In Vitro Molecular Pattern Classification Using DNA-Based Weighted Sum Computation

Hee-Woong Lim[a], Seung Hwan Lee[b], Kyung Ae Yang[c], Suk-In Yoo[a], Tai Hyun Park[b], and Byoung-Tak Zhang[ac]*

[a]School of Computer Science and Engineering, [b]School of Chemical and Biological Engineering,

[c]Center for Bioinformation Technology (CBIT)

Seoul National University, Seoul 151-744, Korea

*E-mail: btzhang@bi.snu.ac.kr

Biomolecular computing enables us to manipulate biochemical information directly and this supports its potential as embedded biological tools and applications. Here we describe a DNA-based weighted sum computation method as a novel quantitative analysis tool for nucleic acid solutions. Whereas conventional quantitative analysis using fluorogenic probes is either single target or multiplexed detection and requires subsequent *in silico* processing for further analysis, the proposed method makes it possible to quantify multiple target DNA or RNA species and calculate the sum of the target quantities with their own weight factors, simultaneously. The computation is performed via competitive hybridization between target molecules and a differentially labeled weight-encoding probe mixture, and the result is detected as a fluorescence signal.

As an application of the weighed sum operation, approaches are presented how to build a linear pattern classifier, where negative weight values can also be incorporated for effective classification of the input patterns. Such a classifier can be used for analyzing and classifying *in vitro* patterns represented as nucleic acid solutions, and thus could be applied to gene expression-based diagnosis. As a proof of principle, we prepared two sets of synthetic oligonucleotide DNA mixtures and demonstrated their successful classification experimentally.