Predicting amino acid functionality from sequence data in a phylogenetic framework.

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Abstract

Outline

Introduction

- incorporating selection is important to for proper phylogenetic estimates, but where to get information about selection?

- Default codon models do not include information on site specific amino acid preference, all amino acids are equally prefered.

- DMS or SelAC as options

- DMS experiments specific to stress factors, do not represent general evolution

  - only applicable to genes which respond to environment that can be manipulated in the lab

  - only applicable to organisms with fast gernarational turnover

  - need library of mutations, making mutations accesible that may not have a functional path (Maynard-Smith 60s)

- SelAC estimates amino acid preferences from sequence data

  - Depends on physico-chemical (PC) properties

  - Rank of prefered amino acids is limited by PC

  - What about observed frequencies?

- Only comparing sequences (aa preferences), not models

Results

- Test various PC properties, can we even produce the observed rank?

- Compare DMS from Firnberg and Stiffler to SelAC and majority under SelAC and phydms

  - Comparison of Frinberg under SelAC (three sequences: DMS, Majority, SelAC)
  - Comparison of Frinberg under phydms (three sequences: DMS, Majority, SelAC)
  - Comparison of Stiffler under SelAC (three sequences: DMS, Majority, SelAC)
  - Comparison of Stiffler under phydms (three sequences: DMS, Majority, SelAC)

- Is there always a valid path from WT to prefered aa in DMS data?

Discussion

- What happends if PC can not produce observed rank?

Introduction

Materials & Methods

Results

Discussion

Supplemental Material