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Structural and Functional Genomics of the Human Gut Microbiome

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The microbiome is a diverse, dynamic, and complex environment important to health. It harbors tens of trillions of microbes represented by more than 2 million unique genes. Through its malleability and links to health - being associated with diseases ranging from obesity, ulcerative colitis, type-1 diabetes, through Parkinson's disease, depression, to modulating cancer therapy response - the microbiome is an attractive target for research and therapeutic interventions. Hindering this is our limited understanding of gene functions and metabolic potential encoded within the microbiome.

Currently, we are able to functionally annotate less than 50% of microbial genes. To address this, we devised a synergistic approach in which through large-scale grid computations we predict *de novo* 3D protein structures of microbial proteins from sequence. Then, using those structures and a combination of LSTM and deep learning Graph Convolutional Networks (GCN), we annotate gene function with higher accuracy and coverage. Finally, those results are used in a custom metagenomic annotation pipeline for high-accuracy and high-coverage annotations of real-world metagenomic datasets.

Thus, we build a gene/protein sequence-structure-function link, which combined with an influx of metagenomic data and the development of machine learning approaches to design individual's microbiome composition opens up new avenues for microbiome-oriented therapies and precision medicine.

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