

## Abstract

**Motivation:** Glycosylation is one of the most heterogenous and complex post-translational modifications, but.  
**Results:** These are the results for this article.

# Application of Network Smoothing to Glycan LC-MS Profiling

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## 1 Introduction

Glycosylation is one of the most pervasive forms of post-translational modification (Varki (2017)).

Table 1: Fitted  $\lambda$ ,  $\gamma$ , and  $\tau$  for *20141101-04-Phil-BS*

Neighborhood Name	$\tau_i$
high-mannose	17.615084
hybrid	13.599120
bi-antennary	0.0
asialo-bi-antennary	13.919251
tri-antennary	0.0
asialo-tri-antennary	12.906467
tetra-antennary	0.0
asialo-tetra-antennary	14.723146
penta-antennary	0.0
asialo-penta-antennary	11.226188
hexa-antennary	0.0
asialo-hexa-antennary	10.696785
hepta-antennary	0.0
asialo-hepta-antennary	3.071313

Fitted  $\lambda = 0.99$  and  $\gamma = 11.12$ .

## 2 Results

The performance of our algorithm is demonstrated on *20141101-04-Phil-BS* and *Perm-BS-070111-04-Human-Serum*. Please refer to section S4 for all other datasets. For each comparison, the unregularized case is not smoothed, effectively  $\lambda = 0$ , the partially regularized case uses the grid search fitted values of  $\tau$  but uses a fixed  $\lambda = 0.2$ , and the fully regularized case uses the grid search fitted values of both  $\tau$  and  $\lambda$ .

### 2.1 Chromatogram Assignment Performance for *20141101-04-Phil-BS*

The fitted parameters for the network constructed for *20141101-04-Phil-BS* are shown in Table 1. The assigned chromatograms and their quantification are shown in Figure 1. The comparison of assignment performance with differing degrees of smoothing is shown in Figure 2. The ROC AUC for the unregularized case is 0.838, for the partially regularized case is 0.987, and for the fully regularized case is 0.921.

Figure 1: Chromatogram Assignments and Quantification for *20141101-04-Phil-BS*

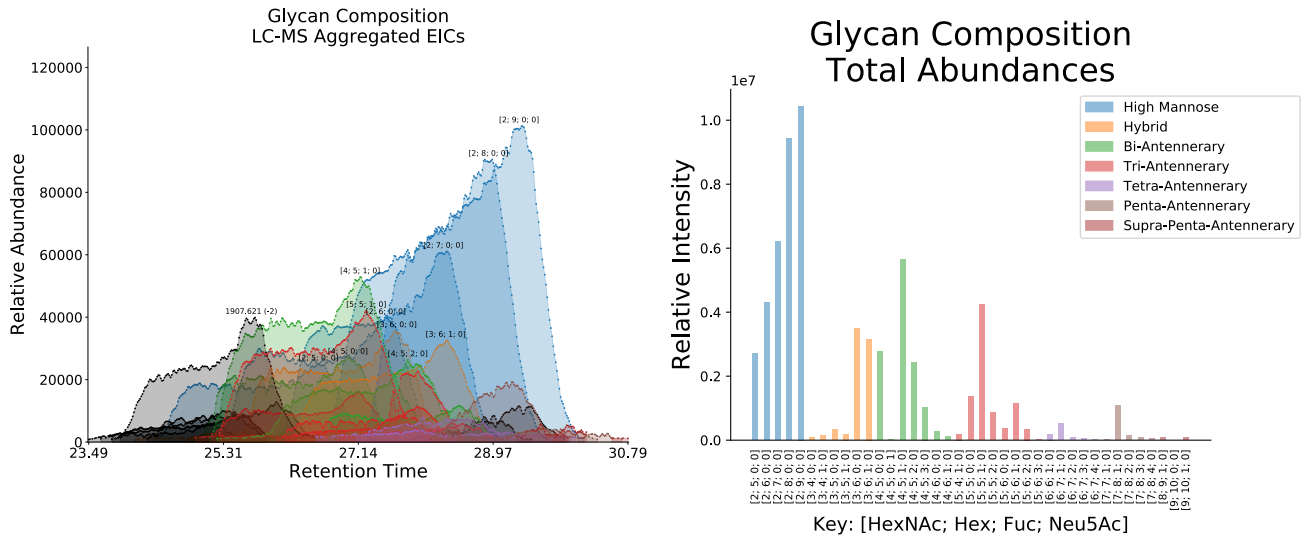
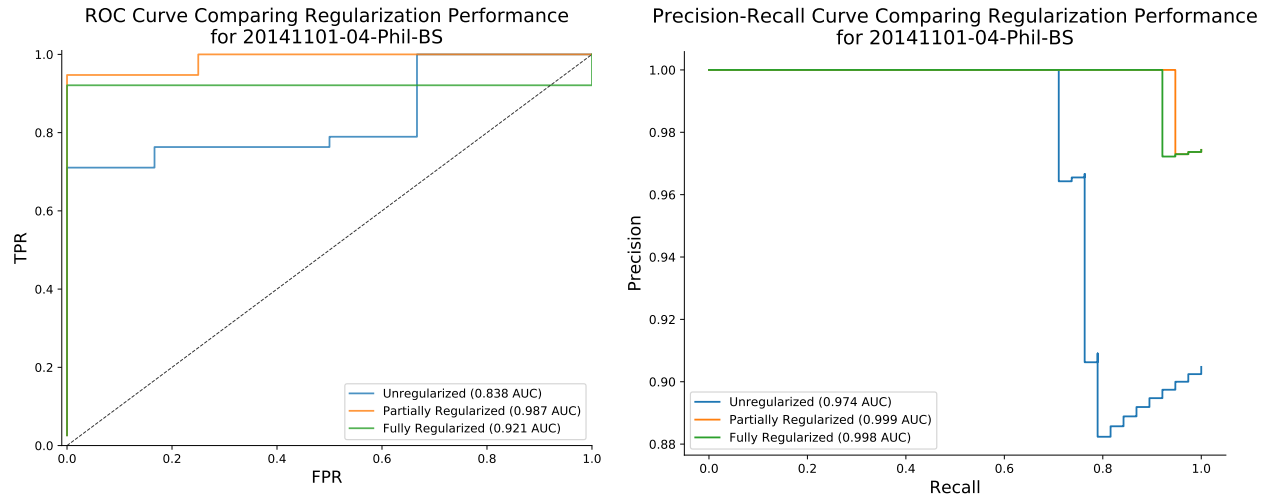


Figure 2: Performance Comparison with and without Network Smoothing for *20141101-04-Phil-BS*



## References

Varki, A. (2017). Biological roles of glycans. *Glycobiology*, **27**(1), 3–49.