

BEAGLE



Science Highlight

Zodiac: a comprehensive depiction of genomic interactions in cancer

Project Duration: April 2013-Present

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Summary:

Complex diseases like cancer are rarely caused by an abnormality in a single gene, but rather reflect perturbations to intracellular molecular interaction networks that attract cells to new malignant and carcinogenic states. Learning the genomic interaction networks is critical to the elucidation of the molecular mechanisms of cancer, identification of cancer genes and pathways, and discovery of network-based biomarkers that improve disease diagnosis and prognosis.

We introduce Zodiac, a comprehensive cancer genomic interaction database, based on integrative analyses of The Cancer Genome Atlas (TCGA) data (<https://tcga-data.nci.nih.gov/tcga/>), which include whole-genome measurements of multiple genomic and epigenomic features, such as DNA sequence, copy number, DNA methylation, gene expression, protein expression, and miRNA expression for thousands of matched cancer patient samples in over 20 types of cancer. We develop and extend novel Bayesian Graphical Models (BGMs) to infer genomic interactions in each pair of genes (total ~200 million genepairs) for every cancer type using the multi-modal TCGA data.

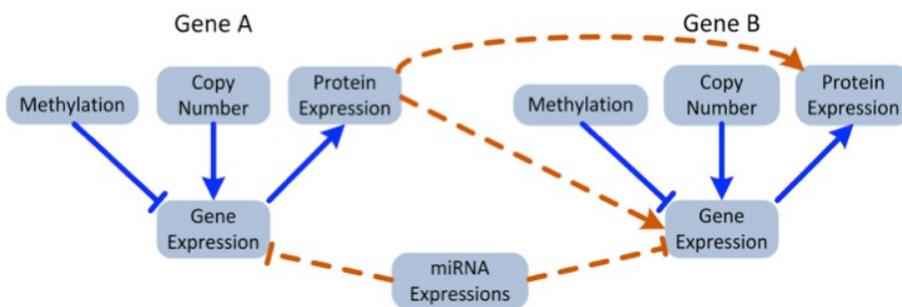
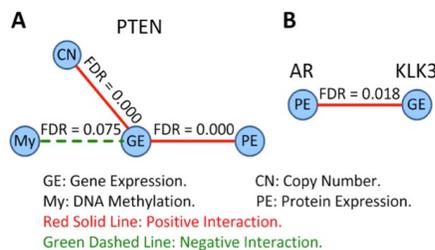


Figure 1. An illustration of some genomic interactions that can be inferred in the analysis of a gene pair. Blue solid lines indicate intragenic interactions. Orange dashed lines indicate intergenic interactions.

Figure 2. Examples of significant molecular interactions identified by BGMs in breast invasive carcinoma. A. The identified intragenic interaction network of tumor suppressor gene PTEN. B. The most significant interaction between Androgen Receptor (AR) and KLK3 inferred by BGM. AR is a transcription factor that regulates KLK3 expression. AR has been demonstrated to be a prognostic factor for breast cancer and is considered a target of endocrine therapies for breast cancer.



Upcoming Training

Python on Beagle

December 4th, 2013 at 10 am, room 240A, Searle building.

The training will cover topics such as:

Techniques for improving Python performance

MPI4PY, NumPy, Scipy, Matplotlib

Python & packing jobs

Python & multiprocessing

Python & MPI

Beagle Intro

November 21st, 2013 at 10 am, room 240A, Searle building.

The training will cover topics such as:

Basic access and navigation operations

Using compilers and applications

Appropriate use of local and network filesystems

Submitting jobs and monitoring jobs

Data transfer

To learn more go to: [Trainings and Events](#)



Additional information can be found at: [Beagle Website](#)

Scheduling Policy and Access to Beagle

- For normal priority jobs, there are no limits to the number of nodes, submitted or running jobs, or walltime used. To find more details about specific queue type: `qstat -q`
- For the new low priority settings, the restrictions are a walltime of four hours or less, and nothing more than 10 nodes. Basically, we're scheduling normal priority jobs first, then filling in the gaps with **lower priority jobs**. The smaller the job, the easier it'll be to schedule, so the quicker it will move from queued to running.
- Nothing needs to be specified in the submit script. Low priority configurations are handled on the server side on a per-project basis. Any project that has been designated as having a low-priority allocation will automatically have those settings assigned when Moab reads the project code/name when the job is submitted.
- Scheduling is based on a fair-share system, with four queues to meet the varying needs of our users. Details can be found at: [Beagle Scheduling Policy](#)

Work done during the last maintenance period:

Software upgrade:

- Installed boost 1.54.0
- Installed python with MPI as MPI4PY, Numpy, Scipy, Matplotlib
- SMW upgraded to the latest version, SMW 7.0.UP03
- CLE upgraded to the latest version, CLE 4.2.UP02
- CADE upgraded to the latest version, 6.24

Change in scheduler:

- **Removed interactive queue** because it was used rarely. We recommend users to ask for a reservation if necessary. Small tests (at most threaded code, less than 30 min) can be done interactively on login nodes.
- **Removed scalability queue** because it was used rarely. We recommend users to ask for a reservation if scalability tests are inefficiently run in the batch (which is often the case then the machine is busy)

Allocations:

- **New allocations are active** and there is no carry over of hours from last year. Some groups might not have an allocation anymore because they either not used their previous one or haven't used the machine in some time, if they want to keep computing on Beagle they need to reapply.

Beagle Related Publications

Please keep sending us your publications that are acknowledging Beagle!

Wave propagation of beta oscillations in motor cortex and its relation to spatiotemporal spiking patterns and behavior
Kazutaka Takahashi in CiNet (2013)

Kinematically defined state dependent changes in functional connectivity of neurons and in local field potentials in orofacial motor cortex during chewing and swallowing
Kazutaka Takahashi in Motor control of feeding behaviors session, at Neuro2013 (2013)

Development of the Charmm Drude Polarizable Force Field for the Study of Ion Interactions in Biological Systems
Hui Li, Karen Callahan, Jr. Mackerell, Alexander D., Benoît Roux in Biophysical Journal (2013)

Discovering RNA-Protein Interactome by Using Chemical Context Profiling of the RNA-Protein Interface
Marc Parisien, Xiaoyun Wang, George Perdrizet, Corissa Lamphear, Ketan C Fierke Carol A Maheshwari, Michael J Wilde, Tobin R Sosnick, Tao Pan

Explaining why Gleevec is a specific and potent inhibitor of Abl kinase
Yen-Lin Lin, Yilin Meng, Wei Jiang, Benoît Roux in Proceedings of the National Academy of Sciences of the United States of America (2013)

N-of-1-pathways" unveils personal deregulated mechanisms from a single pair of RNA-Seq samples: towards precision medicine
Vincent Gardeux, Ikbel Achour, Mark Maienschein-Cline, Gurunadh Parinandi, Lorenzo Pesce, Jianrong Li, et al. in Translational Bioinformatics Conference (2013)

Fast and accurate pedigree-based imputation from sequenced data in a founder population
Oren E. Livne, L. Han, G. Alkorta-Aranburu, William Wentworth-Sheilds, Lorenzo L. Pesce, Carole Ober, et al. in American Society of Human Genetics (2013)

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