Autocatalysis and evolution in metabolic networks

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Autocatalysis is central to biology. Life is autocatalytic: given food, a bacterial cell can grow and divide into two more or less identical bacteria. The same argument can be made at different level of biological organization, like genes, enzymes, cells, multicellular organism, eusocial societies, etc.

The minimal living entity has 3 subsystems, each of which is autocatalytic: metabolism, membrane (compartmentalization) and information storage. During the evolution of life living organism were preceded by infrabiological systems that only had two of the above subsytems. In the widely accepted RNA world hypothesis the infrabiological system consisted of the informational and the metabolic subsystem, and compartmentalization occurred later. The compartmentalization of ribozymes (RNA enzymes) lead to the first living system, and thus this is the first major evolutionary transition.

Metabolism has obligatory autocatalytic cycles. An obligatory autocatalytic cycle is one whose constituents cannot be produced from the externally available (food) molecules. It turns out that ATP, the universal energy molecule of living systems, is universally obligatory autocatalytic. We have so far analysed 24 Bacterial, 4 Archaeal, and 2 Eukaryotic genome-based metabolic reconstructions. In each of them ATP was found to be obligatory autocatalytic. In certain organisms, other cofactors, such as NAD, CoA, THF, was also found to be obligatory autocatalytic.

Plausible metabolic networks can be generated, but then we need to understand how and in what order did reactions in the network get enzymatic catalysis. On one hand, having more reaction catalysed result in higher yield, but more enzymes also require more biomass component to be produced to replicate the whole system. Moreover, side reactions are problematic. We have shown by numerical simulation of an enzyme-catalysed reaction chain that specialist enzymes can appear, but only after the invention of linked genes (chromosome).

There is still much to do. The employed reaction network was very simple, not even approaching the complexity of real metabolic network. Algorithmic, modelling and computational innovation is required to make the transition from toy-models (which are still computationally hard) to more realistic ones.

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