

The Flavour Network

Science Makers

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Molecular Gastronomy

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Techniques such as cooking meat **for three days at 60° C**, making ice cream with **liquid nitrogen**, or **spherification** are now common in many fine-dining restaurants.

An area which has received some attention as well are the **chemical compounds** that give food its **flavour**.

Food pairings

In recent years it has been suggested by several chefs and food scientists involved in Molecular Gastronomy, that **two foods taste good together if they share chemical flavour compounds.**^{1,2}

1)H. Blumenthal, *The Big Fat Duck Cookbook* (Bloomsbury), 2008

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Food pairings

In recent years it has been suggested by several chefs and food scientists involved in Molecular Gastronomy, that **two foods taste good together if they share chemical flavour compounds.**^{1,2}

This allows for the **prediction** of surprising taste combinations.

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Coffee & Garlic

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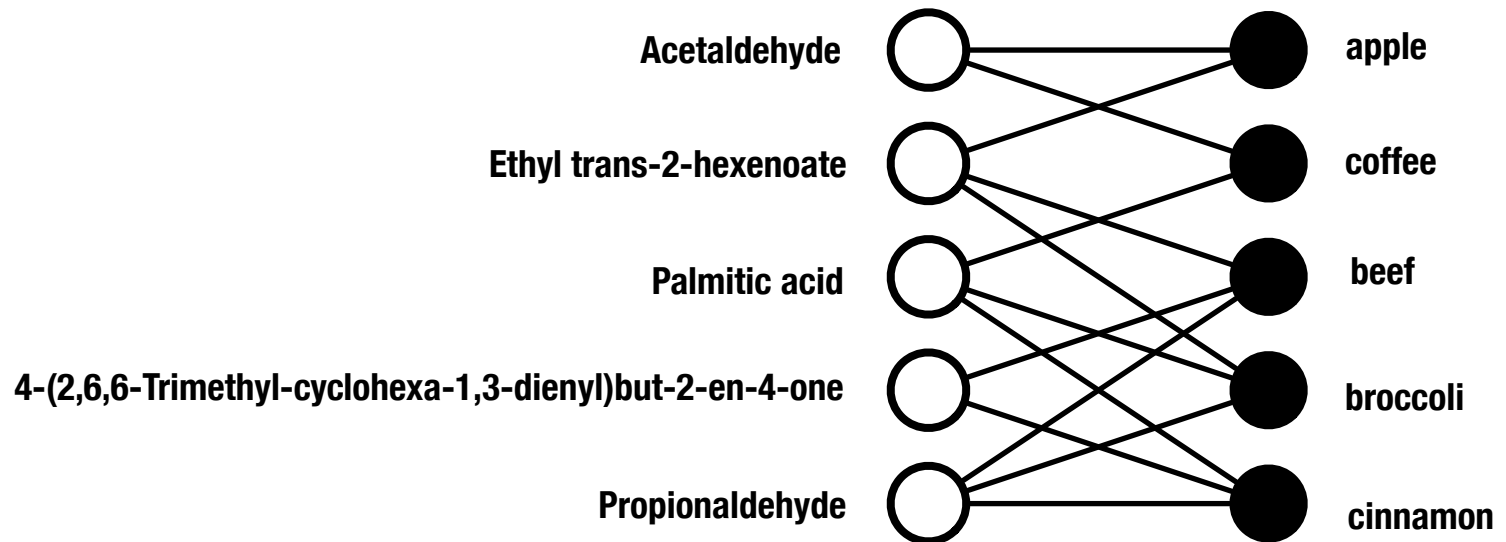
flavour compounds

(e.g. Acetaldehyde, Ethyl trans-2-hexenoate,

and 4-(2,6,6-Trimethyl-cyclohexa-1,3-dienyl)but-2-en-4-one)

Bipartite network

Hence we can draw a so-called **bipartite network**.



Bipartite network

We will analyse this bipartite network using the tools of **complex network research**.

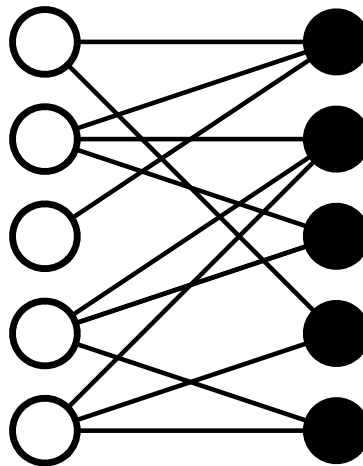
Bipartite network

We will analyse this bipartite network using the tools of **complex network research**.

This is a field that has grown very rapidly over the last decade, after it was shown that **many different real-world networks share common features** and can be analysed using the same tools.

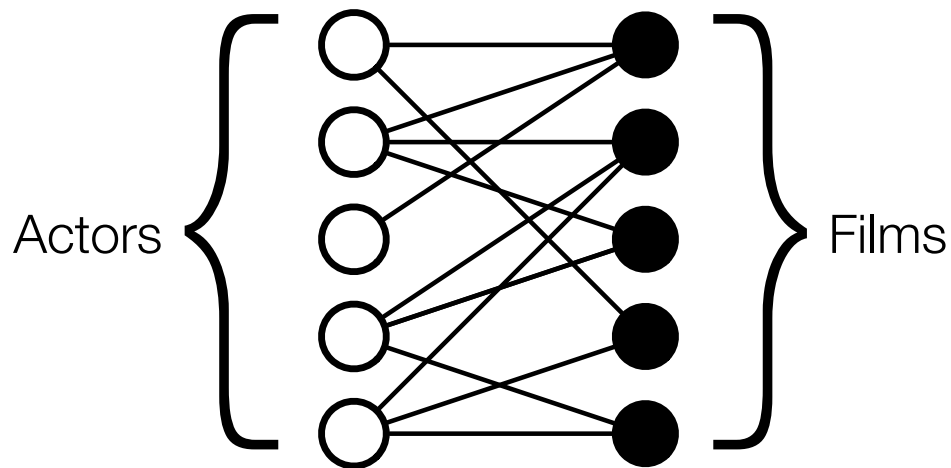
Bipartite network

Bipartite networks are common in everyday life and have been studied in great detail by network scientists.



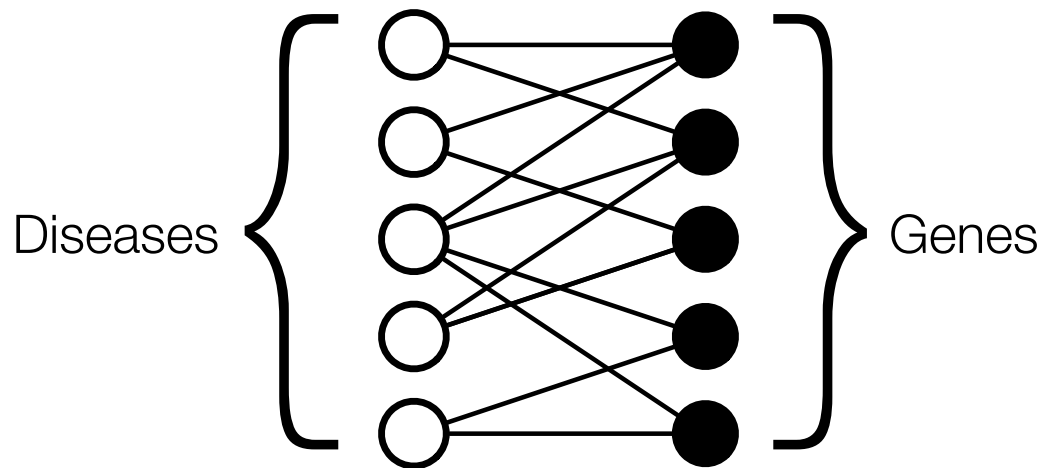
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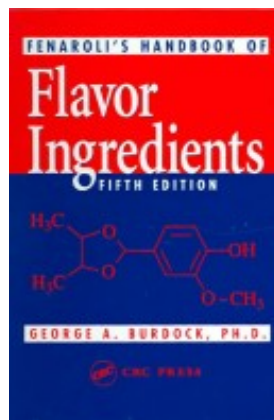
The data

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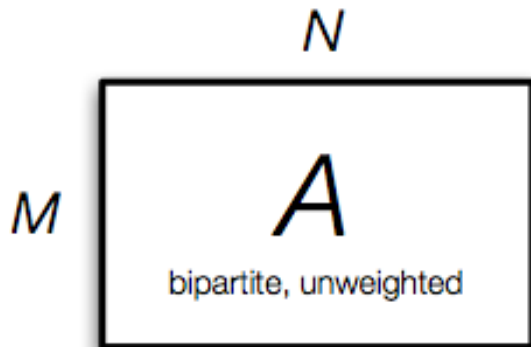
It was compiled from a reference handbook for food chemists [1], by looking up the natural occurrences of flavour compounds.



[1] G. A. Burdock, G. Fenaroli, *Fenaroli's Handbook of flavour Ingredients* (5th ed., CRC Press).

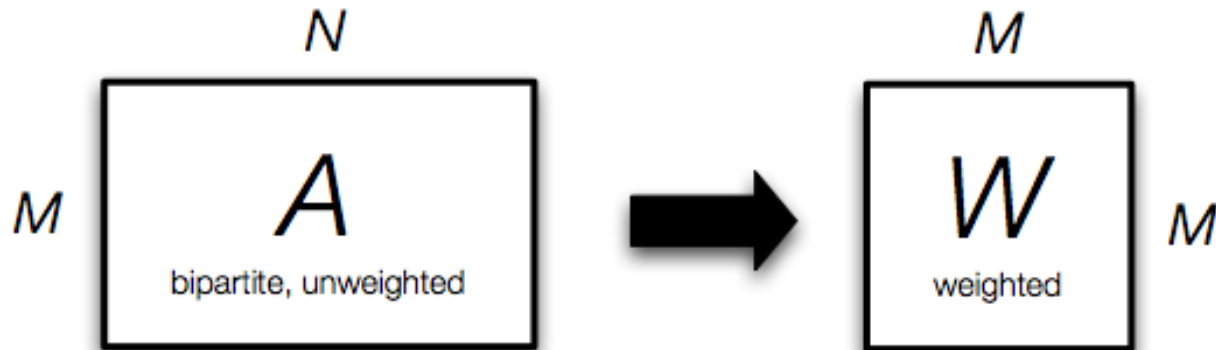
Bipartite network

The unweighted, bipartite adjacency matrix A ,
of M **foods** and N **compounds**



One-mode projection

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can be converted into a weighted $M \times M$ adjacency matrix W
of **foods** only, through a one-mode projection.

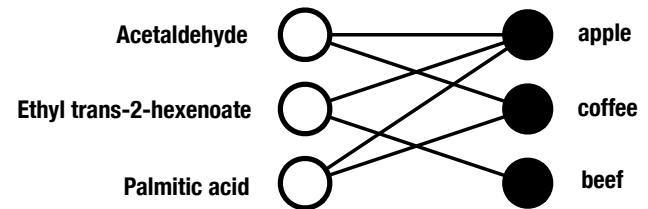
The weights

This means that the entries w_{ij} of the matrix W , given by

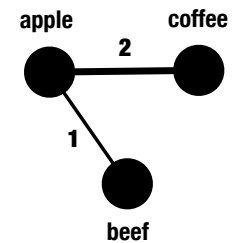
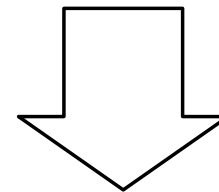
$$w_{ij} = \sum_{k=0}^N a_{ik} a_{jk}$$

indicate the number of **compounds** shared between **foods** i and j .

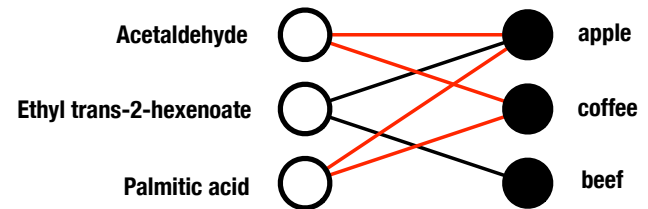
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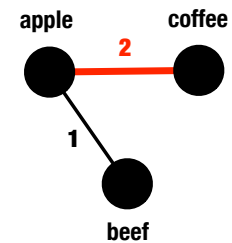
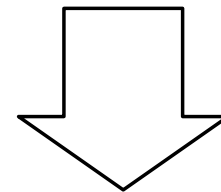
To give a simple illustration:



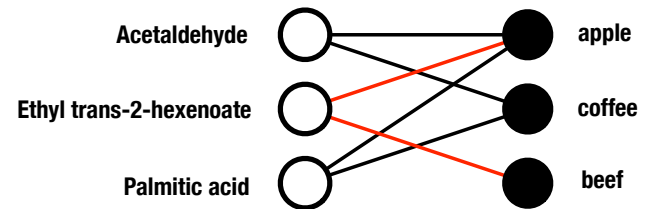
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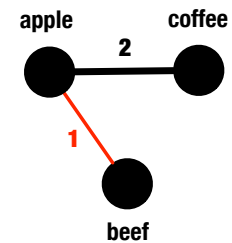
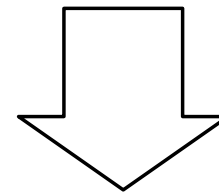
We see that **apple** and **coffee** share two compounds here.



The weights

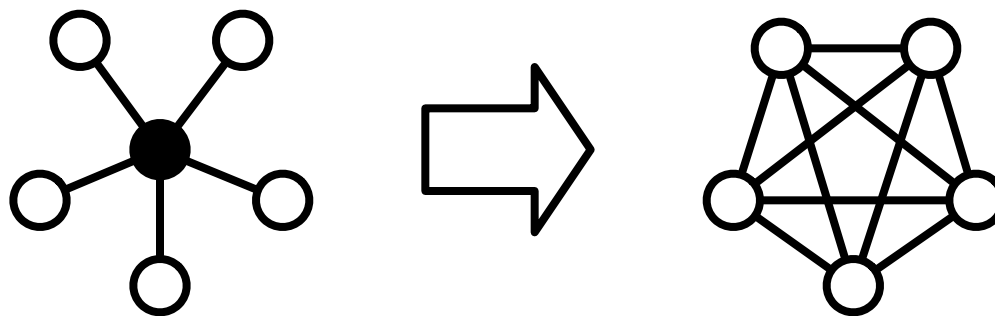


And **apple** and **beef** share one compound.



Too dense!

The resulting network between foods is **too dense** to be drawn in a meaningful way, because several compounds are shared by a large number of foods, which then become a fully connected subgraph.

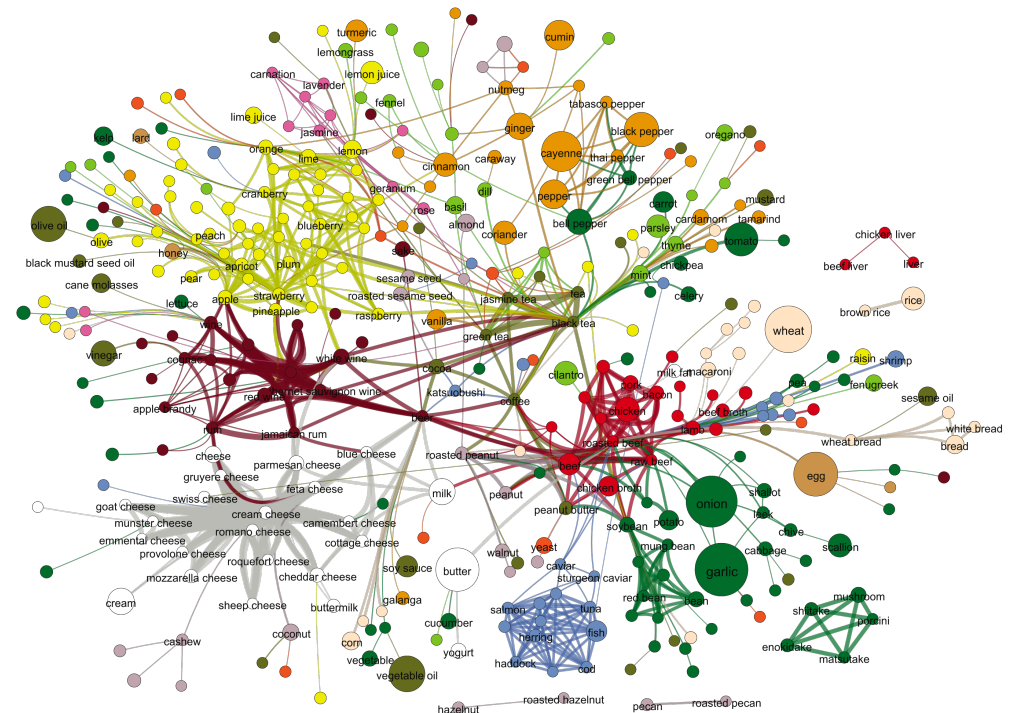


Backbone extraction

In order to visualize the network we extract its **backbone**, using the approach of Serrano et al. (PNAS, 2009).

Backbone extraction

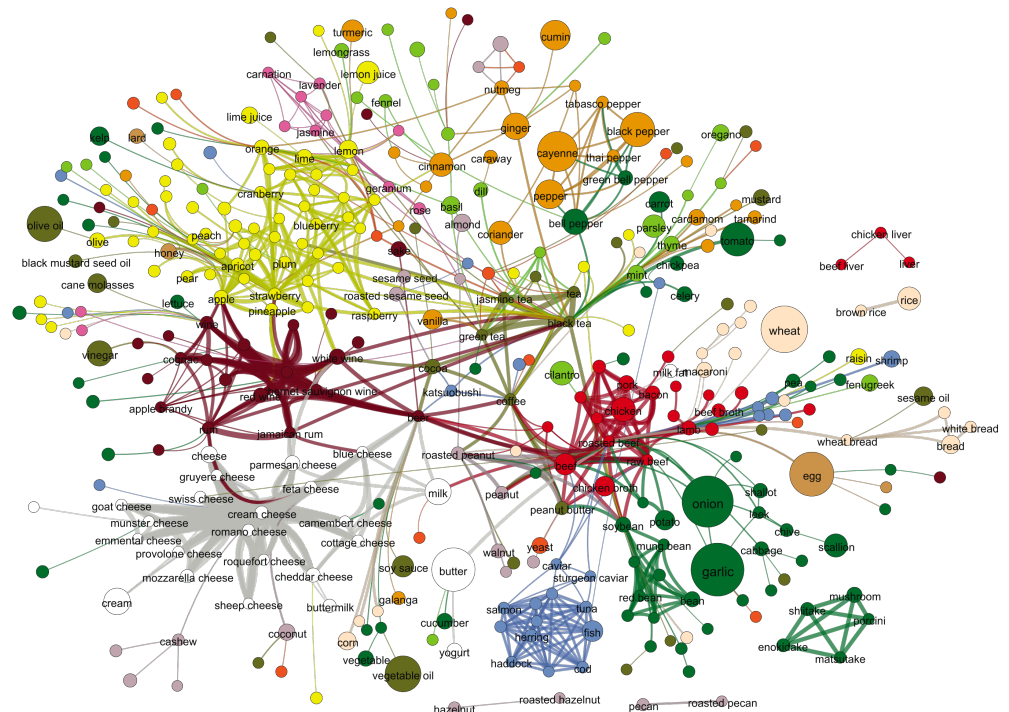
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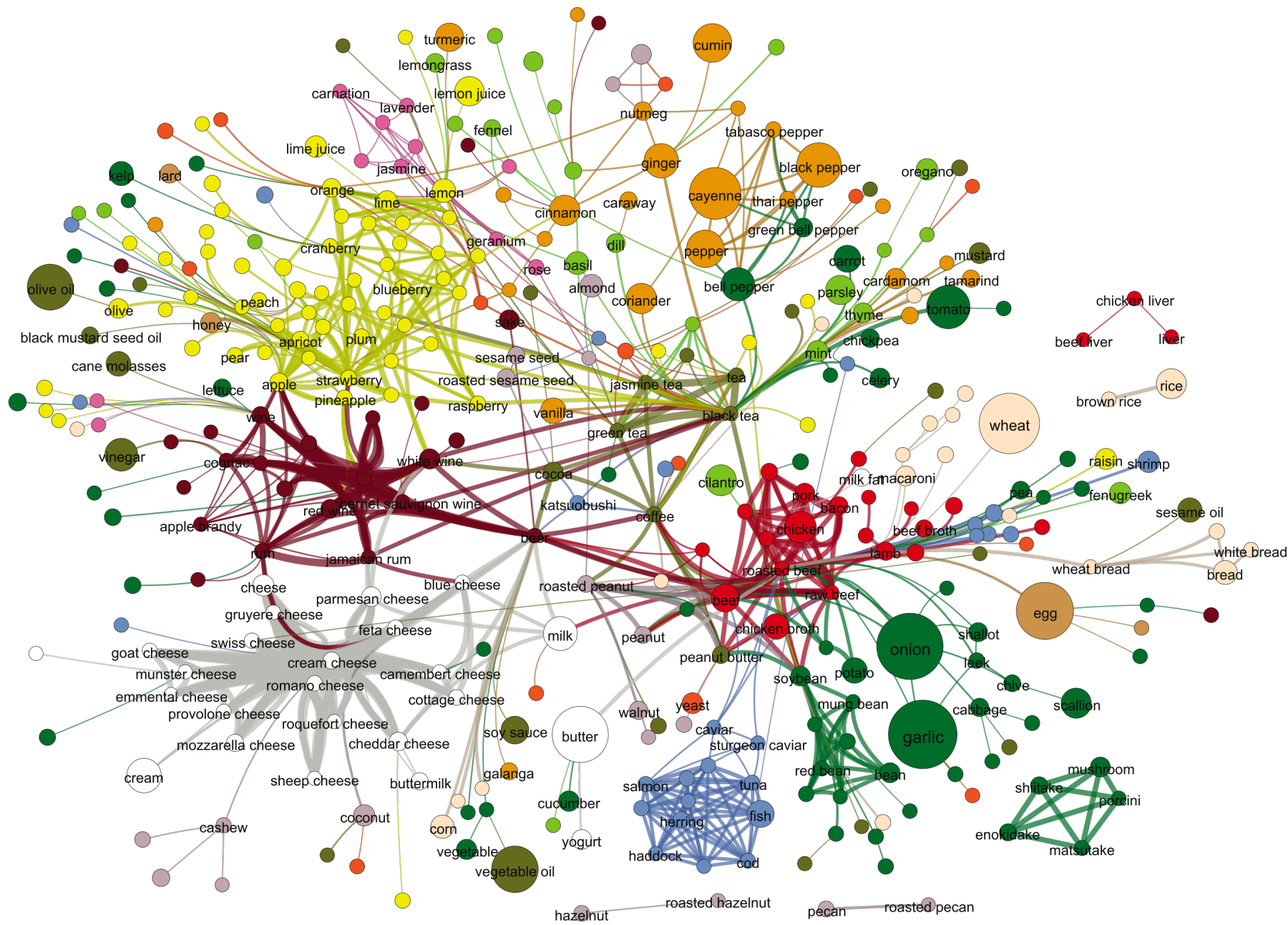


Backbone extraction

In order to visualize the network we extract its **backbone**, using the approach of Serrano et al. (PNAS, 2009).

We see a clear **modular** structure, which strongly correlates with the **food types** (colours), such as meat, fruit, vegetable, etc.





published in Y.-Y. Ahn, S. E. Ahnert, J. P. Bagrow, A.-L. Barabasi, Scientific Reports 1, 196 (2011)

Testing the hypothesis

Let us return to the beginning - the **hypothesis** was that two foods go together if they share compounds, and based on anecdotal evidence it seems to work.

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But can we test this **quantitatively**?

Recipes

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Yong-Yeol Ahn crawled **56498 recipes** from the



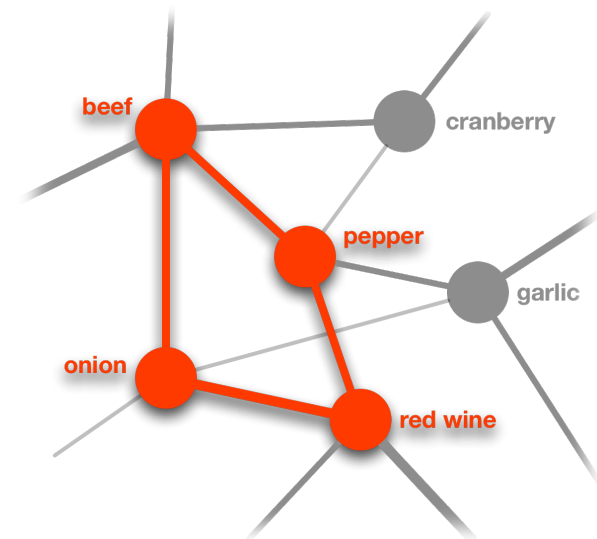
databases.

Recipes

A recipe R is a set of ingredients, and therefore corresponds to a **subgraph** in the flavour network.

To measure whether this recipe confirms the shared compound hypothesis, we can calculate the **average edge weight** in this subgraph:

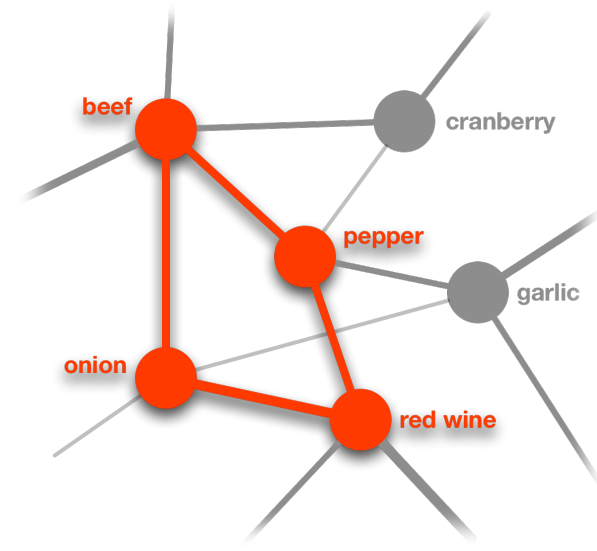
$$N_s(R) = \frac{2}{n(n-1)} \sum_{i,j \in R} w_{ij}$$



Recipes

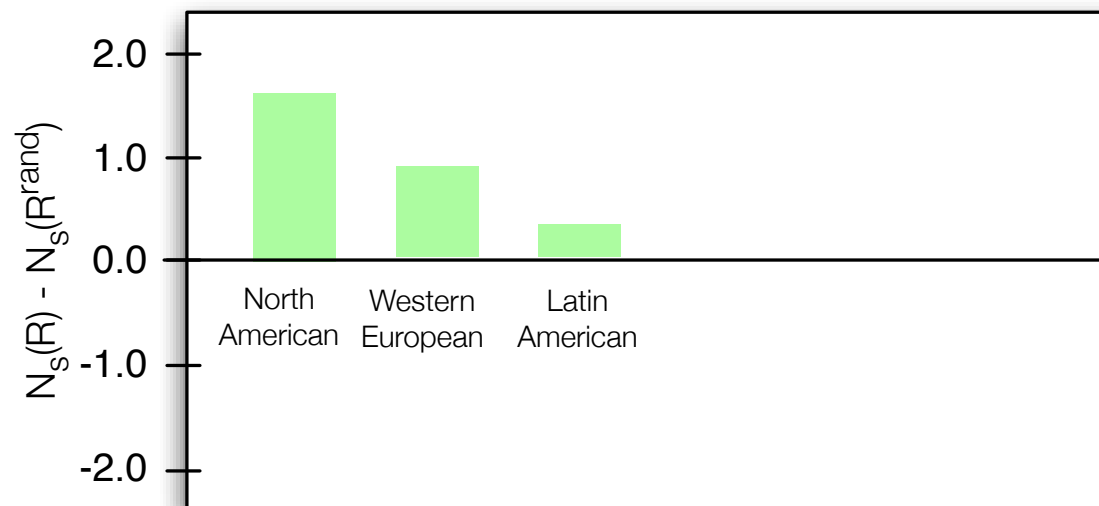
We can then **randomize** the recipes, and calculate:

$$N_s(R^{\text{rand}}) = \frac{2}{n(n-1)} \sum_{i,j \in R^{\text{rand}}} w_{ij}$$



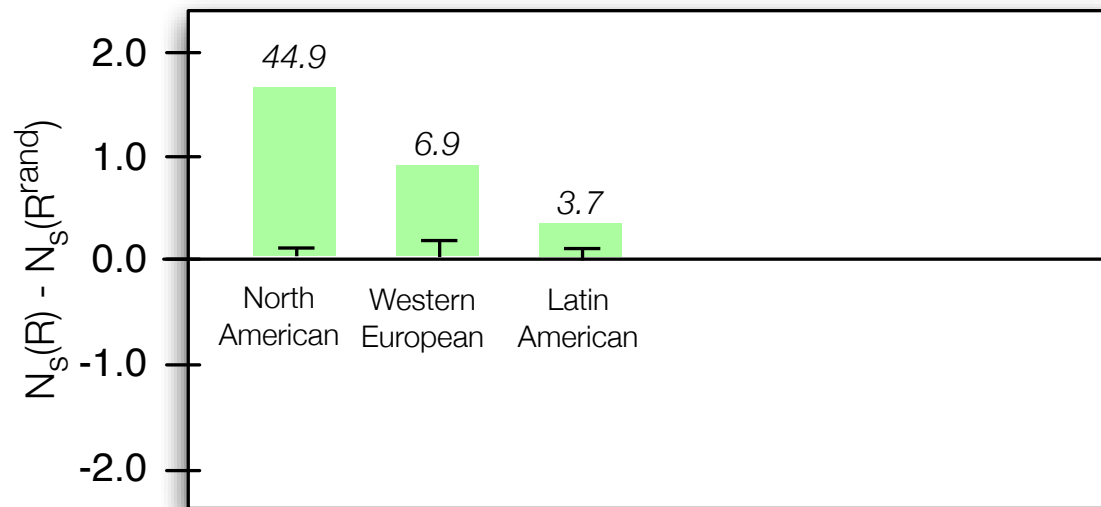
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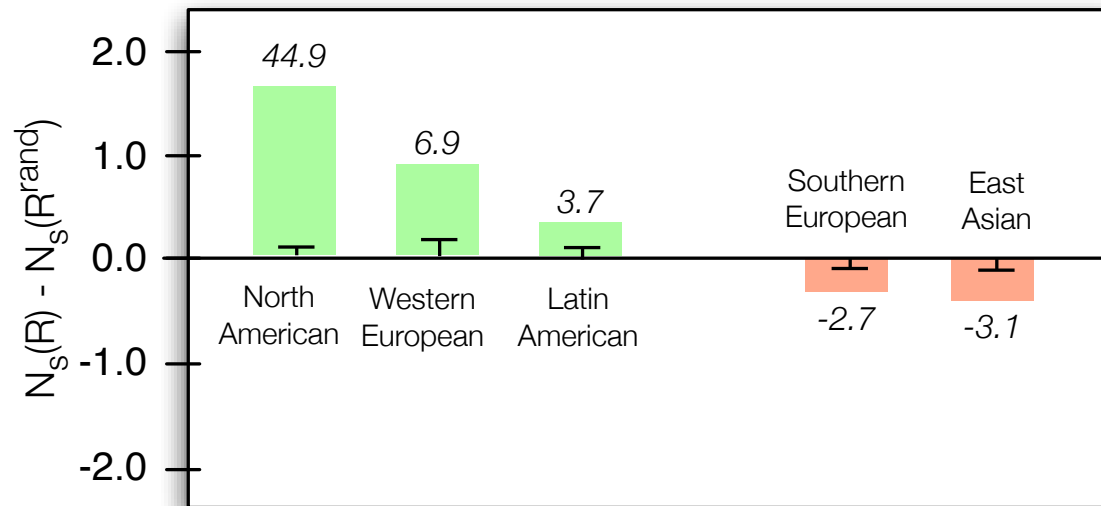
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...and it is significant, but **only for certain cuisines!**

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- there might be **cultural biases** in the compound-ingredient data
- we are not using **concentrations** or detection/recognition **thresholds**

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- East Asian and South European cuisines appear to **deliberately** pair ingredients that **do not share** compounds.
- Both tendencies are **statistically significant**.
- More details: **Ahn, Ahnert, Bagrow & Barabasi, Sci. Rep. 1, 196 (2011)**.

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- Recipe data is problematic, as many recipe ingredients contribute **texture** and **structure** to a dish, not just flavour.

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- Odour and flavour **thresholds**
- Odour and flavour **descriptions** of compounds

The Flavour Bible

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The advantage this data set has over the recipes is that these pairings focus on **flavour**.

Volatile Compounds in Foods

The commercial **VCF** database contains **compound concentration** information on a large number of food ingredients.

We were kindly given access to this databases for research purposes by Ben Nijssen at TNO.

Odour and flavour thresholds

We also purchased a copy of a database containing over 20,000 **odour and flavour threshold** values¹.

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This analysis however is not straightforward, as thresholds vary considerably depending on the medium the compound is in, among other factors.

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Odour and flavour descriptions

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woody-green, piney balsamic odour

1-butanethiol

unpleasant (skunk) odour

OAVs and The Flavour Bible

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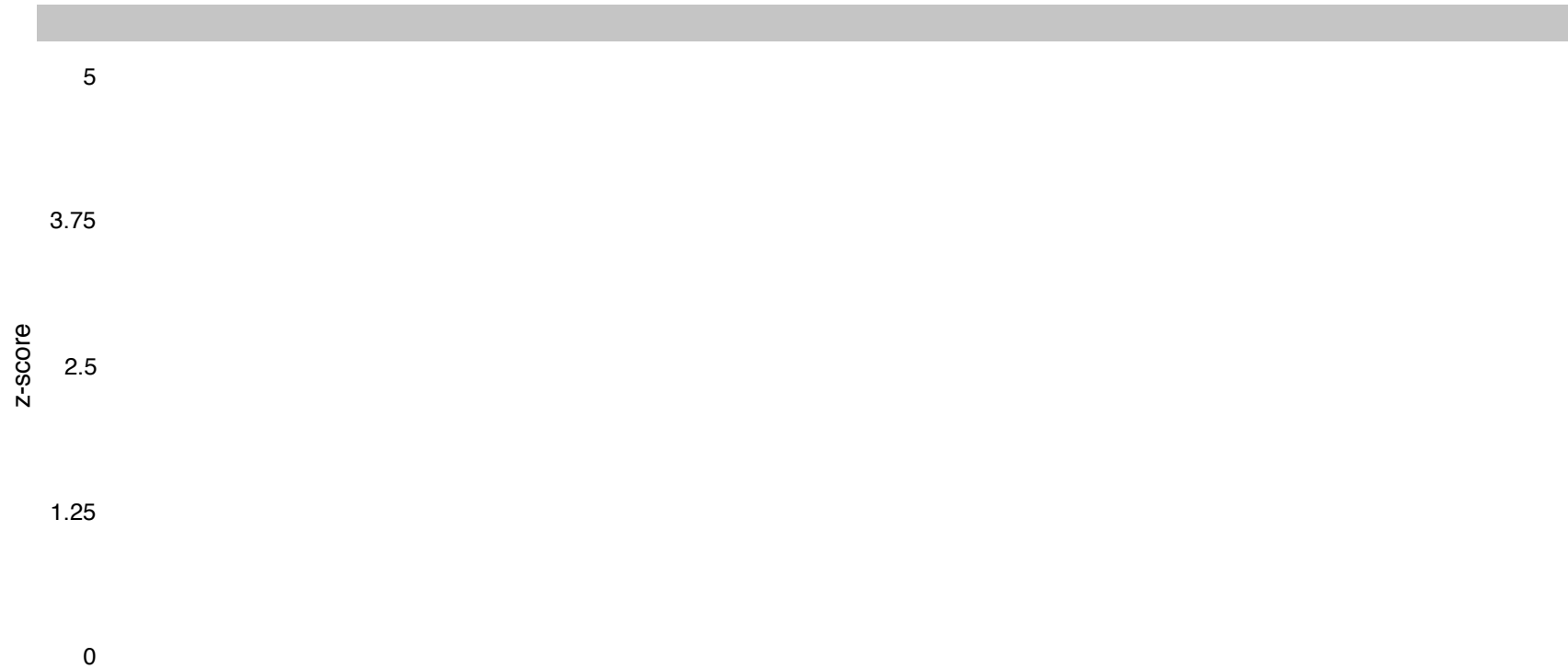
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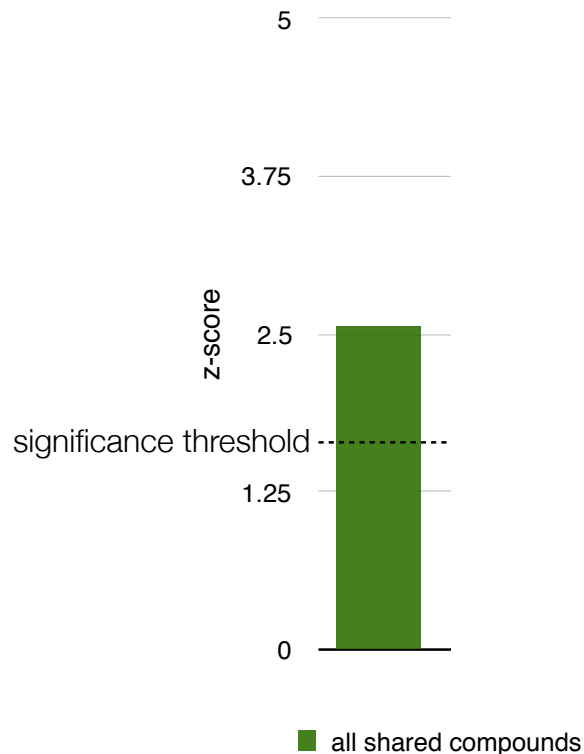
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Like our recipe data, we randomised **The Flavour Bible** in order to see whether compatible food pairs shared more flavour compounds than expected by chance.

OAVs and The Flavour Bible

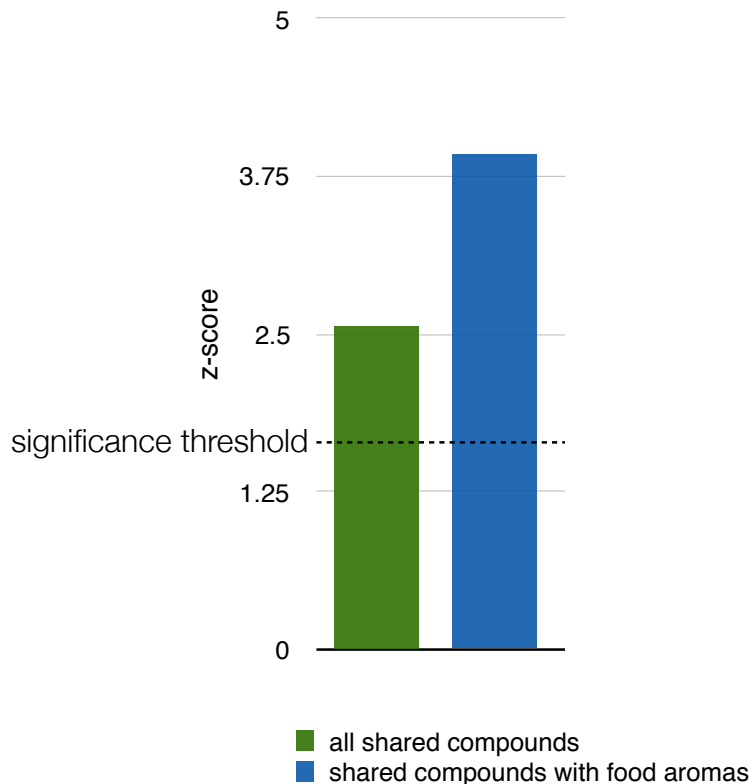


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If we limit ourselves to compounds that have **odours or flavours of foods**, we observe a higher significance score for the shared compound result.

Shared compounds V1.1

We can therefore formulate a modified version of the shared compound hypothesis:

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Two foods are more likely to taste good together if they share **dominant** chemical flavour compounds ($OAV > 1$), particularly if they have **food-related aromas**.

Shared olfactory receptors?

Why does the shared compound effect hold?

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One explanation is that shared compounds lead to the shared stimulation of **olfactory receptor neurons**.

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This is because each aroma compound binds to one or more out of several hundred **olfactory receptor proteins**.

Shared olfactory receptors?

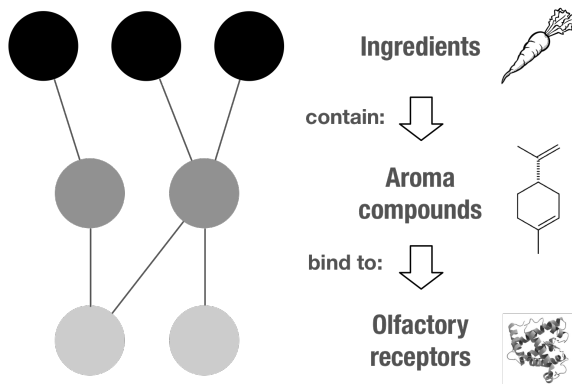
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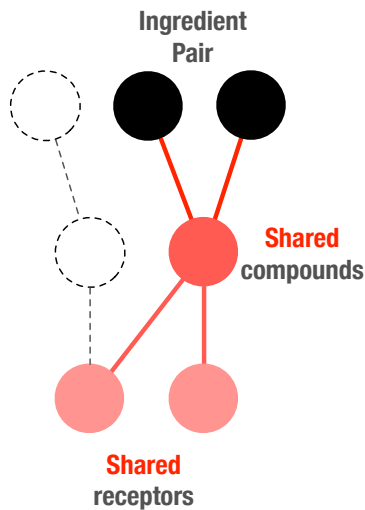
Each of these proteins is expressed in its specific type of olfactory receptor neuron, meaning there is a **one-to-one map** between proteins and neurons.

Shared olfactory receptors?



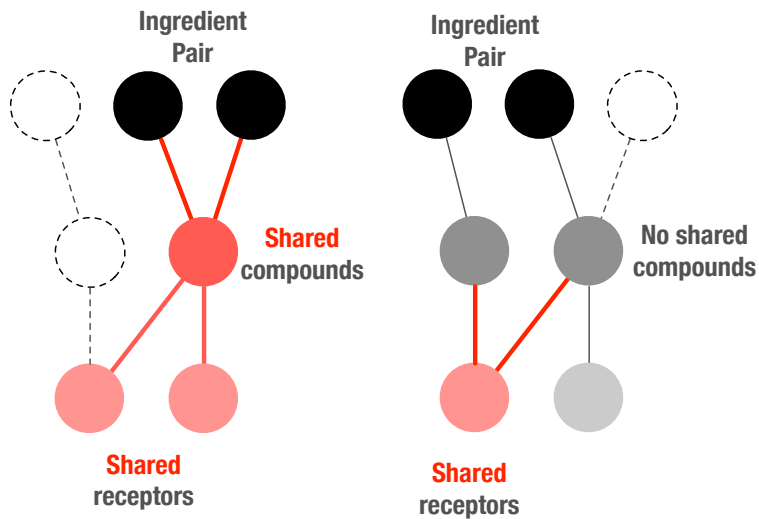
We now have a network with **three node types** – more specifically a tripartite network.

Shared olfactory receptors?



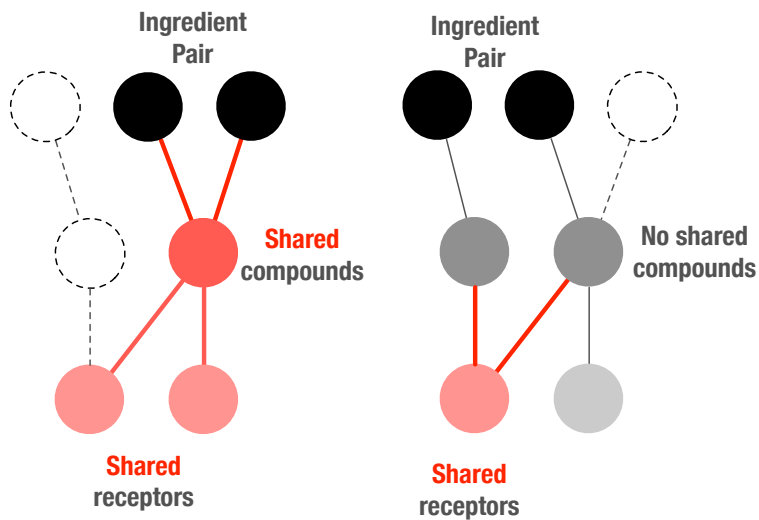
Ingredients can share **compounds**, which means they share **receptors**.

Shared olfactory receptors?



Receptors can be shared **even if compounds are not.**

Shared olfactory receptors?

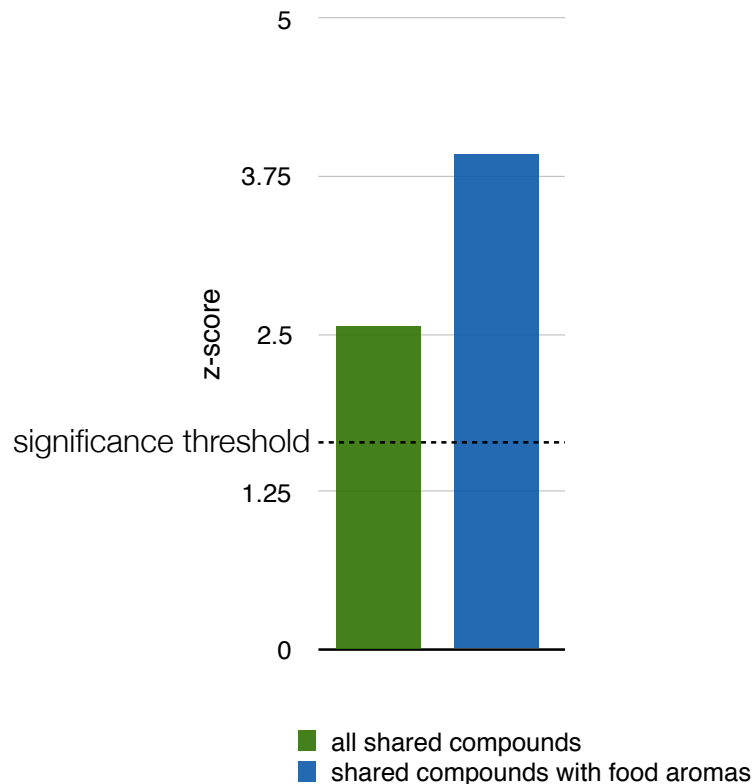


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Data on receptors is beginning to be available.

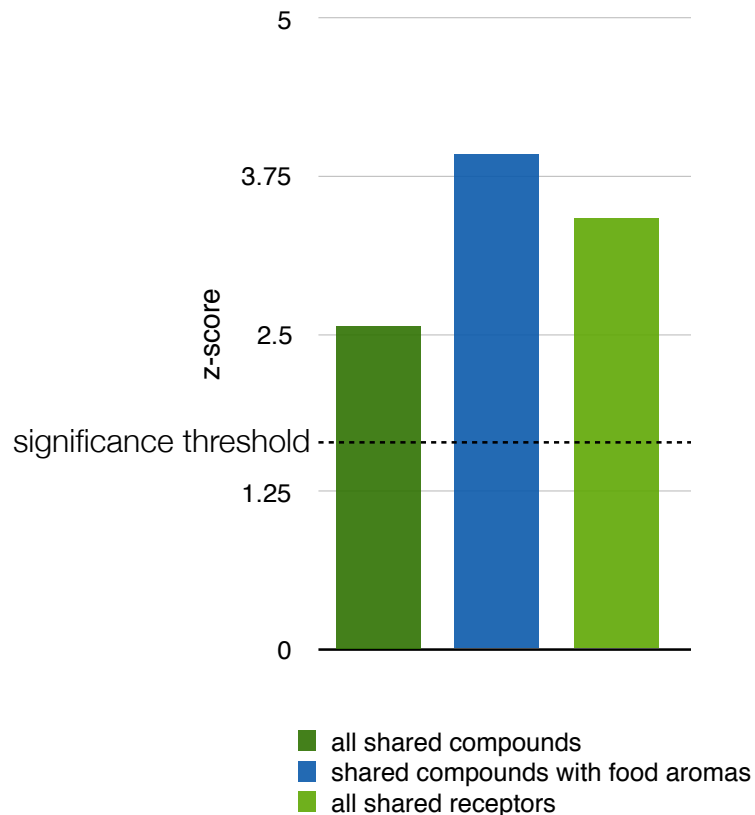
Dunkel, A. et al. *Angew. Chem. Int. Ed.* 53, 7124–7143 (2014)

The Shared Receptor Hypothesis



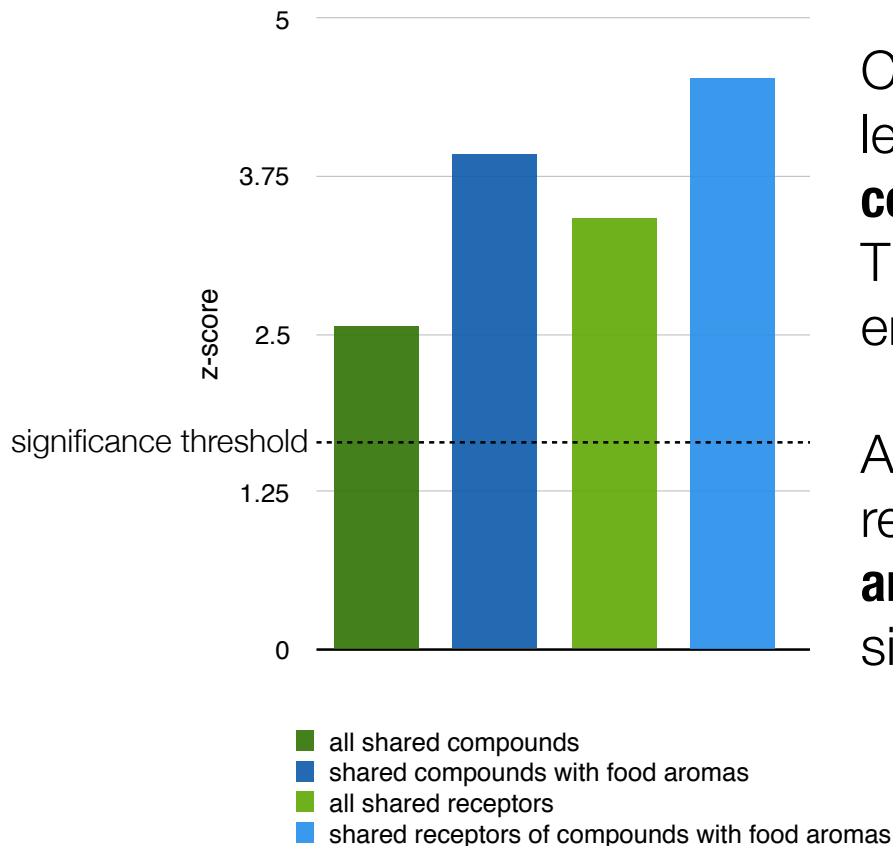
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The Shared Receptor Hypothesis



Comparing to our previous results let us now measure the number of **compound pairs that share receptors**. These are even more highly enriched in The Flavor Bible.

And if we only consider shared receptors for compounds **with food aromas**, the result is even more significant.

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By comparing this network to recipe databases we show that the **shared compound hypothesis holds true** for **some** regional cuisines. In other cuisines, an equally significant **inverse effect** appears to govern the flavour combinations chosen in recipes.

Conclusions

Using new data such as compound concentrations & thresholds, food pairing recommendations and compound descriptions we can show that foods taste good together if they share **dominant** chemical flavour compounds, and particularly those compounds **with food aromas**.

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The mechanism behind the shared compound hypothesis might be the fact that shared compounds mean **shared stimulation of olfactory receptor neurons**. We find some support for this hypothesis by showing that **shared receptors are even more significantly enriched** than shared compounds.

Bigger Conclusions

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So perhaps **computational gastronomy** is next?

Thank you for your attention!

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