How to have Good Ideas Always

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Do me a favour. Think of an airplane. I am thinking of one too right now. This was essentially the task that the first aeronautic engineers were confronted with: Imagining an airplane. The first ever flying machine in serial production was developed by Otto Lilienthal at the end of the 19th century. The apparatus was entirely powered by an initial sprint before take-off. To Lilienthal, flying was like walking, just in the air. His second design iteration used a basic engine to flap the wings of his airplane like a bird. It was only when nautical engineers who had experience building ships changed fields to design airplanes that other propulsion systems were considered.. This is also where we derive the term aero*nautics* from and the reason why pilots are still called "captains". How does a shipbuilder power an airplane? Through a propeller. After all, an airplane is just a ship without the water.

The mode of power you were most probably thinking of, however, is the jet engine. Unlike these other types of propulsion, jet engines really were first and foremost developed with airplanes in mind.[1] The man behind the patent for the jet engine is himself at least as strange as his invention seemed to the people of his time. Fritz Zwicky, born 1898 in Varna, Bulgaria to a family of Swiss cloth merchants, was one of the 20th century's most prolific, as well as overlooked inventors, scientists and thinkers.

After moving to Switzerland, Zwicky studied mathematics and physics at a little-known federal institute in Zurich where he also obtained his PhD. In 1925, he became a professor at the California Institute of Technology where he would teach until his death in 1974. In Pasadena, he would start a career as a prolific astronomer being the first person to posit the existence of dark matter (a name he came up with himself) by applying the virial theorem. You know the virial theorem in a different form as the equipartition theorem – stating that every degree of freedom contributes $\frac{1}{2} k_B T$ to the average energy. Its astronomical equivalent is the statement that the kinetic energy equals half of the potential energy $E_{kin} = \frac{1}{2} U$. Zwicky made the – admittedly bold – assumption that a galaxy is simply a large ball with a radius R and mass M moving at a speed of v. The corresponding kinetic energy in all three directions and its gravitational potential energy[2] are easily found with simple Newtonian physics:

$$\frac{1}{2} M \cdot 3v^2 = \frac{1}{2} \Gamma \frac{M^2}{R}$$

Reordering this equation gives the predicted mass for a known radius and speed of a galaxy. Zwicky applied his equation to the *Coma Cluster* and predicted a mass of 10^{15} times the weight of the sun. Because the mass of a galaxy is proportional to its luminosity, Zwicky knew that the *Coma Cluster* was not producing enough light to have that mass. Thus, there must have been *dark* matter slowing down the galaxy without producing light.

Zwicky was also the first to predict and then experimentally verify the existence of neutron stars. He organised summer schools where high school students could help him analyse thousands of space images to detect neutron stars with an approach we would call *citizen science* today. In 1957, he was the first human to accelerate an object beyond Earth's gravitational field – only twelve days after the (much more useful) Sputnik mission launched the world's first satellite. Among his many ingenious ideas and predictions are also some less practicable ones like turning asteroids into habitable planets or colonising the moon. In any case, Fritz Zwicky is among the most original and productive astronomers who have ever lived. Shri Kulkarni, Zwicky's successor as director at the Mount Palomar Observatory, measures the scientific excellence of astronomers in the unit of "Zwickys". To him, the world seems filled with micro-Zwickys, even a milli-Zwicky being a rare phenomenon.[2]

Fritz Zwicky was very likely a genius. But calling him that also does him injustice. Zwicky had unique talent and creativity, but he also had a very stringent methodology to come up with new ideas. A method that anyone could learn,[3] and that he would spend most of his later career trying to advocate: The Morphological Method.

The morphological method is meant to avoid the pitfall of design we have encountered with the airplane. When tasked to draw up the propulsion system, an engineer will base their blueprint on what seems cognitively closest to them. For a nautical engineer it is the propeller, for a biologist it would be the flapping of two wings. What humans are very bad at is to systematically sample the solution space.

This, however, is precisely what distinguishes the tinkerer from the engineer: the search for optimality. During most of our evolution we humans mostly had to tinker, i.e. locally search for a good solution. When deciding on where to set up camp

1 Interestingly enough, most ships today use some version of submerged jets for steering or propulsion. Apparently, proving that the inverse holds true as well: Ships are just airplanes in water.

2 Vibrational degrees of freedom and NMR transitions do not really size up to an astronomical scale, so we can safely neglect all other forms of potential energy.

3 In 1971, he even wrote a book about it (*Jeder ein Genie*).

at night, a caravan will not first cross the entire desert to find the best camp site but will settle for an ideal solution close to where they are. They will choose the valley of a sand dune for its protection from sandstorms over the peaks, but they will not search any further. The power of engineering (and its mathematical formalism) is to extend search space *on paper* to cover the entire space of possible solutions. The caravans of today have a map at their disposal to find the ideal camp site, not only for tonight, but for each night of the entire trip. The engineer's task is to find this globally optimal solution.

Zwicky used the morphological method to systematically go through all possible designs. This is how he came up with the jet engine in the midst of the Second World War. Instead of locally optimising an already existing solution such as the propeller, he clearly defined the problem (how to efficiently power an airplane) and mapped out all the relevant parameters. The parameters make up the columns of a matrix which Zwicky calls the "morphological box".

You can apply the morphological box to anything. I, for example have recently tried to optimise my daily muesli with its help. Step one is to define the problem and the goal clearly: how to make myself a tasty, healthy and efficient muesli every morning. The problem is that I want to simultaneously achieve multiple things with my breakfast. These are the parameters (or issues) we try to cover. More abstractly, they are also the dimensions of the solution space. Some of the parameters are: Carbohydrates, Proteins, Fibres, Healthy Fats, Vitamins, Solvent (Milk, Yoghurt, …), Additions (spices, sweets, etc.).

The parameters make up the columns of the morphological box. It is very important that we truly consider all relevant parameters here, which will require some prior knowledge. In this case, I had to know what a "healthy" diet consists of. Once this was done, I continued with step three, which is listing all possible values for each parameter. You can find the example I worked through in Figure 1.1. I tried my best to include even solutions that felt immediately wrong. As solvents I wrote down orange juice and coffee (real things people put in their muesli!), even though I could not imagine ever using them.

The last step is to now find all combinations of values, i.e. picking any allowed combination of values from the columns. A possible muesli solution could be: cornflakes, almonds, raspberry, milk. Note that some of the values appear in multiple columns (i.e. the dimensions are not independent):

Figure 1.1: Be as creative and permissive as possible in admitting possible solution values. The whole point of the morphological method lies in the elimination of bias and with the courage to find novel solutions. Maybe your muesli should also be powered by jet engines?

milk is a solvent, as well as a source of proteins. In my case, I also allowed for multiple values from each column to be included. Another solution could be: cornflakes, almonds, raspberry, milk *and* yoghurt.

You *must* go through all possible solutions in this step, lest your biases guide you awry again. Otherwise I would not have considered the combination of two solvents (milk and yoghurt), given my own bias that such a muesli would be "too complicated". In practice you can exclude some solutions based on consistency (e.g. orange juice and milk will not work as co-solvents). In my case, I excluded solutions which do not cover all vital nutrients, i.e. which did not have at least one value in every column. Every solution will be evaluated based on the criteria defined *beforehand*: taste, time, cost. I am happy to report that tomorrow's muesli will consist of apples, oats, cornflakes, milk, and yoghurt with cinnamon as the globally optimal solution.[4]

This approach is easily extended to any chemical reaction, where, if anything, the

[4] Anybody in disagreement is invited to send a letter of complaint to the editor.

parameter space is typically even smaller. Just like those original aeronautical engineers, we chemists are also heavily biased by our experience. Who would have even considered doing Diels-Alder reactions in water before click chemistry came along? Today's expeditions into uncharted chemical space are often through machine learning (ML) models. One such project having been recently presented this semester by a good friend of our institute, Prof. Scott Denmark.[3] His surprising finding was that even after the first iteration of the model, his group had already found a catalyst for a specific transformation that outperformed any previously reported one. Denmark, too, is convinced that the big advantage of ML models in chemistry is to challenge the chemist to consider truly all solutions. Even better, if one does not have to produce all of them synthetically.[1]

The limitations here are clear as well: defining the parameter space for a morphological box or a ML model can also introduce biases. As Denmark realised himself, when he used a ML model to optimise a thionyl catalyst, only to then discover that phosphoric acids are much better suited. It is extraordinarily challenging to parametrise all of chemical space, or, in other words, to make chemistry *embeddable*. A ML model can relatively quickly learn to optimise across all thionyls, but it will not by itself consider all phosphoric acids as well. This is part of the elegance of the morphological method. Even though it can never *quantify* performance like a ML model, the morphological box effectively projects a *n*-dimensional solution space down into a manageable 2D representation. My muesli was 6D in effect, but I could find possible solutions just by combining values in a 2D table that furthermore forced me to consider outlandish solutions. Perhaps Denmark would have been well served with a morphological box to find all possible molecular patterns before optimising them by ML?

So do me a favour. The next time you imagine an airplane, also think of the fact that every component you see first had to be imagined by someone, too. Everything we see around us is a testament to the creativity and prowess of mankind. The morphological method is extraordinarily powerful in producing new ideas. Truly anyone can be creative, simply in the sense of *creating* novel solutions. Fritz Zwicky truly believed that *everyone is a genius*. During his many stays in Switzerland he gave lectures on his method both at ETH as well as the Migros Klubschule. In one of his speeches, which is probably the most concise introduction to his work, Zwicky

laments that "because of the emergency actions which we had to fight […] against nazis, fascists, and communists, it is doubtful whether the older among us will see the day again when we can freely choose our problems".[4] Zwicky always applied his morphological method for the betterment of humanity: first to destroy the Germans in 1945, and then to send scientific journals to their war-stricken libraries. We, once again, are free to choose our field of work, and there are more than enough problems that require new solutions. All you have to do is pick one.

I want to thank Lara Turnherr for being the first to point me towards Fritz Zwicky and his morphological method.

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