beijing campaign (described above), this produces a layout, (Figure 1.8) where (a) shows the graph-based representation including links, and (b) shows the density distribution for all nodes. Figure 1.8b shows that primary emitted species (orange dots) are uniformly (radially) distributed for angles and Figure 1.8a reveals that influential nodes with a high degree (highly connected) are located close to the centre of the graph. Although the

Mercator embedding does reduce the ‘hairball’ problem experienced by other layouts, it does not take edge weight/direction or self-loops. This means that it works well for the representation of the general network layout, but cannot be used for advanced data exploration concerning simulation results.

1.2.2.3 Force-Directed

Force-directed graph layouts are the results of the Spring-Electrical model. This was first introduced by [Eades, 1984] and further improved by [Fruchterman and Reingold, 1991]. Force-directed layouts are, in essence, a simple physics simulation of like-charged particles representing the nodes. These particles act similarly to protons which experience Coulomb repulsion and try to get away from each other. If there is a relationship between two nodes, an attractive spring-like force is introduced, drawing the nodes back together.

In the case of a weighted graph, where each link (or relationship) has a value associated with it, we can adjust the spring coefficient of the attractive force to reflect this. This results in a layout where strongly connected objects are drawn together, and weakly connected ones further away. Uses for this type of representation have been shown biology, social networks, and with this thesis atmospheric chemistry [Muelder et al., 2014; Kohlbacher et al., 2014].

Next, we describe the Barnes-Hut algorithm, a mapping algorithm which builds a hierarchical tree of the data by splitting a plane into quartiles. This is used within the many force-directed graph layouts, including those of Force Atlas 2 and Yifan Hu, described shortly. Once this has been done a selection of four different layout algorithms shall be discussed.

Barnes Hut Algorithm

Since calculating the attractive/repulsive forces for each node of a large graph can be computationally intensive, many force-directed layouts rely on the Barnes-Hut approximation. This solves the N-body problem of pairwise reactions between nodes, $O(n^2)$, by approximating long-range reactions by grouping such nodes and applying a single action on their centre of mass- reducing the computational time to $n \log n$.

To do this, first, a spatial index of each node is constructed (see below). This can either be done using a quadtree (2D) or octree (3D). Following this we calculate the centre(s) of mass, allowing us to approximate the repulsive forces of a force-directed graph.

Quadtree Construction: A quadtree is the recursive partitioning of two-dimensional space into a set of quadrants (a set of 4 squares). This process is repeated, with each square then being divided into four itself, until there is only a single point within a cell. This converts a network, into a hierarchical

tree representation of the nested quadrants in which each point resides (a quadtree), Figure 1.9.

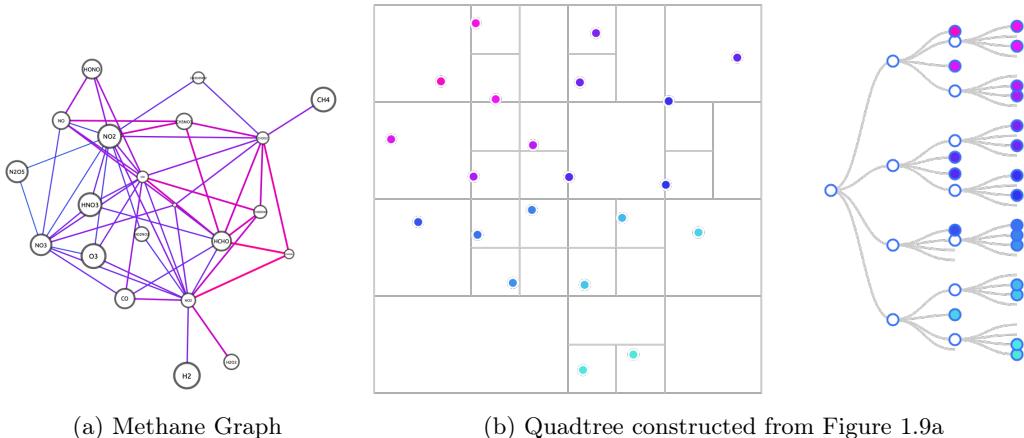


Figure 1.9: Demonstration of the formation for a quadtree from a force directed graph of Methane (including inorganics). (a) shows the force directed graph of Methane from which the quadtree has been constructed- edge colours represent the flux between species. Here we partition the area into 4 and start at the top-leftmost cell. This is then partitioned into 4 itself in a recursive process until there is only one point per cell. We repeat the process to any remaining cells in a clockwise manner (b). The hierarchical tree (b right) shows the containing structure for each node. Here the colours represent the order in which nodes have selected (starting at pink and ending in blue).

Having defined this, we move on to looking at the graph layouts.

Force Atlas 2

The force atlas two [Jacomy et al., 2014] algorithms is a force-directed layout designed primarily for scale-free² network spatialization. It is primarily designed for the use of networks consisting of 10 to 10,000 nodes and uses barnes-hut approximation for the calculation of forces. Attractive forces are derived from the spring-electric model ($F_a = -k.d$), where k is the spring constant and d is the distance between the two nodes. Optional features for the graph include dissuasion by degree (separating nodes with a high number of total links/reactions), logarithmic attraction forces, adjustable gravity (attraction the centre of mass of the system to prevent disconnected components from drifting away) and collision detection to prevent overlapping nodes. Finally, an adaptive cooling scheme is applied, where the overall energy of a system is gradually decreased, allowing the nodes to settle into a low energy state.

Yifan Hu

The Yifan Hu graph layout [Hu, 2004] is a multi-level graph drawing algorithm which uses the Barnes-hut algorithm with an octree layout. As with the force atlas algorithm, Yifan Hu also has an adaptive

²A network whose degree distribution follows a power law (7 degrees of separation). This is described in Chapter 1.

cooling aspect to it - meaning that as the algorithm is run its energy is progressively reduced, allowing the system to settle within a low energy state.

The main difference within the algorithm, however, is the use of the multilevel approach. This has been applied to graph partitioning [11,12,23], matric ordering [24] and the travelling salesman problem [5]. This works by graph coarsening (coalescing neighbouring nodes and weighting them), running the algorithm on the coarse graph, prolongation and then refining the results. This produces an algorithm that runs faster than the Force Atlas, however, is constrained to only working on un-directed edges.

OpenOrd

A force-directed graph algorithm capable of scaling to very large graphs [Martin et al., 2011]. OpenOrd uses simulated annealing (see below), which has five distinct phases. These are each run for a fraction of the total number of iterations and mimic the different states experienced when heating/cooling a physical object (liquid, expansion, cool-down, crunch and simmer) - here each state describes the amount of energy assigned to the nodes within the force simulation. In addition to this, the OpenOrd algorithm applies a degree of edge-cutting to remove a percentage of edges experiencing the most stress within the physical system. This allows the network to open out into a more aesthetically pleasing layout.

Simulated Annealing

Most iterative layouts are updated interactively from some initial configuration in an attempt to reach the lowest energy state of the system. In most cases this results in a minimum configuration; however, this is generally a local minimum rather than the desired global minimum (the optimum low energy state of the entire system) [Davidson and Harel, 1996]. To overcome this, the work of Metropolis et al. [1953], which was later formulated in general terms by [Kirkpatrick et al., 1983], was used to lay the foundation for simulated annealing algorithms.

Annealing is usually used to describe the slow cooling applied to liquids for them to reach a crystalline (totally ordered, minimum energy) form. It can be shown that if the atoms(nodes) are cooled too rapidly (losing energy quickly and coming to a quick stop), they will form amorphous structures representing the local minima, as opposed to the desired global one. If cooled slowly, our graph is allowed to find a thermal equilibrium at every temperature. A slow cooling constant is applied, whilst occasionally supplying the system with short bursts of energy, that may allow it to overcome local minima.

tsNET

t-Distributed Stochastic Neighbor Embedding (t-SNE) is a dimensionality reduction technique which mimics the style of a force-directed graph (this is discussed in ??). tsNET³ is a graph drawing algorithm which leverages the non-linear dimensionality reduction capabilities of the t-SNE algorithm [Maaten and Hinton, 2008a]. This works by first computing the shortest-path distances between all nodes to produce a distance matrix. This distance matrix is then used to construct a cost matrix which consists of the sum of three terms:

1. A measure of the divergence between picking pairs of low- and high-dimensional data points.
2. A compression factor, known to reduce the t-SNE optimisation time, taken from [Maaten and Hinton, 2008b].
3. A repulsion term to prevent nodes clumping together.

Node positions are then determined by the minimisation of the cost matrix using gradient descent - an optimisation algorithm used to minimise a function by iteratively moving in the direction of the steepest descent.

Note: Although tsNET makes for an excellent alternative to classical graph layouts, it does not take link direction into account.

1.3 Selecting The Best Graph Drawing Layout.

Subsubsection 1.2.1.1 explained the importance of removing overlapping edges and Subsubsection 1.2.1.2, the desire of having a well-distributed graph layout. This subsubsection builds on those criteria, assessing all the graph layouts described within this section (Mercator, Force Atlas 2, Yifan Hu, OpenOrd and tsNET). These all use the chemical mechanism representing species within the APHH campaign in Beijing [?]. Here we look at the distribution (Subsection 1.3.1) and density (Subsubsection 1.3.1.3) as they affect a users ability to isolate the shortest path (fastest flux).

Force-directed graphs place a greater emphasis on node positions,

Criteria, such as the ability to isolate the shortest path (in this case the fastest flux), are essential in determining the usefulness of a graph. Comparing different layouts [Pohl et al., 2009] found 68% of user-chosen routes to reflect the shortest path between them.

³A play on t-SNE and network.

This is due to the force-directed layout placing a greater emphasis on node positions and distance than other layouts. For comparison, the same study found this to be 40% for hierarchical layouts and only 2% for orthogonal ones. This section compares a number of graph layouts, and their effect on user readability.

1.3.1 Graph-Node Distribution

Subsubsection 1.2.1.2 explained the importance of node distribution within a graph visualisation. Additionally, Purchase et al. [2003] explains that if we partition the viewing medium into quartiles, and populate each quadrant with an equal number of nodes (homogeneity), this drastically improved the usability and symmetry of a graph.

The problem is that for complex real-world graphs is that they often contain nodes with many reactions between them (Figure 1.10). Such regions of dense, indecipherable links (often referred to as hairballs [Ma and Muelder, 2013]), obscure nodes and edges within a region, making it impossible to read.

Methods such as edge pruning [Dianati, 2016] (removing unimportant links) can be used to reduce complexity. This process may be done either post computation (syntactic representation) - resulting in a loss of information, or during the algorithmic approximation (e.g. within the OpenOrd algorithm) - where any removed edges are then re-introduced in after the final layout has been generated.

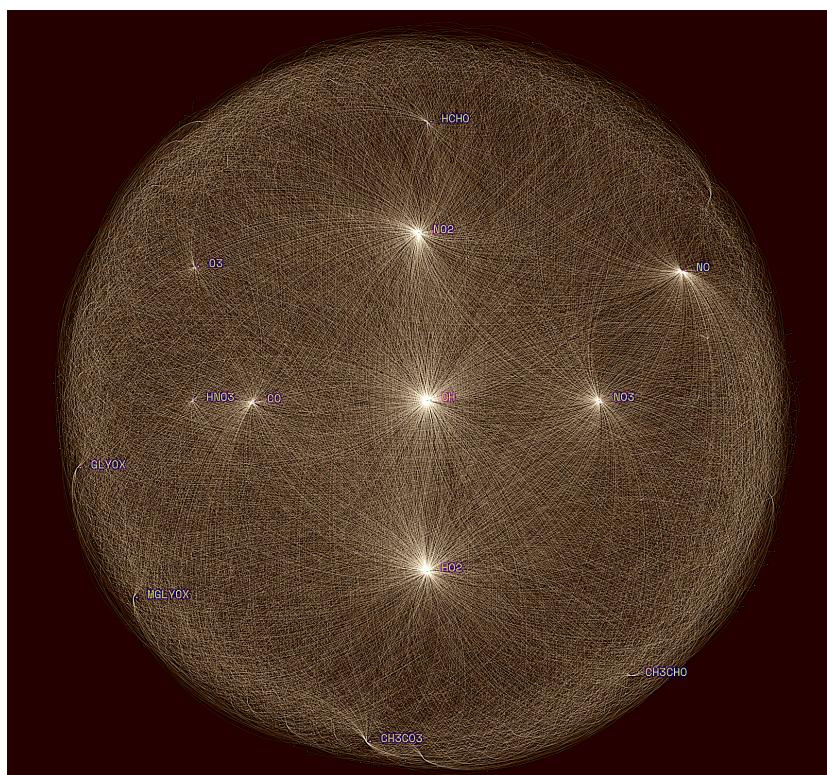


Figure 1.10: **A graph of the full MCM - a hairball.** The high number of nodes and edges (especially those to inorganic species), causes a high degree of obfuscation, rendering the graph unusable. Species with a large number of reactions (links) are labelled.

1.3.1.1 Evaluating Node Distribution For The Beijing Mechanism

In deciding which layout algorithm produces the best graph-node homogeneity, a kernel density approach is used to compare node distributions across 2D space in Figure 1.11, and the Mercator density plot from earlier (Figure 1.8b).

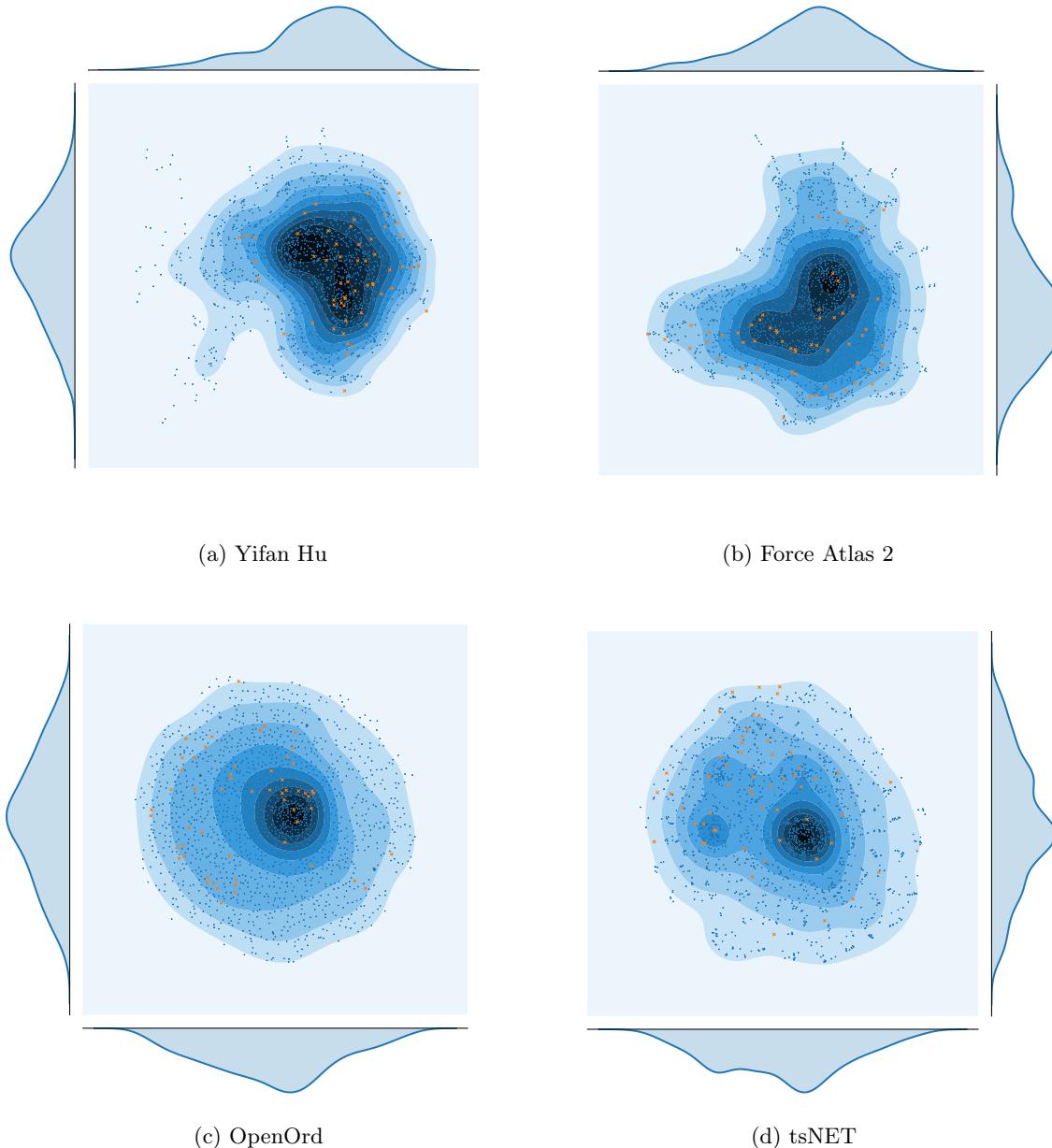


Figure 1.11: Contour and kernel density plots showing the node distribution for different graph layouts. Line charts show the distribution of nodes in the x and y directions, while the contours represent density with respect to the location of each node (the crosses). Primary emitted species are coloured orange, and the darker contour polygons show areas of higher density.

This style of plotting allows for the easy location of areas containing a large number of nodes (high density) through the use of the contour-colour gradient. In an ideal graph, we would have groups (clusters) of high density, all of which would be evenly dispersed around the 2D plane. Additionally,

the use of x/y kernel density can show us the homogeneity of a graph - a perfectly homogeneous (lattice) graph will have a uniform distribution across both axes. For a modular graph of evenly dispersed groups, we would expect an oscillatory distribution of similar amplitudes. Using this criteria, the Mercator (Figure 1.8b), tsNet (Figure 1.11d) and Force Atlas (Figure 1.11b) score the highest, where the OpenOrd and Yifan Hu graphs containing a gaussianesque distribution across both axes - a distribution conducive to the production of a hairball.

1.3.1.2 Distribution Of Primary Emitted Vocs

Within the construction of an atmospheric chemical mechanism, a chemist first begins with a primary emitted species. This is then broken down to produce other species, depending on its structure and functional groups (??). This process suggests that in constructing a network from such a mechanism, this structure will be prominent. Knowledge dictates that a chemical graph should start from a large emitted species, and aim towards carbon monoxide (and ultimately CO₂ although this is not included in the MCM). To show such a structure we expect any primary emitted species to be evenly distributed and the chemistry tending towards the location of CO (the centre). In searching for a layout that satisfies this requirement, the tsNET graph (Figure 1.11d) is found to be the best, followed by the OpenOrd and ForceAtlas2. Yifan Hu (Figure 1.11a) and Mercator (Figure 1.8b) both contain areas where many of the primary emitted (orange) species are grouped, and are therefore unsuitable for the representation of the MCM structure.

1.3.1.3 Calculation Of Spatial Clustering

Subsubsection 1.3.1.1 explains that the ideal (modular) graph consists of many groupings of like chemistry evenly scattered across the graph. This requires a degree of regular anisotropy to produce ‘clusters’ of densely connected nodes, sparsely separated in space. To calculate this we can rely on Voronoi tessellation.

Voronoi Tessellation

Voronoi Tessellation is the process of finding the largest area closest to a specific point. It can be thought of as a container bubbles at the location of each node, where each bubble collapses to fill the largest area possible.

Here we begin by partitioning the graph plane into the same number of cells as our nodes. Next each cell polygon boundary is calculated such that all the points on it lie closer to its seed (origin) node, than any other. Mathematically these are referred to as the perpendicular bisectors of the lines

between all points.

Finally we calculate the areas of each polygon and use it to represent the density distribution between neighbouring nodes of our graph. To simplify the visual analysis of each graph, these are also coloured in Figure 1.12.

Visual study of node clustering

The method of using Vornouli tessellation for the calculation of density has been used in the study of neurones [Duyckaerts and Godefroy, 2000] and areas of fixation when viewing images [?]. We apply it to the nodes of a set of force-directed graphs to determine the graph layout which provided the best high-low density ratio for the atmospheric chemical mecahnism of a Beijing environment.

Using Vornouli tessellation in Figure 1.12 we find that the OpenOrd and tsNET (Figure 1.12d,Figure 1.12c) layouts have the highest isotropy - containing cells of similar sizes and consequently a small colour gradient. This suggest that these are spatially efficient layouts as they do not reveal any additional information about nodes of similar chemistry.

In contrast the Mercator layout, despite having a high $x - y$ node distribution, contains large areas of unoccupied space due to its non-linear density distribution. Using this measure of spatial modularity we find that the ForceAtlas2 and YifanHu (Figure 1.12b,Figure 1.12a) graphs have distinct modules of high density distributed across the entire graph, which is what is what we expected from the MCM network.

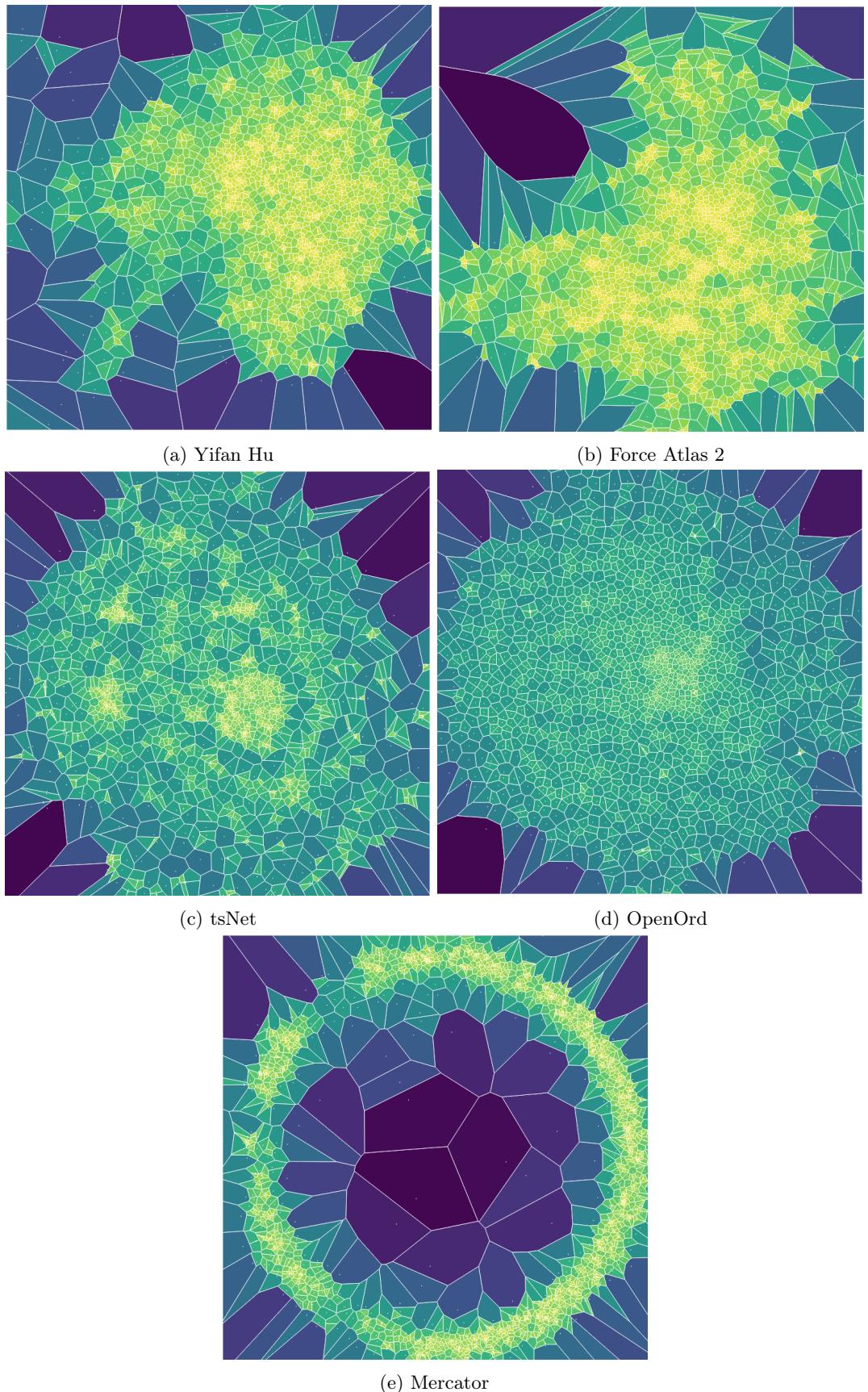


Figure 1.12: **A visual analysis of node-cluster density using Voronoi tessellation.** Each polygon is centred on a node, and their area represents the space between a node and its nearest neighbours. Colours follow the normalised size of the voronoi cells/polygons.

Mathematical Analysis And Layout Selection

In contrast to the qualitative analysis of the visualisation, it is also possible to calculate the distribution of polygon areas (and this node dispersion) of each graph through the use of a boxplot (Figure 1.13), in addition to the minimum, maximum and outlier properties, a boxplot allows for the comparison for the inter-quartile range (IQR) between graphs. If these values are large, they signify a bigger distribution between sparsely and densely grouped nodes (a commodity that is desired). The medians location within the IQR can also be used to indicate the dominant size of polygon within the graph. Here a larger number of smaller polygons is desired, and can be seen by a median approaching the lower box boundary (25^{th} quartile).

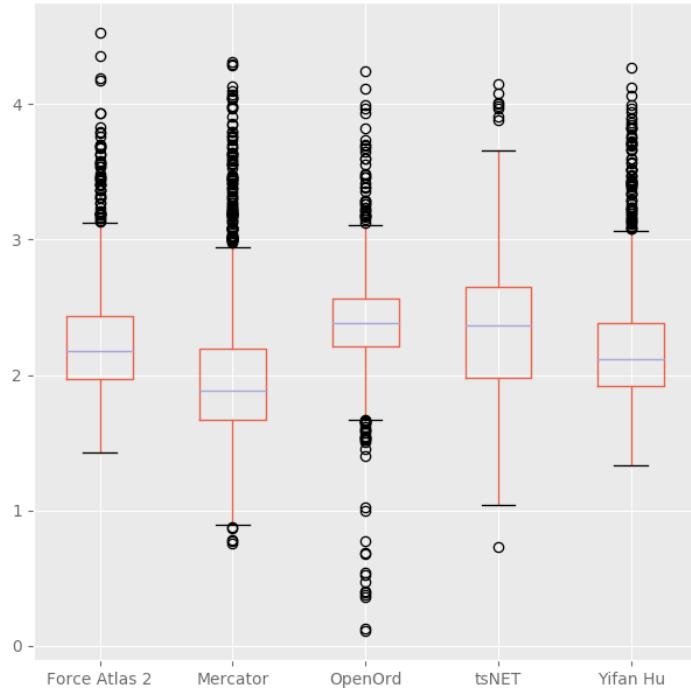


Figure 1.13: **Voronoi** $\log_{10}(\text{Area})$ BoxPlot for all plots in Figure 1.12. This provides a mathematical analysis for the areas around each node within a graph.

Figure 1.13 shows Mercator to provide the best result, however it is noted that although the boxplot contains the best ratio, its radial shape is not conducive to the representation of modularity within a chemical network. tsNET contains the largest IQR, however since it is not able to handle the directed edges of an atmospheric chemistry graph, this again has to be ignored. Finally, although OpenOrd can reduce the number of hairballs within a graph by using simulated annealing and edge-cutting, its homogeneous isotropic node distribution (small IQR with a large median value) make it not most effective at highlighting the structure of the MCM. Yfan Hu layout fares better with regards to the box plot, yielding an overall lower box, with a similar IQR and median ratio. Here its lower median suggests more high-density nodes, with a similar distribution to the ForceAtlas2. This makes sense

since the two algorithms share many similarities, however the inability to handle directed edges makes it unsuitable for our application.

By process of elimination this leave the ForceAtlas2 algorithm as the best candidate for representing a chemical mechanism. Its directed nature coupled with intuitive design make it applicable and easy to explain, while maintaining the ability to produce a clear representation of any underlying structure. In addition to this, its uniform spatial distribution (Subsection 1.3.1) makes it a better candidate than the Yifan Hu graph (which fared slightly better in the boxplot).

1.4 Graph Semantics

Deciding the correct semantic (relating to meaning) representation for visualisation is often just as important as the selecting the correct syntactic (structure) style. Semantic features are often applied post generation [Bennett et al., 2007] and are used to encode additional information and clarify the data. As a means of achieving both an aesthetically pleasing outcome, and an easy to understand visualisation, we must first consider what features we, or the reader, are most interested. Once this has been decided, we begin to explore various methods for representing them.

1.4.1 Limitations

Before selecting any semantic features, we must inform ourselves of the visual, cognitive and technological limitations of the visualisation, medium or user.

Visual

In visual analytics the most significant bottleneck falls on the resolving power of the eye - this is known as an acuity (shapness or clarity of vision at a distance). Acuities are a measure of the angle of an observed object with the viewer's eye using arcs (one arc minute equates to $\frac{1}{60}^{th}$ of a degree). This provides a unit of measurement for the total amount of information density we can feasibly perceive [Ware, 2013].

In ophthalmology there exist four types of acuities:

- **detection:** The smallest size an object can be whilst still being shown
- **recognition:** The smallest size an object can be to be recognised
- **resolution:** The smallest distance between two objects before they begin to merge

- **localization:** The smallest amount of visual change that can be measured between two objects

These provide a set of considerations which may be used to assess a visualisation. Depending on what encoding we use, it is possible to improve/hinder the readers ability to percieve information, (Figure 1.14). An example of this would be that for a Macbook Pro retina screen⁴, where at 87 pixels/cm we can resolve at most 2 million resolvable nodes (at 57 cm from the screen). If we wished to add links between nodes, the total items idenified is reduced to one million [Jankun-Kelly et al., 2014].

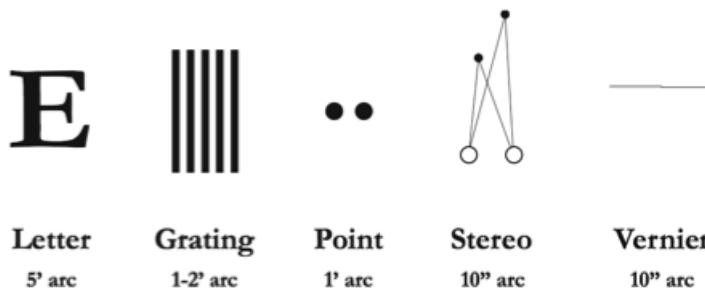


Figure 1.14: **Important acuities in visualisation.** Here a double prime " represents an arc minute which equates to an angle of 1/60 of a degree. A single prime ' is that of an arc second with is 1/60th of an arc minute (or 1/120 of a degree). For comparison the maximum angular resolution of the human eye is stated as 28 arc seconds [Deering, 1998] - this means we can only ever see up to 28 nodes or 2 verneers (disjoint lines) at any one time. Source: [Jankun-Kelly et al., 2014; Ware, 2013]

Cognitive

Although it may be possible to distinguish 1 million nodes and links visually, interpreting and understanding these presents another problem. The visual thinking laboratories [VTL, 2019], have a range of publications exploring how presentation can improve though, cognition and communication between info-graphic and reader. Steven Franconeri [2018], explains that the time required to interpret a visualisation is directly related to the encoding used to highlight the data within it. Also ‘intentional blindness’⁵ and misinterpretation are problems which are often occurred with poorly thought out encodings.

In considering the cognitive load of a visualisation Norman [2005] provides a list of three categories which should be explored:

1. Firstly we have the visceral level, a subconscious process where decisions are made rapidly based on sensory inputs to the body. This is usually due to our inherent ability to locate patterns and

⁴A retina screen, is half the maximum possible resolution of the human eye at a 30cm distance. Additionally the operating system interpolates in sets of 4 pixels, such that the image displayed may not be at full resolution.

⁵The failure of a user or audience to notice a fully visible feature because their attention was engaged by something else - e.g. misdirection in magic tricks.

changes due to semantic properties which shift the focus of the user.

2. Next follows the behavioural level (mostly subconscious). These are often learned reaction to changes noted as part of the visceral level. Here reactions may be honed on and influenced by past experiences and events.
3. Finally we reach the reflective level. Here the user collates all sensory input from the previous two levels and makes an informed conclusion about the underlying data. Conclusions drawn here can be used to bias the methods used within the behavioural level in future events.

Technological

In addition to human limitations, there may be restrictions due to the medium a visualisation is created/presented. In addition to monitor resolution, much scientific research is constrained by the size, resolution and colour quality of the presentation mediums used for talks, printing or posters. Ware [2013] explains that a printer capable of producing 1200 dots per inch squared, can only do this for black/white binary images. If for instance 256-greyscale is used, the resulting resolution is then at-least 10 times smaller. This is because printers use a Monet (dot matrix) style approach to create shading and colour. It therefore follows that at full colour⁶, the output resolution will be worse.

It is also essential to have a graph fitting the same overall shape of the canvas on which it is presented [Taylor and Rodgers, 2005]. This not only makes optimal use of any space available, but also reduces the visual complexity as it minimises the number of distinct shapes available to the user.

1.4.2 Node Encoding

Within a graph the nodes or vertexes are representation for the set of items we have an interest in. In addition to the relationships between them, items often contain a multitude of features which describe them. Examples of these may be user information for a person, categories of characters or the chemical composition / concentration for a species in the MCM.

Each of these additional properties can contain valuable information for the interpretation of the graph, and the interactions between nodes. It is for this reason that graph convolutional neural networks [Klicpera et al., 2018] require a ‘feature matrix’ describing each node, in addition to the network structure and edge weightings.

This subsection addresses a number of ways in which additional information can be encoded in the representation of a node, Figure 1.15. Each different category colour matches the title description in

⁶CYMK (Cyan Magenta Yellow Black)

the text.

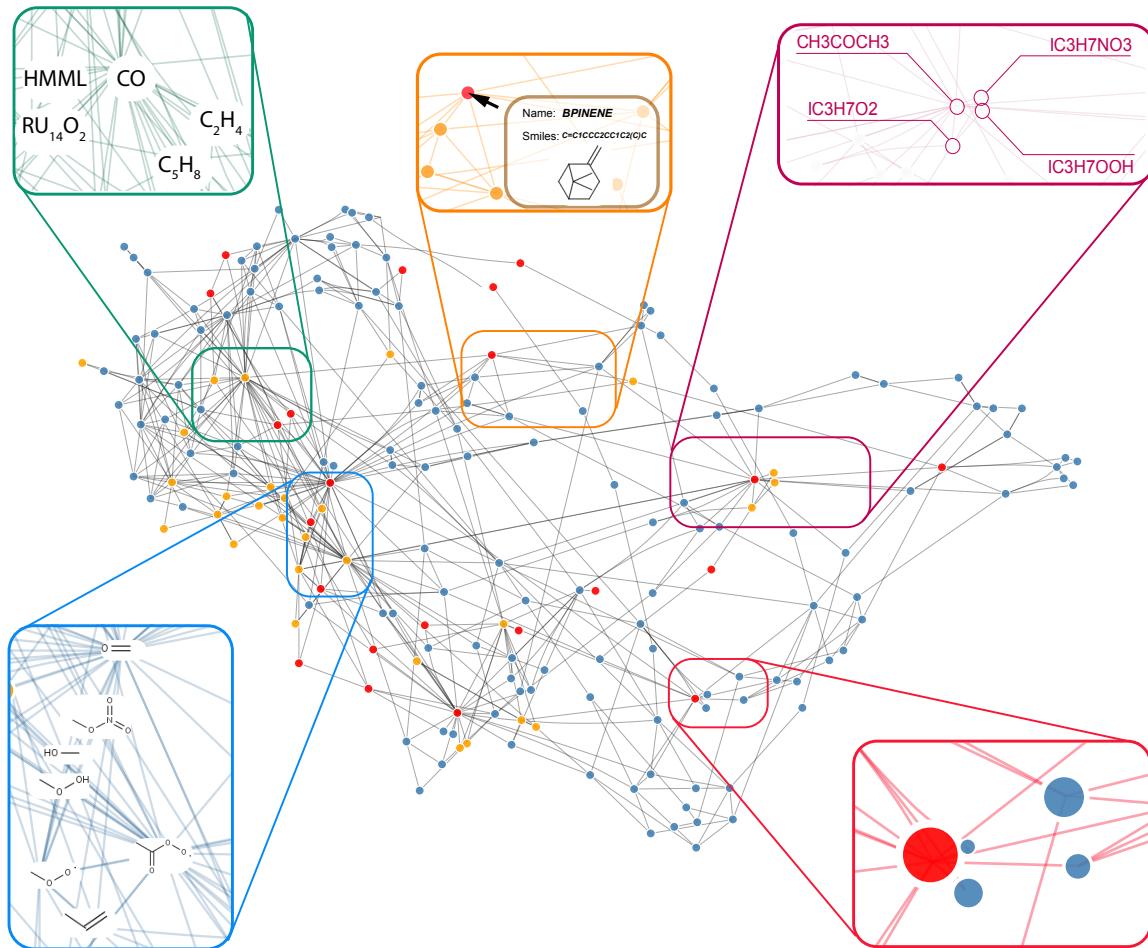


Figure 1.15: **A graph showing 5 different node encoding methods.** These are Circle Attributes (red), Chemical structure (blue), Species Name (green), External Labels (maroon) and interactive selection (orange). The network shows the Common Representative Intermediate species [Jenkin et al., 2008] mechanism. Node colours represent primary emitted VOCs (red), MCM species (orange) and lumped CRI-only species (blue).

Circle Attributes

The simplest of these range from the use of colour, shape, size, thickness and stroke (outline) to indicate a group. Here it is possible to provide information such as a species concentration based on its size, its importance with its colour, its degree with its opacity and its category with its stroke colour [??]. Such decisions depend on what properties the user is trying to show. For instance red species in Figure 1.15 are primary emitted VOCs, orange species exist between both the MCM and the CRI (see figure caption) mechanism, and blue ones are lumped species which do not appear as part of the MCM.

Chemical Structure

Traditional chemical diagrams use the chemical structure to depict the node (Figure 1.2). This makes it intuitive to extract information about functional group and potential bond changes within species. Such a method of representation, is indeed useful, however when visualising hundreds, or thousands of nodes on a page, it results in occlusion, or labels being too small to resolve visually.

Species Name

Much like the chemical structure, a species name is proven useful in explaining to the user its chemical structure or properties (often due to prior knowledge, or the ability to look this up). Unfortunately since names have differing lengths, this can cause problems, especially with large numbers of closely located nodes. A solution to this may be to adjust the font size to fit in within the circle radius of the node. However this does come with its problems - for instance tiny nodes may have text smaller than a pixel, or the misleading notion that longer names are less important, since they are represented by a smaller font.

Interactivity

Ben Shneiderman, one of the first, and most prominent, researchers in human-computer interaction coined the phrase '*overview first, zoom and filter, details on demand*' [Shneiderman, 1996]. This is the philosophy behind most data orientated interaction design, and can be applied to graphs. One example is the selection only of reactions relative to a node of interest, as is shown in Figure 1.16.

For complicated systems, interactivity plays a vital role in unraveling complexity and reducing clutter [Shneiderman, 1997]. This is a method which lessens the cognitive load (Figure 1.4.1) on the user, allowing them to query only items of interest, whilst still displaying all the information in a single location [Görg et al., 2007]. This fits in Ben Shneiderman [1985]s 8th rule of interface design, which explains that people only ever remember '*seven plus or minus two chunks*' of information.

A comprehensive list of all available interaction types and styles are provided by Wybrow et al. [2014]. Some examples of interaction are:

Hi-lighting

- Hovering
- Brushing and Linking
- Magic Lenses (see hidden objects)

Navigation

- Pan / Zoom
- View Distortion (fisheye)

Visual Structure-Level Interaction

- Selection
- Changing layout/mapping attributes
- Changing representation

Data Level Interactions

- Adding / Filtering
- Search / Query



Figure 1.16: **Using mouseover edge-selection to hilight all links related to a node.** This figure shows how in using interactivity it is possible to reduce clutter and filter the information presented by a densely populated graph. In this case the mercator projection (Subsubsection 1.2.2.2) is used, with reactions relating to Carbon Monoxide (centre) highlighted. Orange lines represent reactions producing CO whilst the red (some of which may be hidden) are of reactions with CO.

External Labeling

In cases where interactivity is not possible, such as papers, books and this thesis, an alternative approach to data selection has to be employed. Here nodes which are central to the explanation of a certain point are filtered by the author, and displayed through the use of external labels. It is found that having links at 45 and 90 degree angles (such as in transport maps) lead to a clearer layouts and better distinction from the links already within the graph. Automatically generated labels within the thesis are made using Lu [2019].

1.4.3 Edge Properties

Defining the purpose of force-directed (graph-energy) models as: a means for creating a visualisation from which the viewer can infer properties of the data [Noack, 2004], it can be shown that this criterion is easily met in small and sparse graphs. However non-planar examples with high edge density (lots of links) can easily result in tangled results with impractical running times [Kumar and Garland, 2006]. In most cases attaining an optimal solutions here seems to be computationally infeasible [Davidson and Harel, 1996]. This is generally because graphs primarily focus on hi-lighting a specific purpose or following a set of aesthetic heuristics [Pohl et al., 2009].

1.4.3.1 Muti-Variate Edges

Since there are multiple relationships between species, it is important to decide if simplifying the network would be of benefit. Although it is possible, multiple edges may cause unnecessary clutter for larger networks. Instead it is often useful to simplify the number of edges in the network, and encode the edge properties within the vector object. This allows the user to retrieve any additional information by hovering over the edge or connecting nodes, as required. Should the topic of interest require a specific property, then it would also be possible to remove, or hide, all edges which do not contain it. This produces an interactive graphic containing all the required information, as and when needed, without the unnecessary clutter of having every reaction shown.

1.4.3.2 Edge Direction

When using a directional graph it is convention to use arrow heads to represent the direction of flow. However in high density regions it is often found that arrow heads take up precious real estate in the drawing area [Dwyer et al., 2006a]. As an alternative, colour and line-type can be used to represent the direction instead - this was seen in Figure 1.9a (the quadtree example). This example can be shown in the routing networks presented by [Di Battista et al., 2004]. One example applicable for chemistry would be the use of dashed lines to represent mono-directional relationships, and continuous lines for bi-directional ones.

1.4.3.3 Edge Shape

Edge shape is essential, as it is the medium we use to represent relationships within a graph. For orthogonal graphs (Subsubsection 1.2.1.1), multiple lines are used to simplify the complexity of a graph and reduce edge crossings [Di Battista et al., 1994]. In increasing the number of lines within an edge, these multi(poly)-line graphs can be modified to give drawings with nicely curved edges. In a

similar manner it is possible to replace the edges in a straight-line graph with Lombardi-style curves or cubic beziers [Chernobelskiy et al., 2012; Goodrich and Wagner, 1998].

Using a mechanism describing the reactions of Butane in the MCM, we compare a number of edge shapes (Figure 1.17). In this graph each node has multiple edges between nodes (multi-link). Each edge represents a different reaction between the species. Figure 1.17a shows the straight line representation of each graph. Since each edge represents the shortest distance between two nodes, any additional reactions pairs between similar nodes are hidden from view. If using this type of representation it is advised to take the net edge direction and weight between the values. An improvement to the straight-line graph comes from the use of quadratic cuves (Figure 1.17b). This allows for the symmetric distribution of edges within the graph. If instead an asymmetric representation for each edge is required it is possible to use a bezier curve (described below) instead of a quadratic edge (Figure 1.17c). These can provide additional information through the use of control points, which can alter the shape, steepness and asymmetry of each link.

Bezier Curves

Bezier curves are named after Pierre Bezier who used them in the bodywork design of Renault cars in the 1960s [Hazewinkel, 1997]. Since then they have been widely used in graphs, computer graphics, font design and animation/interactivity response [Goodrich and Wagner, 1998; Hazewinkel, 1997; Mortenson, 1999]. Bezier curves come in a range of possible dimensions, cubic beziers are the most commonly used within network visualisation. These contain four control points respectively which can be used to determine the shallowness of the curve through design. In general, relatively shallow curves are preferred, as these do not introduce unnecessary edge crossing or abrupt changes, which have been shown to hinder a users ability to isolate items of interest [Purchase et al., 2003].

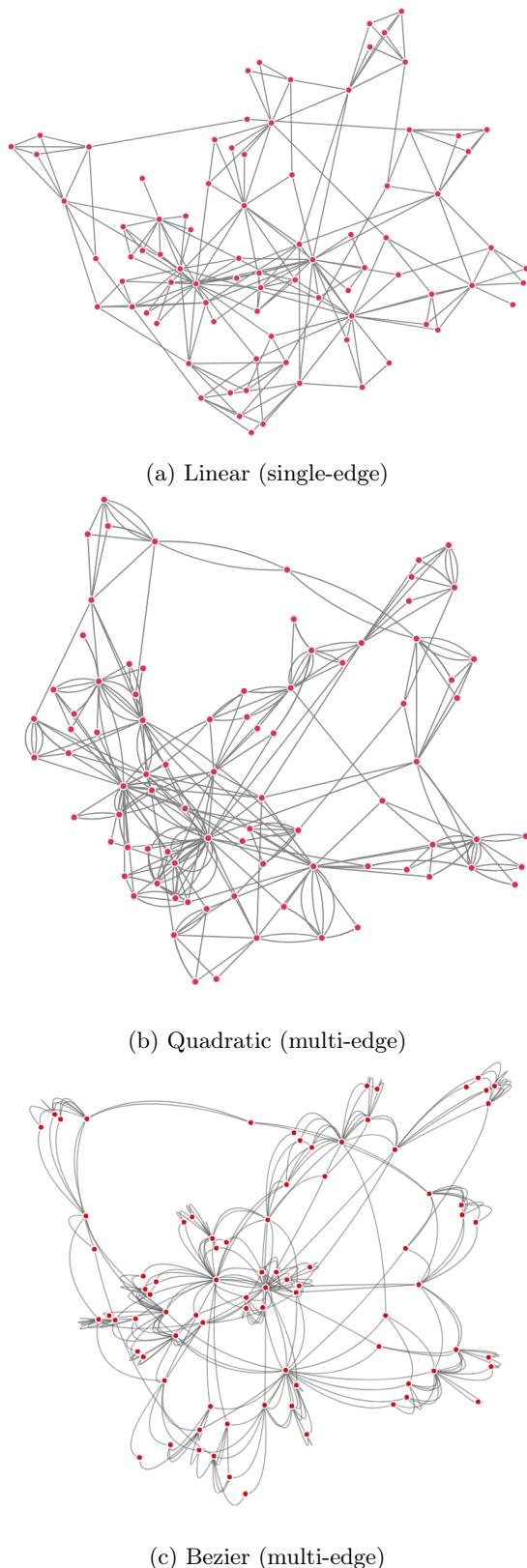


Figure 1.17: **A selection of edge shapes for the butane network.** These show linear (a), quadratic (b) and bezier (c) edge shapes for the same network. In general the the bezier curves appear to provide the most aesthetically pleasing graphs shapes.

1.4.3.4 Edge Bundling

Pioneered by Holten [2006], edge bundling techniques are an effective way to reduce visual clutter. Much like a force graph, edges are represented as a string of lined points. This allows for edges to be pulled together (attracted to one another) and produces a visualisation akin to moving water droplets on a hydrophobic surface. Figure 1.18 shows how in changing the amount of attraction between edges, it is possible to reduce clutter in a visualisation.

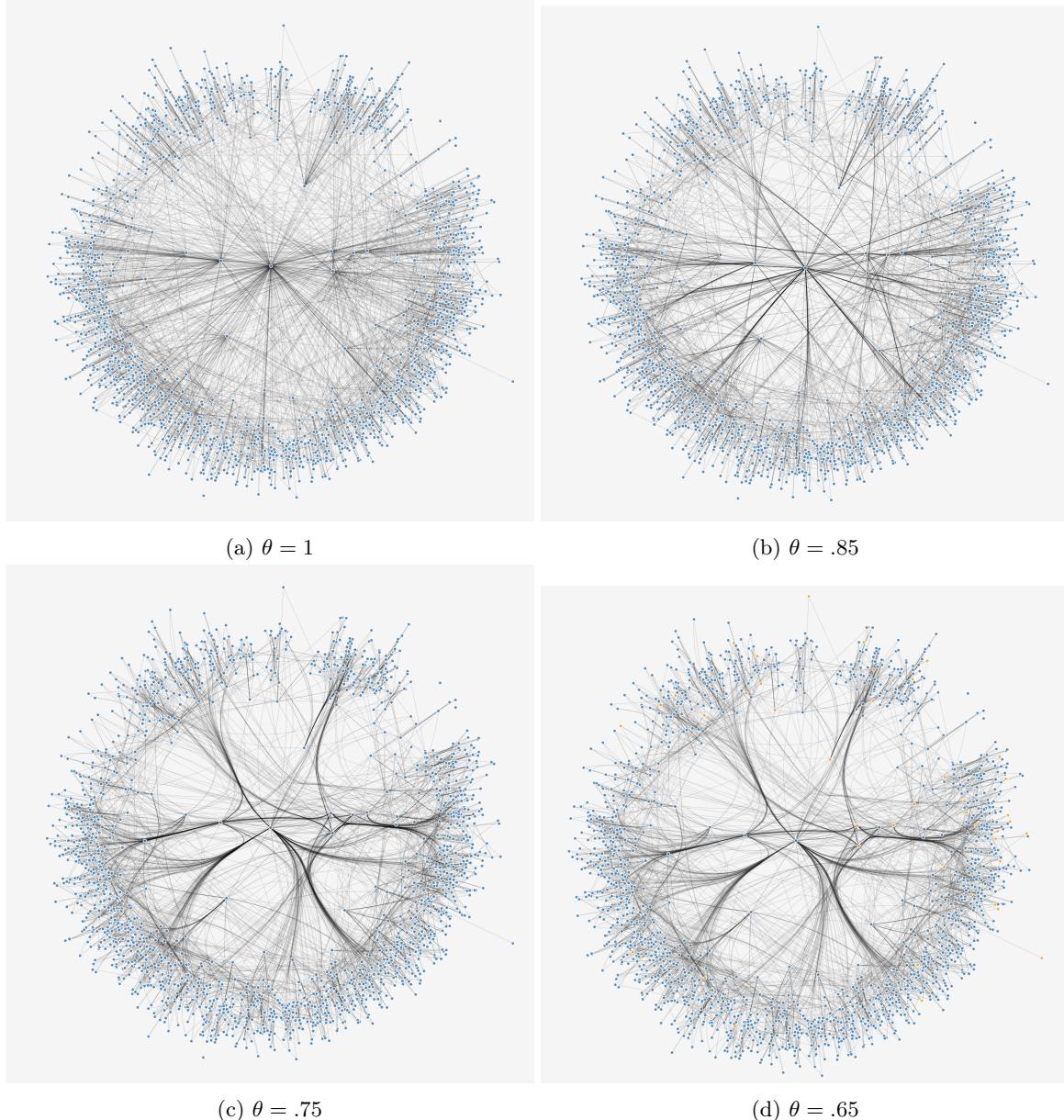


Figure 1.18: **How the compatibility threshold affects edge bundling using the Mercator graph from Subsubsection 1.2.2.2.** In increasing the amount edges are attracted (θ) it is possible to improve the clarity of a graph. However there reaches a point where this distortion can worsen the result, confusing the reader, or creating a false positive. For this reason, I generally use only a slight bundling value > 0.7 .

1.4.3.5 Power, Routing And Confluence.

Confluent graphs use a graph drawing method in which edges are not drawn as individual distinguishable geometric objects, but rather as a crossing free system of arcs and junctions. [Förster et al., 2019]. Their design is similar to that of the edge bundling algorithm, except that rather than bundling edges spatially (a design which may introduce ambiguity), the bundling is done based on connectivity and can help reduce clutter by grouping multiple edges where the all target nodes are also connected to all the source nodes (Figure 1.19) [Bach, 2020].

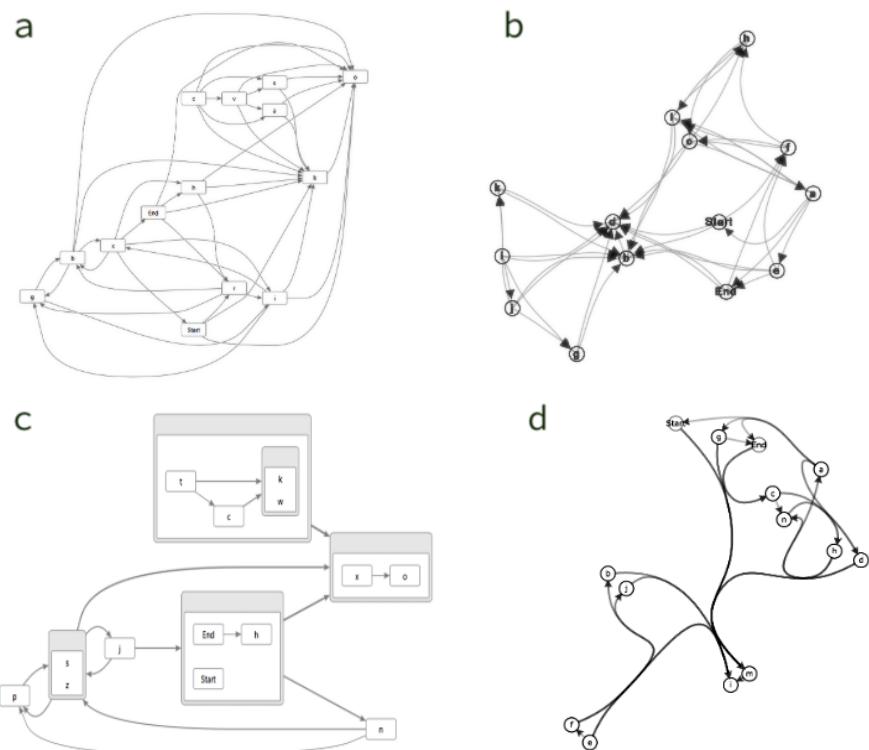


Figure 1.19: **An example of confluent bundling.** A traditional network (a), Edge bundling (b), Power Graph (c) and Confluent graph (d) representations. Source: [Bach, 2020]

Using the oxidation of butane as an example we shall explore the construction process of a confluent. Starting with the network presented in Figure 1.17, we create a power graph - power graphs are a representation of complex networks where sets of items identical source and target links are lumped or grouped within a single item. Next multiple edges which follow the same path are bundled through a ‘routing’ node to create the routing graph in Figure 1.20. The newly created routing nodes are now used as control points for the mapping of the graph using basis-splines⁷ (Figure 1.21). Finally any crossing links are removed leaving the confluent graph in Figure 1.22.

Confluent drawings have been found to have many applications (e.g. the ego-centric author network

⁷These are similar to bezier curves but require a degree (p), $n + 1$ control points, and a knot vector of $m + 1$ points. Knots are the things that make the curve continuous

and social interaction graph), they generally perform best in sparse networks with locally dense clusters of a tree like structure [Bach et al., 2017]. Although sparse, the cyclic nature of atmospheric chemistry does not allow for a sufficient reduction in complexity to make them a suitable improvement over traditional graphs. The use of very close fitting basis-splines in addition to a routing graph (confluent graph with crossing artifacts), may however help to simplify specific layouts or mechanism subsets with a certain amount of tweaking.

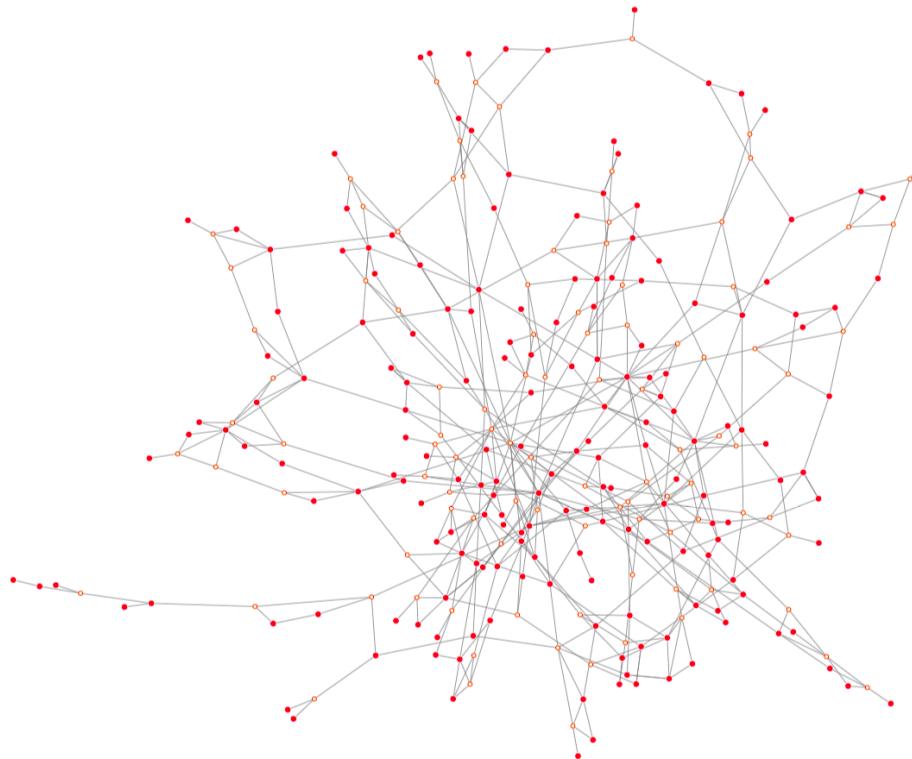


Figure 1.20: **The routing graph of the butane mechanism.** Here paths which contain two or more bundles have an extra ‘routing’ node introduced (orange stroke)

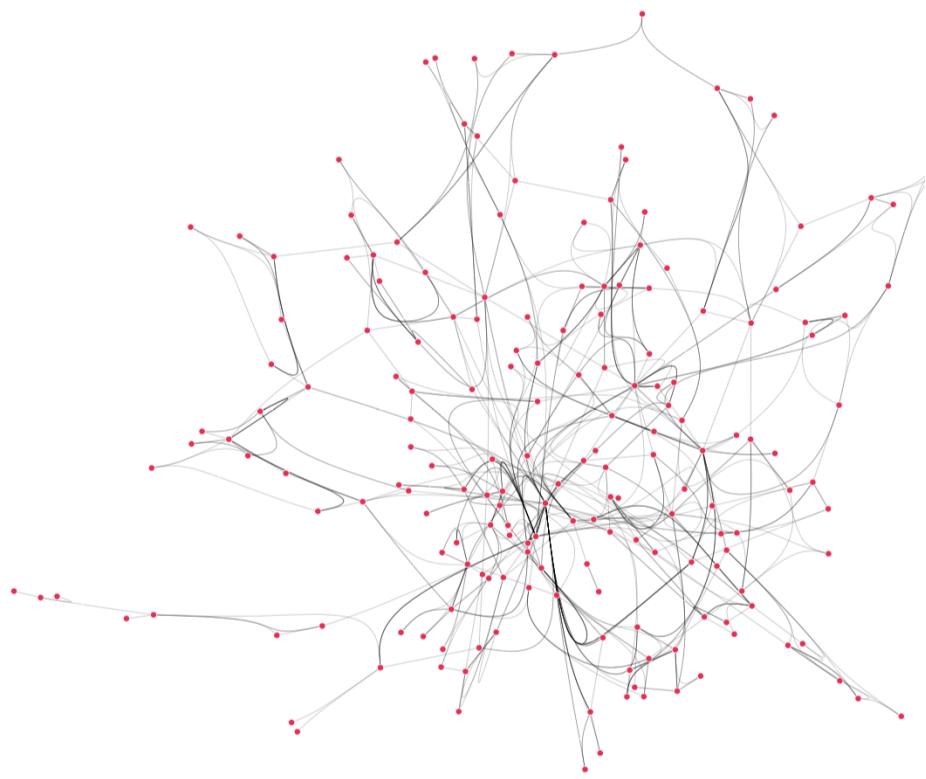


Figure 1.21: **Confluent graph with crossing artifacts.** The routing graph with the addition of basis-splines using the orange routing nodes in Figure 1.20 as control points.

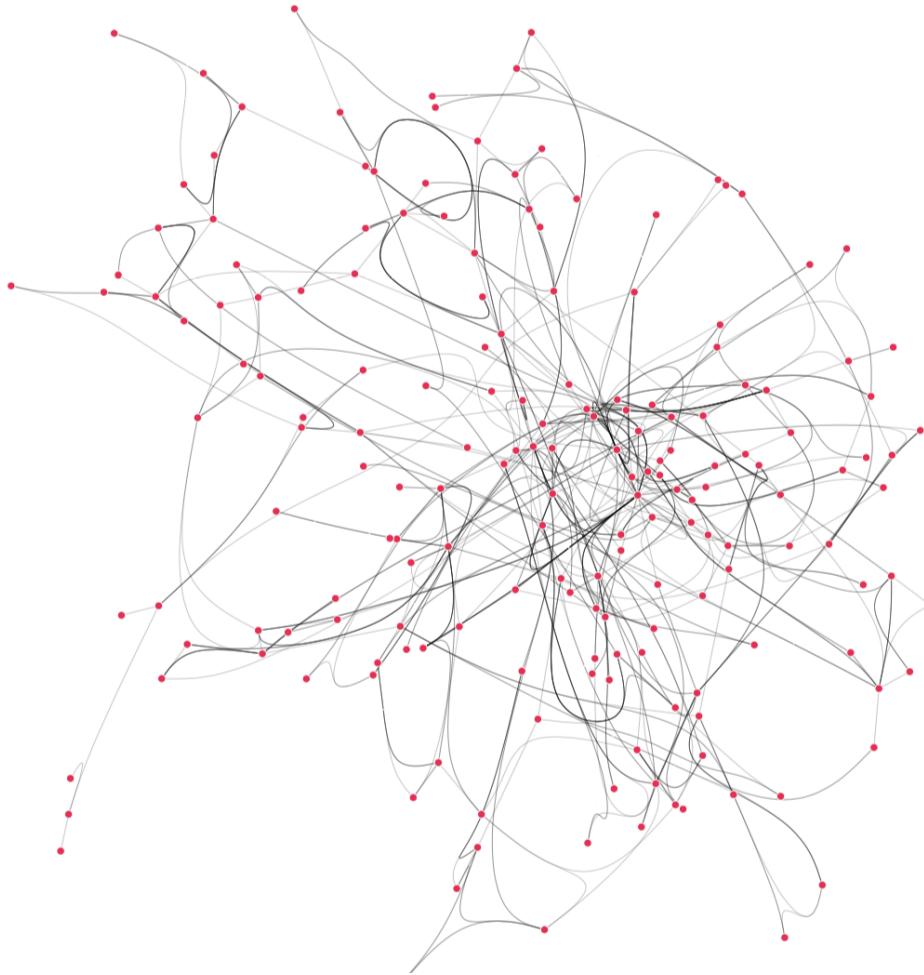


Figure 1.22: **Confluent graphs without crossing artifacts.** The remaining confluent graph with crossing edges removed.

1.4.3.6 Angle / Continuity

Visual representation utilises our conscious and unconscious pattern recognition and intuition abilities [Dixon, 2012]. To avoid apophenia (finding patterns where they do not exist), careful consideration has to be placed in the design of a graph layout. Although edge crossing is often thought of as the most important aesthetic metric, finding a continuity between inward and outbound edges of a node was found to be of equal importance [Ware et al., 2002].

Reducing the angle between related edges increases readability and allows the behavioural process to infer information about a graph correctly. This process can be compared to predicting the direction of turbulent vs laminar flow. In addition to this edges should be spaced evenly around node, maximising the minimum-edge-angle between all edges of a node [Bennett et al., 2007].

1.4.4 Temporal Projection

Story-telling has been an effective method to convey information, experience and cultural values for almost as long as people have been around. Many real-life physical processes occur over time and thus allow the use of a story-telling analogy. Gershon and Page [2001] provides a generic structure which begins with creating a general overview of the subject. Events are then animated in order of occurrence and defined as we go along. Finally any remaining conflicts and uncertainty is addressed, and these are rectified. Using this as a template for our graphs, we find that the content is usually given in the form of a title or figure description, the evolution as the visualisation, and finally the reflection and resolution through the use of user interaction (e.g., node hi-lighting, zoom or animation).

Since very few graph layouts support dynamic time-varying graphs [Kumar and Garland, 2006], several methods of visualising temporal events have been developed. Although storylines can be useful for drawing the evolution of simple systems, these break down when dealing with large numbers of dependent variables. Force-directed layouts may be adapted, to suit these better, whereupon the initial positions of the previous node endpoints are used as the initial positions for consequential simulations. Three methods of representing these are shown in [Ellis, 2018] - screenshots of which are shown in Figure 1.23.

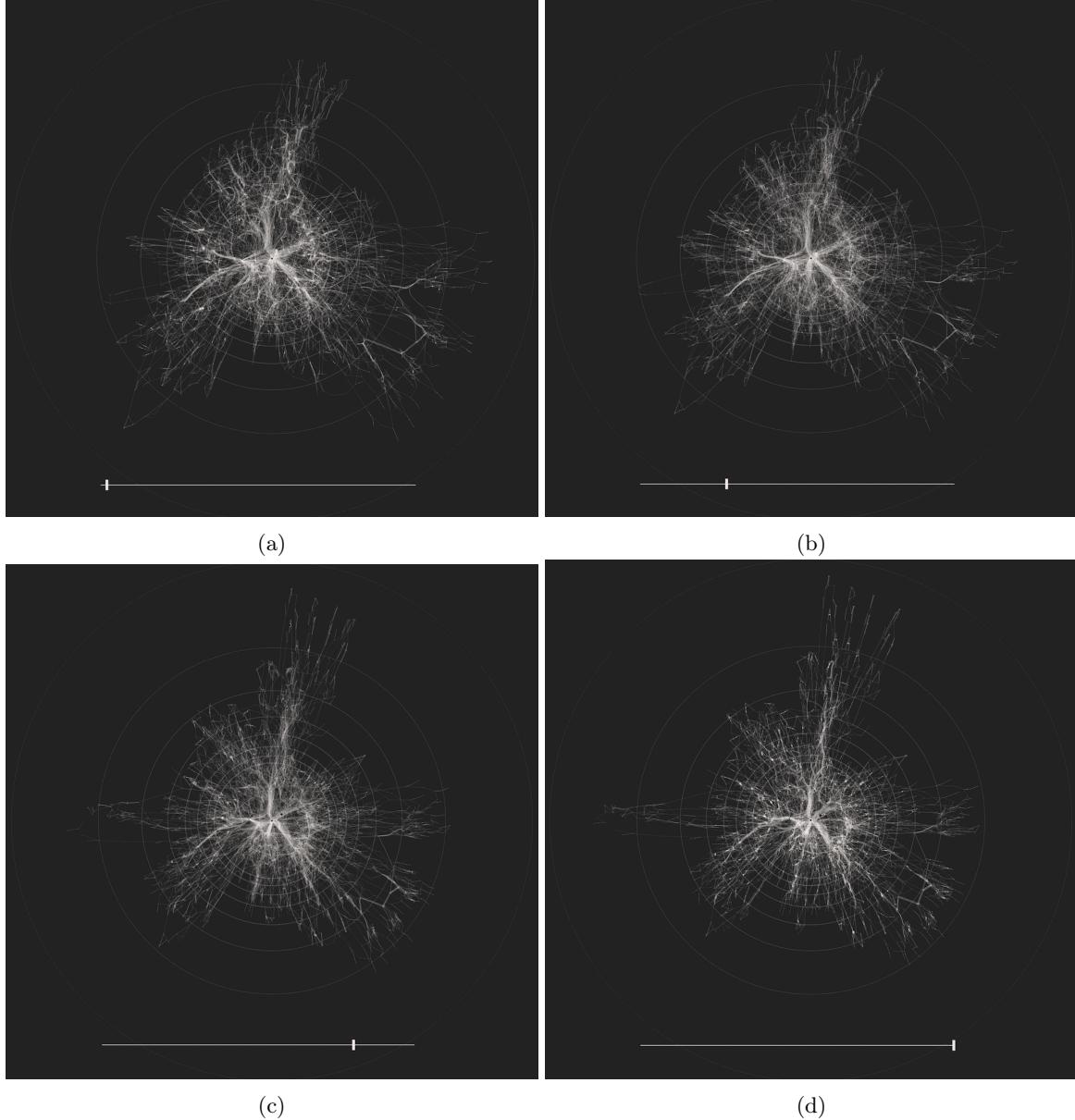


Figure 1.23: Film style representation of temporal changes in a network. Showing the temporal changes from a model simulation of the beijing atmosphere. (a) shows a weighted graph at midnight. With the addition of daylight, the chemistry speeds up causing the force graph to contract, changing the overall network shape (the faster reactions have a stronger attractive force). The animation of this can be found at https://github.com/wolfiex/DanEllisThesis/blob/master/daynight_26mb.gif

Finally, user-interaction such as hi-lighting key nodes/links, zoom and animation⁸ may be used to clarify information at the reflection stage.

⁸[Archambault et al., 2014] notes that animation poses high demands on the users visual memory, and that snapshots are likely to miss underlying patterns. For this reason an interactive techniques that can allow retrospective selection of timesteps allows for a good compromise between these.

1.4.5 Additional Dimensions

Additional dimensions can be used to emphasise certain aspects of our graphs. For instance multiple layers may be used in a directional graph to separate the importance of the nodes [Dwyer et al., 2006b]. Figure 1.24 shows the first, second and third generation species of a mechanism containing isoprene in three dimensions, where each layer in the third dimension represents a different generation of species. Such a visualisation may be explored interactively, with the aid of a computational input device (a mouse, keyboard or device gyroscope), or with the aid of red-cyan 3D glasses (for non-interactive mediums such as print).

Different layers can be used to separate primary VOCs, from species which result in their production (+1 layers) and loss (-1 layers). Temporal data (e.g. Figure 1.23) can also be presented in this format. The only drawback is the high possibility of obfuscation which may result from many layers of overlapping information.

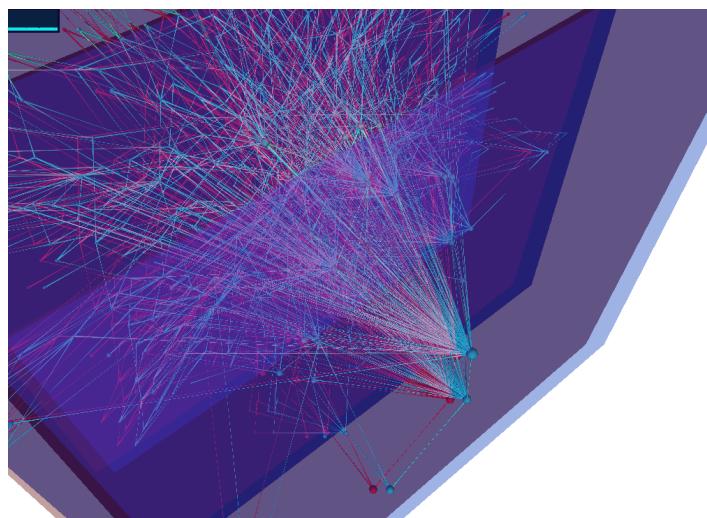


Figure 1.24: **A 3D representation of a graph to highlight certain features.** The first, second and third generation species of isoprene shown as an interactive 3D anaglyph.

1.4.6 Summary

In this section the different semantic methods have been explored. It is found that additional information such as concentration or functional groups may be represented as node size/colour and that there are a range of edge plotting styles that may be used to reduce clutter.

In the next section we combine both semantic and syntactic representation and apply it to an atmospheric chemical mechanism. Using the graph visualisation tools described above we access the quality of information which may be inferred through representing a mechanism in this way.

1.5 A Chemistry Case Study

To conclude we apply many of the tools described above to a simple case study. We select a MCM subset representing the VOCs measured as part of the APHH campaign in Beijing [?]. The chemistry of the mechanism is initiated using the conditions in ??, and propagated by the Dynamically simple model of atmospheric chemical complexity (DSMACC) [Emmerson and Evans, 2009; ?]. We run this forwards to steady state and extract the flux between species on noon. The edge weight is the net flux (product of the species concentration multiplied by the rate of reaction for all reactions between those species and products), normalised to a value between 1 and zero.

1.5.1 Semantic And Syntactic Considerations.

1.5.1.1 Syntactic Representation

Since we shall be using simulation data, we require a layout which deals with both direction and edge weights. The spring-like description of the ForceAtlas2 is chosen from Section 1.2 . This feature highlights fast reactions by bringing nodes together. Such a property has been observed to help users select the shortest path within a network [Pohl et al., 2009]. Here users picked the shortest path an average of 68% for force directed graphs, compared to 40% for hierarchical and 2% for orthogonal layouts. Such properties can help us locate any trends in fast reactions which may control the chemistry within a system.

1.5.1.2 Example Semantic Representation Using A Methane Mechanism.

Since the graph generated by the methane mechanism contains only a handful of species, our screen real-estate allows the listing of names for each node. Node sizes are scaled to represent the concentration of each species at that time point, and edges are coloured to represent the strength of each relationship between them. Here pink edges represent a fast flux and blue ones a slow one. In comparing the the change in graph shape between a weighted Figure 1.25b and unweighted Figure 1.25a graph, we can see that nodes connected by a high edge weight (fast flux) are drawn closer to each other than those with a slow flux.

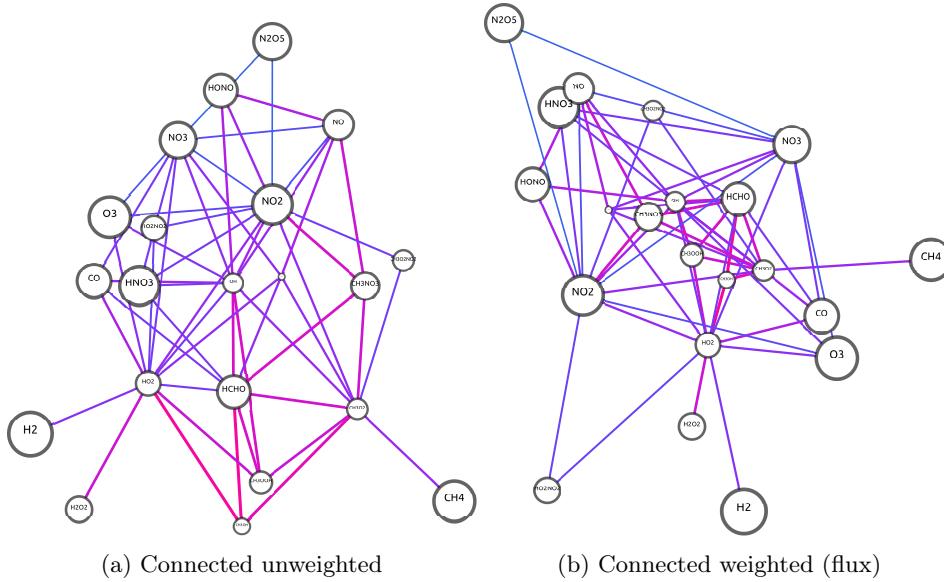


Figure 1.25: A weighted and unweighted force diagram of the methane mechanism. Here it is seen that upon weighting, edges with a faster flux (pink) are drawn closer than those of a weaker one (blue).

1.5.2 A Model Of Beijing

To perform a sensitivity study on the initial positions of nodes within the force atlas algorithm, a graph consisting of links and weightings is constructed using a box model simulation of the Beijing summer environment (mid-day) and feed it the gephi software [Bastian et al., 2009] - an open source software designed for the exploration of networks. We then script the java code to perform the functions in Figure 1.26. As part of this, nodes are initiated with a random position, the force atlas 2 layout is then run and then the graph is rotated and translated such that it is centred around carbon monoxide and has a 45 degree angle between this and formaldehyde. This step constrains the general orientation of the graph, allowing us to analyse the generated graphs for global and local minima. The final step is to save a copy of the generated graph layout and repeat to generate a data set, a subset of which is shown in Figure 1.27. These are discussed further in Subsubsection 1.5.2.1.

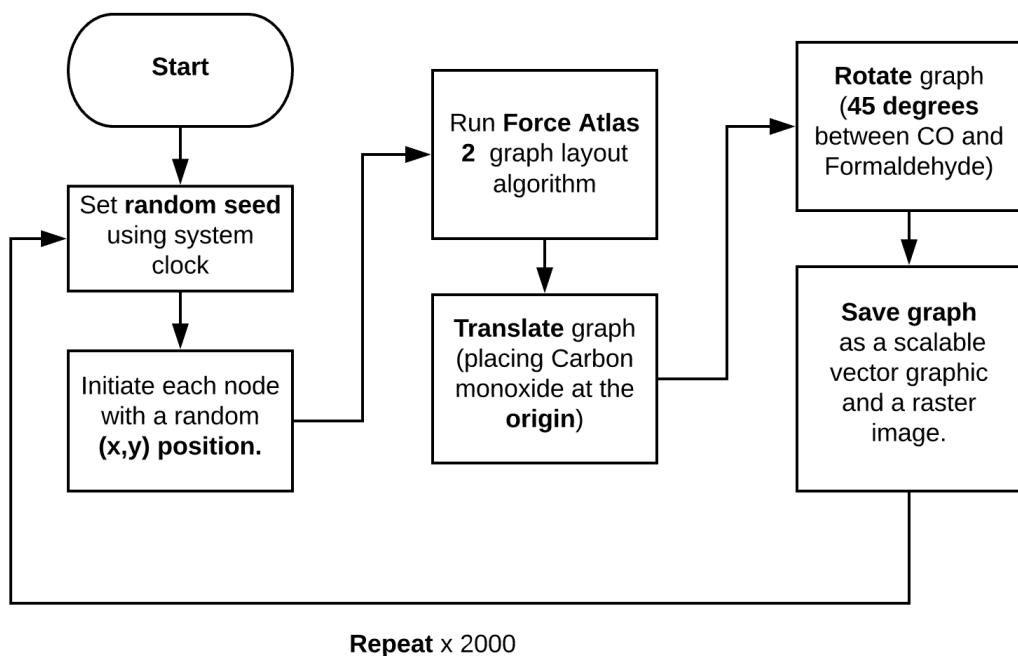


Figure 1.26: A flow chart of the process performed by the custom Gephi script used to generate the data set

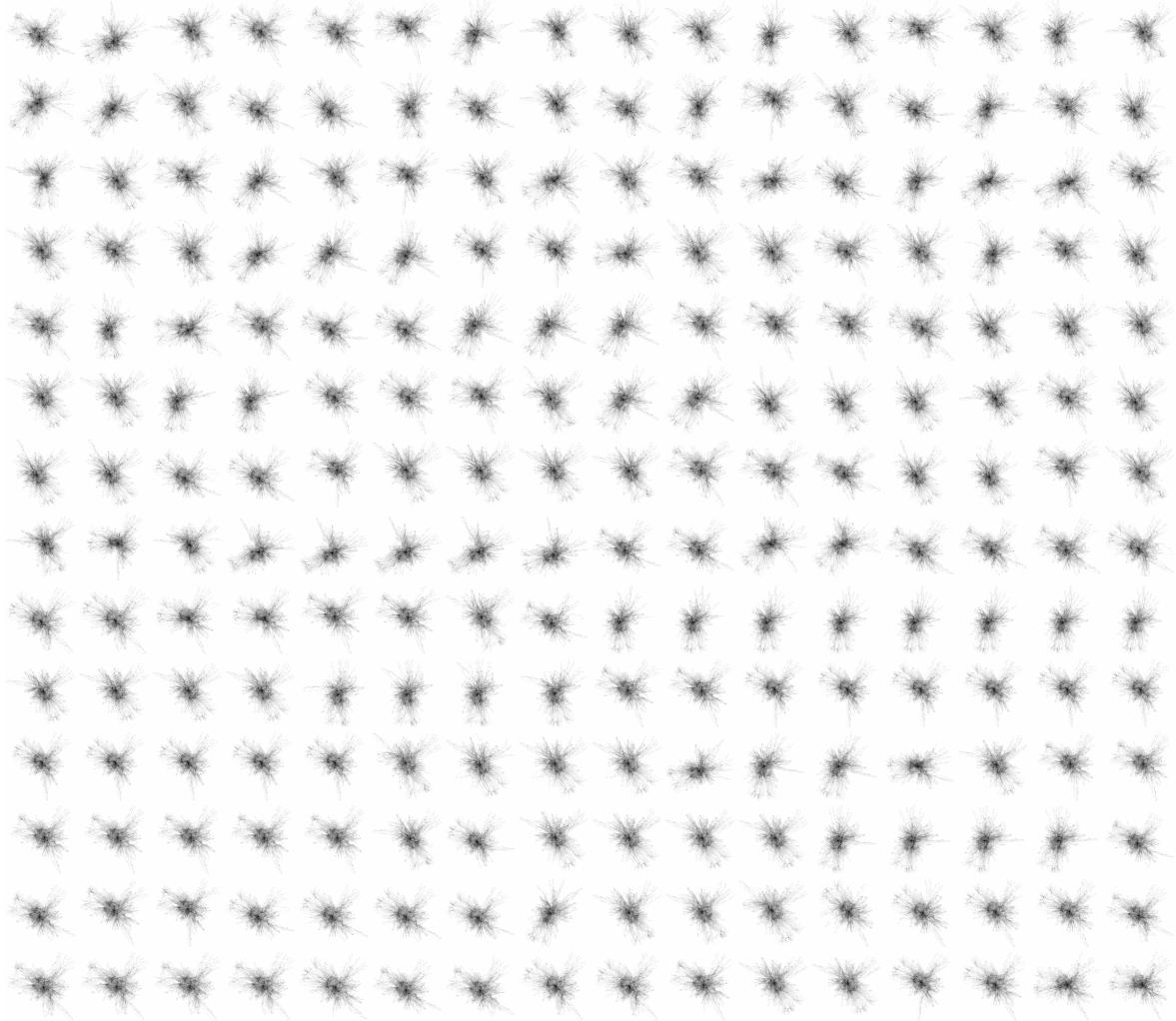


Figure 1.27: A sample of 224 (out of the 2000) graphs generated using the ForceAtlas2 algorithm. These represent the conditions of a spun up simulation of Beijing at noon. The shapes of each graph, and general shapes are discussed in Subsubsection 1.5.2.1 and Subsubsection 1.5.2.2.

1.5.2.1 Similarity Between Graph Shape

Although, through the use of manual intervention, it is possible to perform a superficial level of shape analysis, our cognitive capabilities do not allow us to perform this task for all the simulations of Figure 1.27- less so the entire 2000 graphs in the dataset. To overcome this problem we rely on a method of machine learning called t-Distributed Stochastic Neighbor Embedding (t-SNE) - described in ??, and is the foundation of the tsNET layout algorithm. This is a dimensionality reduction technique used in automatic categorisation of images or photographs [Stefaner, 2020; Sangkloy et al., 2016].

The input for the t-SNE for each dataset is a flattened (1 dimensional) representation of the pixels in the image - we start by taking a binary matrix representing each image, split it up into rows, and glue these together. The pixelmap for each image is then fed into the t-SNE algorithm from the

Scikit Learn package [Pedregosa et al., 2011]. This reduces the logical list of pixels for each image into a two dimensional representation of their similarity. We plot each file, for its (x, y) coordinate, and isolate clusters of similarity using density contours in ??.

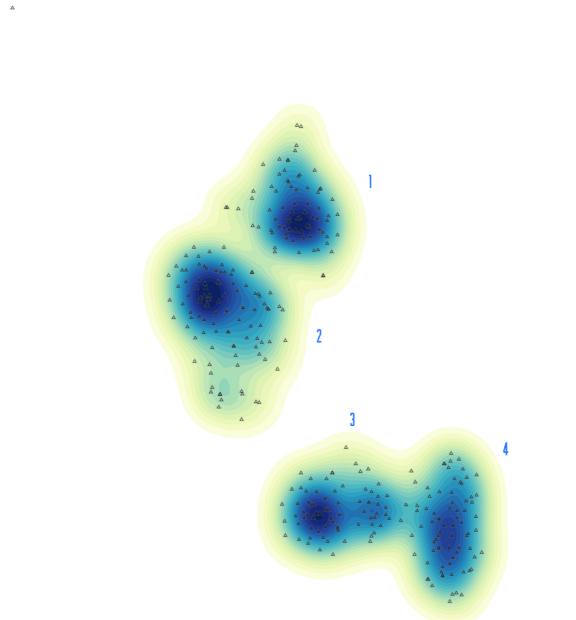


Figure 1.28: **A normalised scatter plot of 2D space produced by the t-SNE algorithm.** Each triangle represents a different arrangement of the MCM nodes shown in Figure 1.27, and the colours/density contours show the regions in which we find similar images/graphs.

Using interactivity and/or vector cluster detection techniques it is possible examine which files contribute to an area of high density. Figure 1.29 shows a sample of four graphs from each of the four corresponding clusters. Although individual node locations may vary, patterns on the macro scale start to emerge, with similar groups exhibiting symmetrical symmetry, e.g. groups 1/2 and 3/4. This suggests a constraint in the overall degree of freedom can be attributed solely to the network structure, and consequently the chemistry which forms this. The non-random nature of the produced graph layouts mean that it would be possible to juxtapose a variety or mechanisms using the force atlas 2 layout.

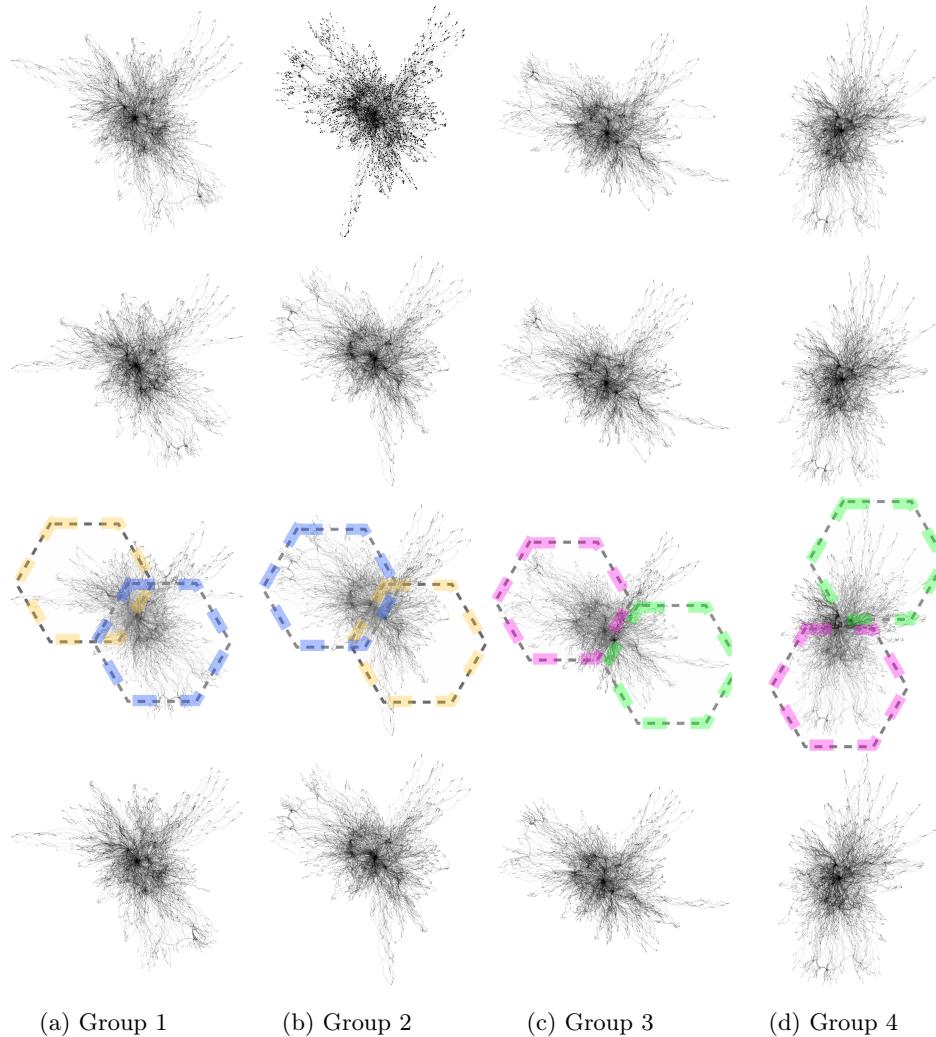


Figure 1.29: **A selection of graphs corresponding to the labeled clusters in Figure 1.28.** These reveal that symmetric similarity between like-positioned points within the t-SNE output.

1.5.2.2 Network Branch Classification

In Subsubsection 1.5.2.1 it was seen that there exist a certain branch pattern that emerge from the structure of the MCM (Figure 1.29). Upon manual inspection of the simulations (Figure 1.27) many graphs appear to contain three branches for each graph - using this it may be hypothesized that these are a result of the mechanism, and by consequence the chemistry it describes.

To test for this we categorise all primary emitted species into Alkanes, Alkenes, Aromatics and Terpenes. All nodes and links in close proximity are regarded as products of these species, and are placed within the same group. Using a randomly selected graph from the dataset, the network is separated spatially and nodes within the voronoi cell (These are described in Subsubsection 1.3.1.3) of a primary emitted species are coloured similarly.

?? shows a split in the MCM chemistry for the Beijing mechanism. Here it is found that

- Using this it is possible to separate the MCM network into an aromatic branch, a terpene branch, an alkane and straight chain alkene branches. Such branches not only help us identify changes of chemistry due to biogenic or anthropogenic sources, but also emphasise the path taken to carbon dioxide and water.

Since the MCM does not contain CO₂ we see all the different groups converge on Carbon Monoxide (white, centre).

Using this format, we may now compare the orientation of the many automatically generated layouts.

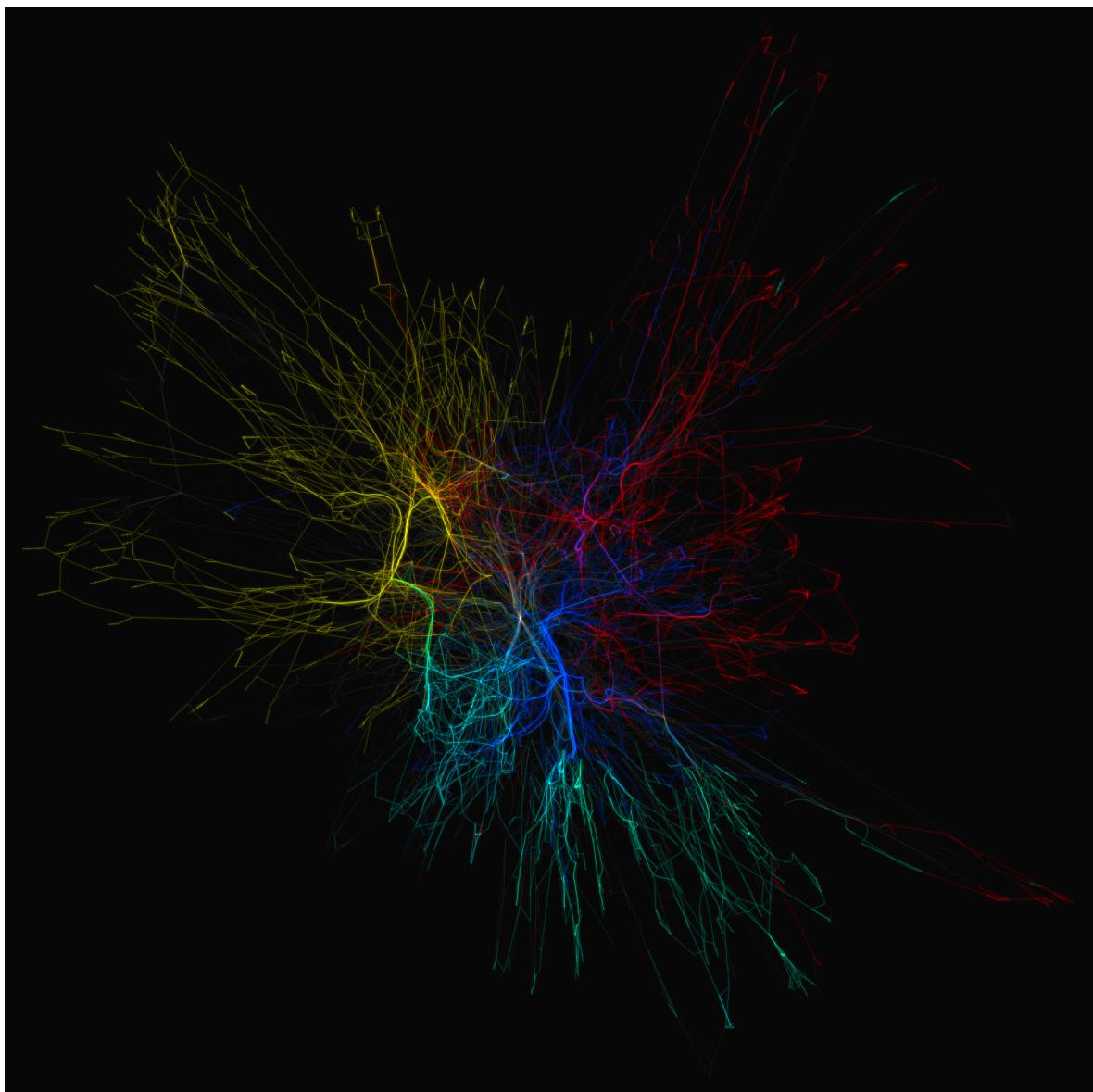


Figure 1.30: Hi-lighting the groups of species, and their products within one of the MCM network graphs from Figure 1.27 These are Aromatics (gold), Terpenes (turquoise) and Alkane/Alkene carbon chains (red/blue)

1.6 Summary

Representing data in a visual format can be used to (utilise) the pattern recognition side of the human brain and alleviate the cognitive strain produced by numerical data. This is a technique used by the Samaritans (YEAR) with the use of cuneiform, and proved useful throughout.

In designing a visualisation it is important to use storytelling and select metaphors familiar to the reader. This should be paired with the correct encoding, as to reduce the time spent trying to comprehend a figure, and increase the knowledge transfer. [ref chapter 1]

When considering relationships, one such analogy lies in the ball and stick analogy. Much like holding hands, this symbolises a similarity between connected items and is the basis of a mathematical graph, or network. Such representations can be applied to the chemical complexity shown in species within the atmosphere.

In representing the chemistry within a mechanism as a graph we may visualise it with the use of a force-directed layout. These are in essence a simple physical simulation, whereupon each graph node is repelled (like-charge), and connected nodes joined by a spring-like attractive force. It is found that the force atlas 2 algorithm not only produces the best visual aesthetic, but also conceptual understanding. Using this it is possible to see patterns such as the the partitioning of each network into aromatic, terpene and straight chain chemistry.

Although graph layouts have a range of local minima, the overall network structure of the MCM is constrained by its construction protocol (due to the allowed chemical reactions), and thus can be used to produce comparable graphs. This method of visualisation, in combination with interactive querying techniques, can aid in the comparison and understanding of large/complex chemistry simulations. This can be particularly useful in the explanation of specific interactions within a mechanism, or the exploration of temporal changes within a simulation.

In the next chapter, I shall extend the graph metaphor for atmospheric chemistry systems beyond that of just visualisation.

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