Work Log for November

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November 10, 2014

Contents

1 Goals for the Month

As of October 31st

1. Use Preston's Simulated Yeast, compare to REU yeast

   look for estimated $\approx$ 4*true

2. Parallelize the Code

   mclapply, getOption("mc.cores")?

3. Wei Chen's Yeast / Real Yeast Genome

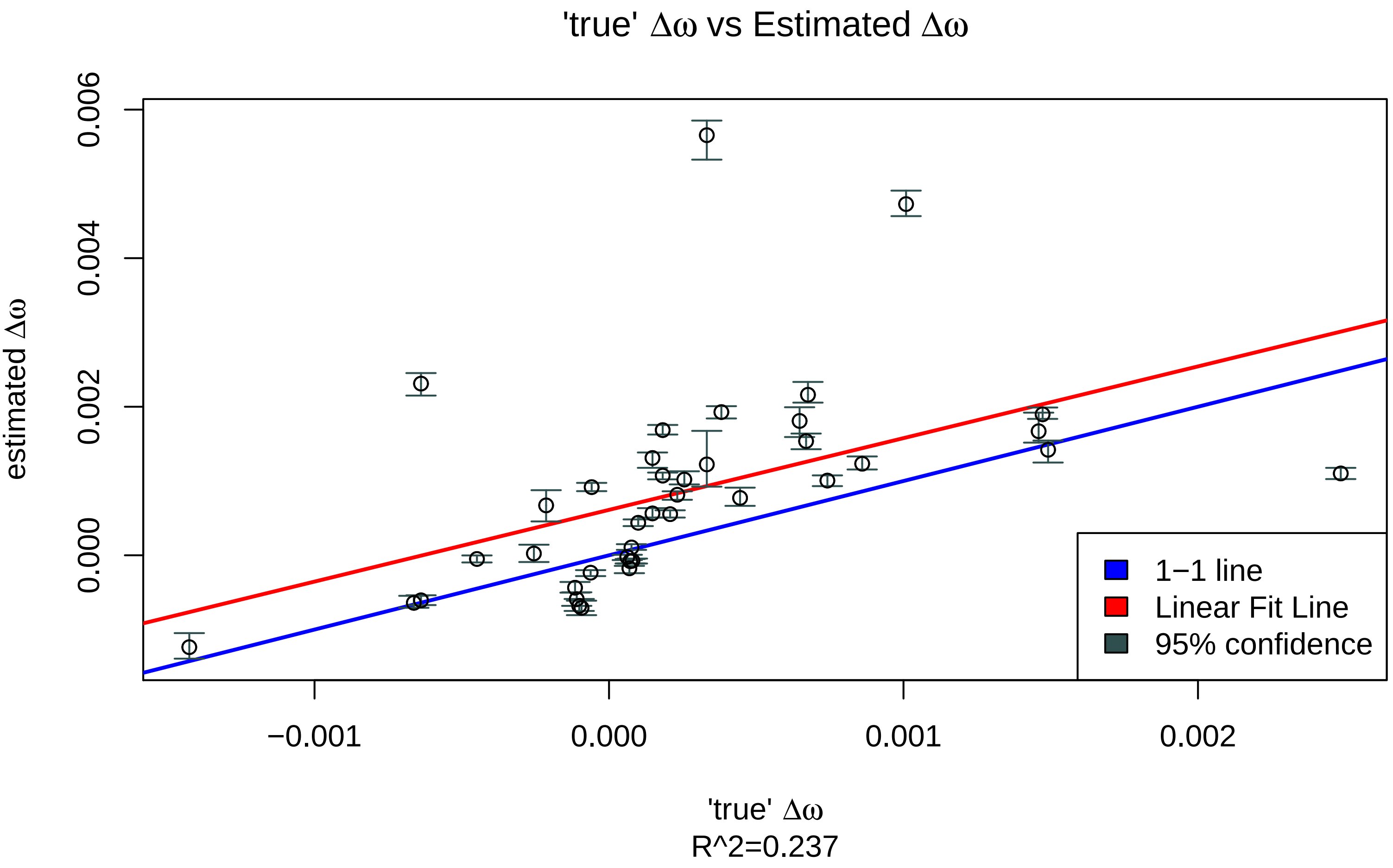
4. Generate my own simulated yeast, using a reverse engineered cubfits

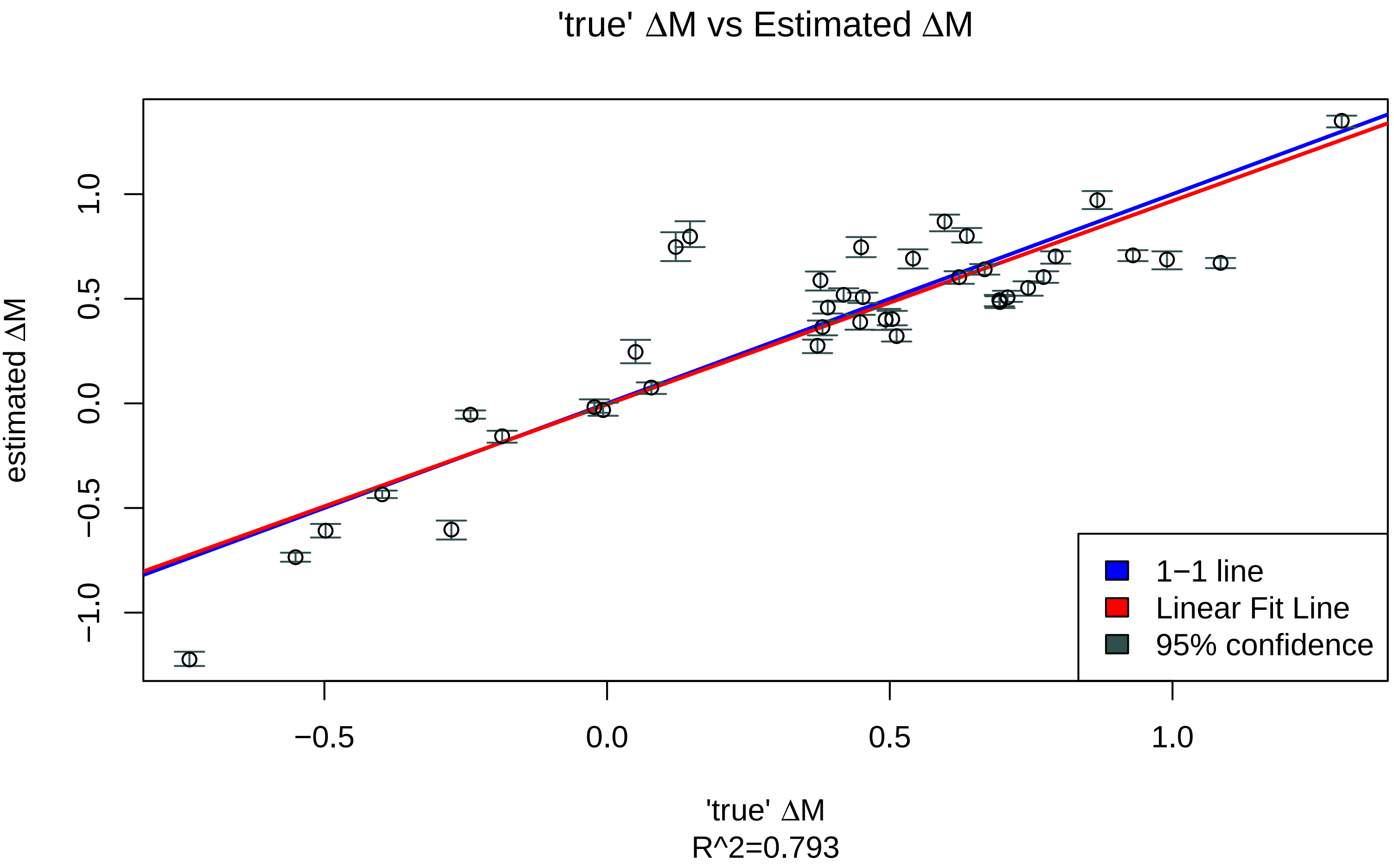
2 Progress/Notes

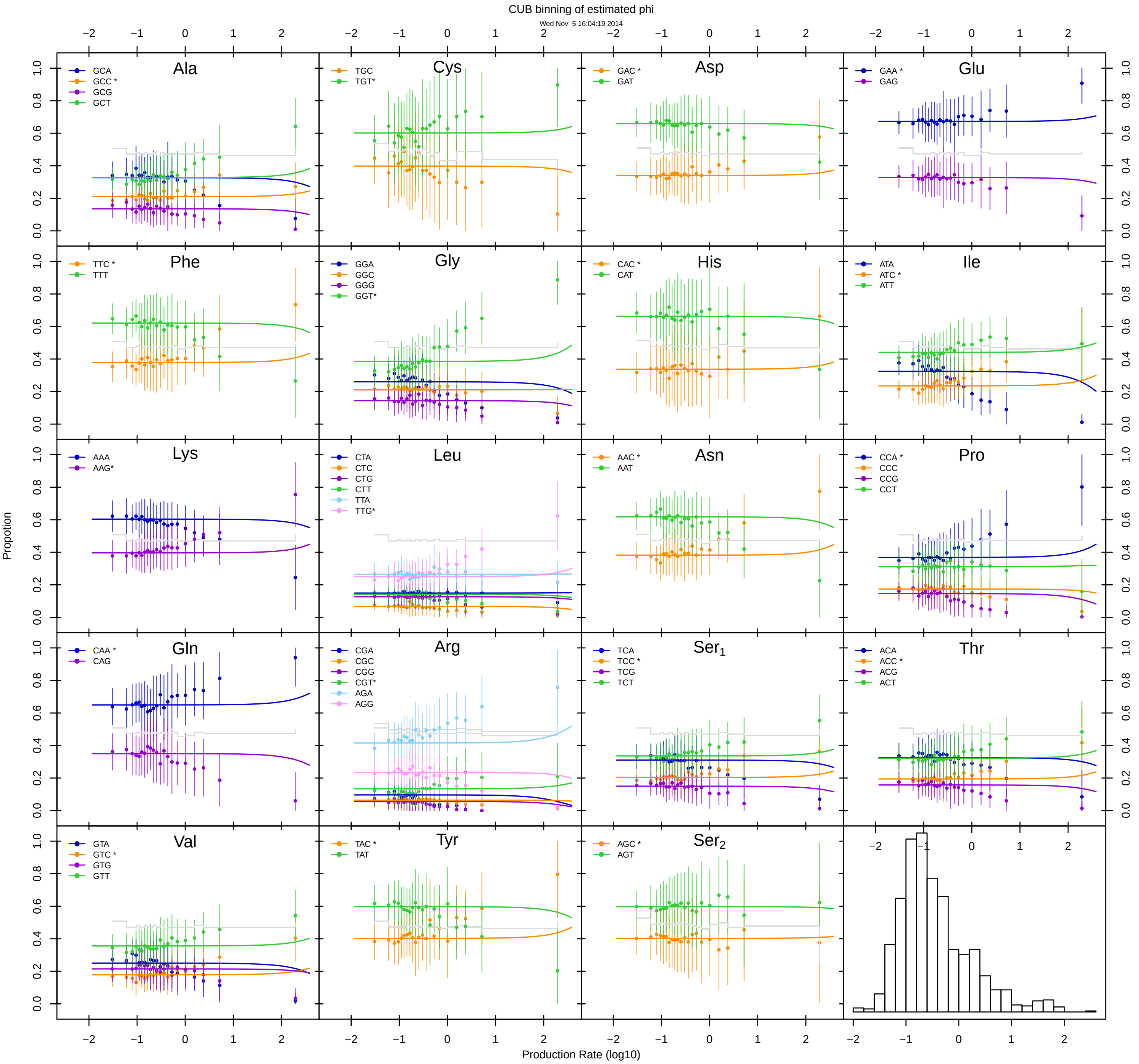
2.1 Use Preston's Simulated Yeast, compare to REU yeast

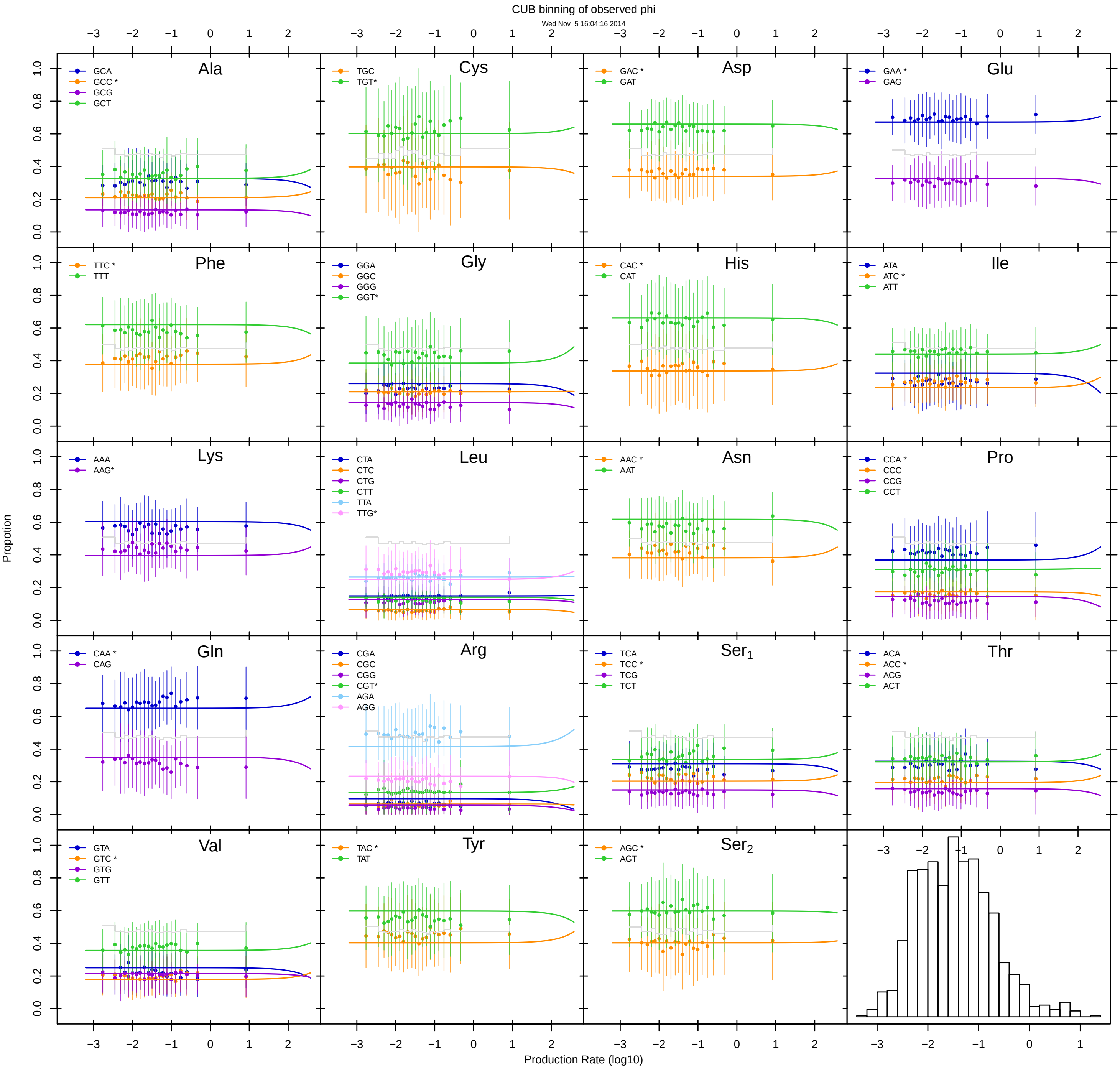
Here are the results from Preston's simulated yeast...

Notice that the $\Delta\omega$ values are not off by that ≈ 4 factor. We got a pretty good correlation on the $\log\mu$ values, but the ϕ is pretty lousy, and the ω values leave something to be desired.


'true' Δω vs Estimated Δω
estimated Δω
0.006
0.004
0.002
0.000
−0.001
0.000
0.001
0.002
'true' Δω
R^2=0.237
🟦 1−1 line
🟥 Linear Fit Line
■ 95% confidence

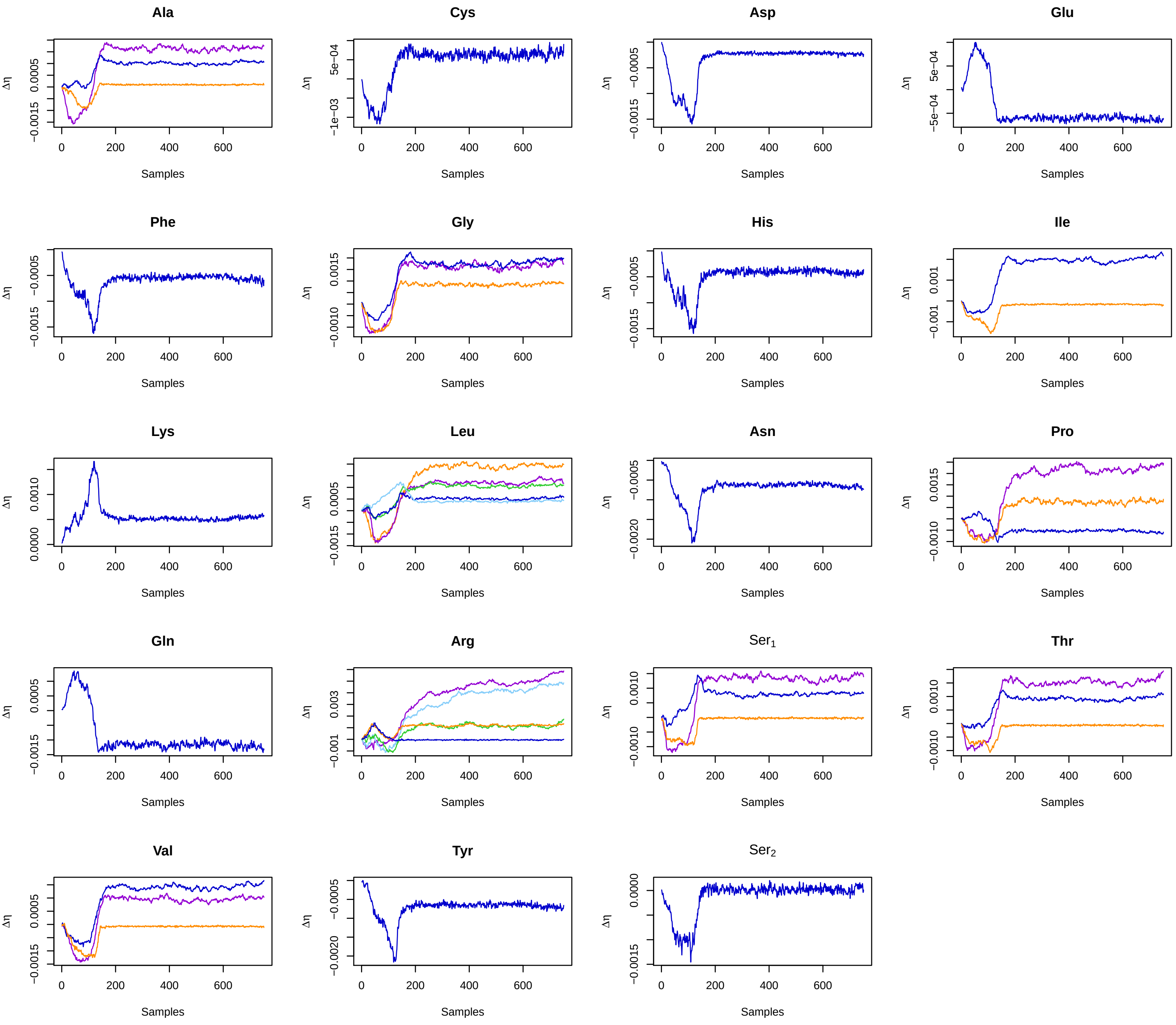

'true' ΔM vs Estimated ΔM
estimated ΔM
1.0
0.5
0.0
−0.5
−1.0
−0.5
0.0
0.5
1.0
'true' ΔM
R^2=0.793
🟦 1−1 line
🟥 Linear Fit Line
■ 95% confidence

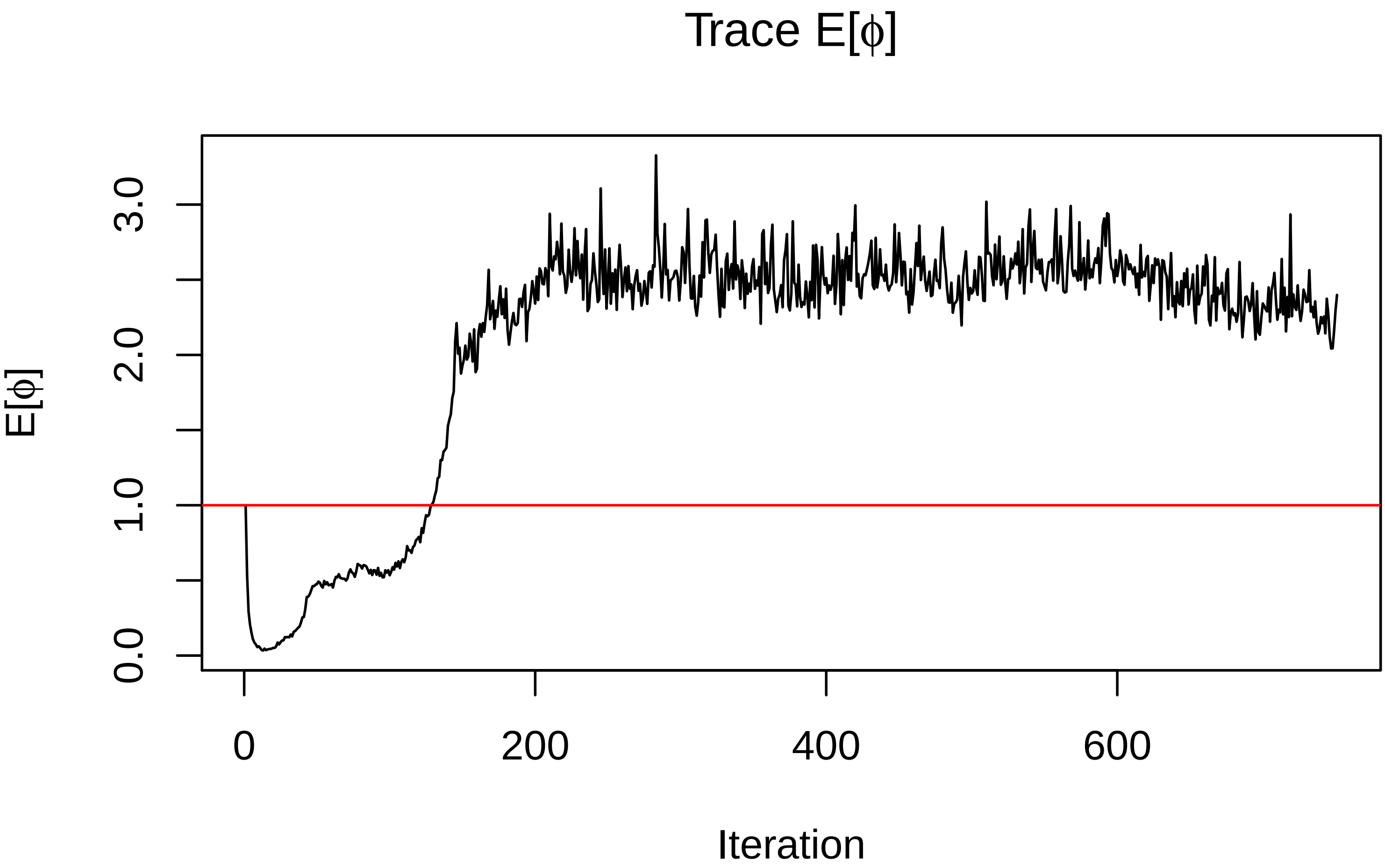

CUB binning of estimated phi
Wed Nov 5 16:04:19 2014
Ala
GCA
GCC *
GCG
GCT
Cys
TGC
TGT*
Asp
GAC *
GAT
Glu
GAA *
GAG
Phe
TTC *
TTT
Gly
GGA
GGC
GGG
GGT*
His
CAC *
CAT
Ile
ATA
ATC *
ATT
Lys
AAA
AAG*
Leu
CTA
CTC
CTG
CTT
TTA
TTG*
Asn
AAC *
AAT
Pro
CCA *
CCC
CCG
CCT
Gln
CAA *
CAG
Arg
CGA
CGC
CGG
CGT*
AGA
AGG
Ser_1
TCA
TCC *
TCG
TCT
Thr
ACA
ACC *
ACG
ACT
Val
GTA
GTC *
GTG
GTT
Tyr
TAC *
TAT
Ser_2
AGC *
AGT
Propotion
0.0
0.2
0.4
0.6
0.8
1.0
−2
−1
0
1
2
Production Rate (log10)

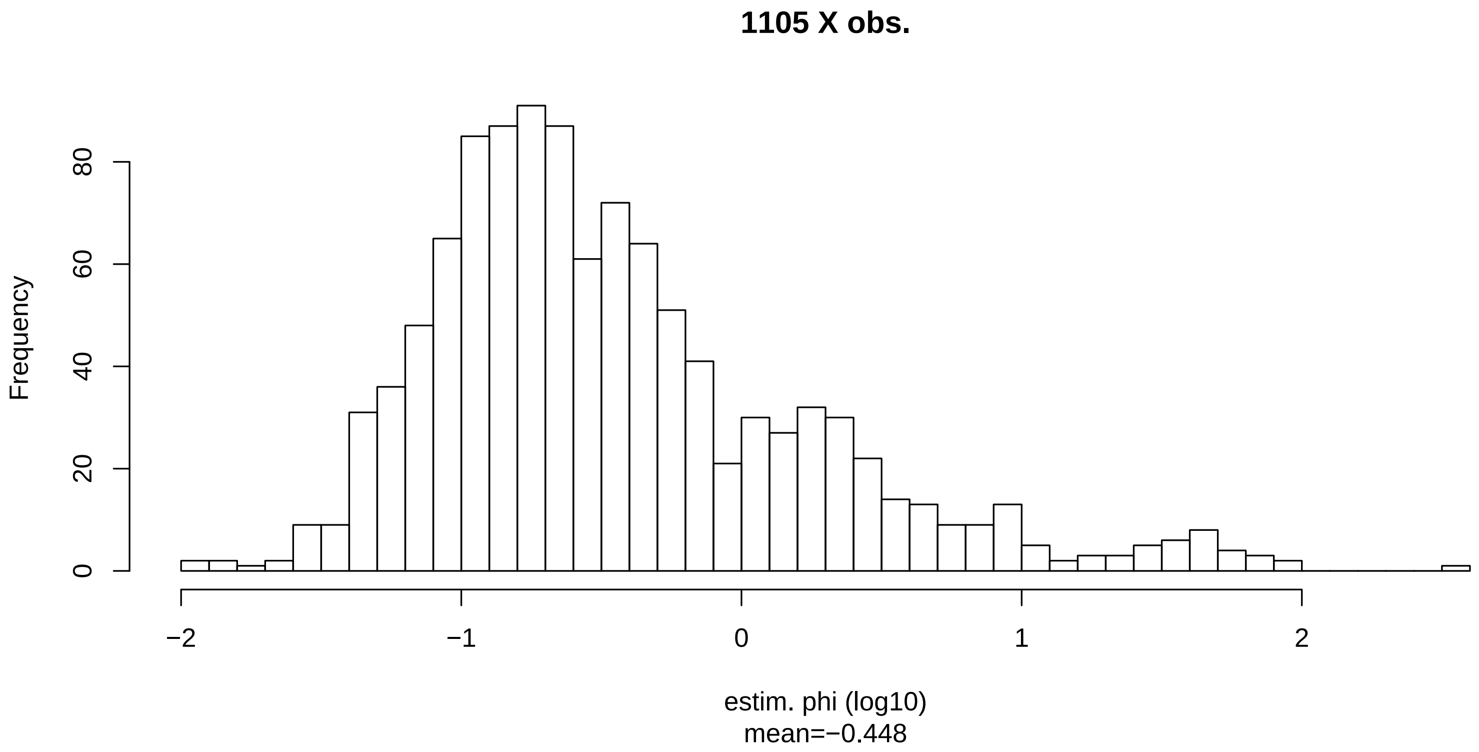

CUB binning of observed phi
Wed Nov 5 16:04:16 2014
Ala
GCA
GCC *
GCG
GCT
Cys
TGC
TGT*
Asp
GAC *
GAT
Glu
GAA *
GAG
Phe
TTC *
TTT
Gly
GGA
GGC
GGG
GGT*
His
CAC *
CAT
Ile
ATA
ATC *
ATT
Lys
AAA
AAG*
Leu
CTA
CTC
CTG
CTT
TTA
TTG*
Asn
AAC *
AAT
Pro
CCA *
CCC
CCG
CCT
Gln
CAA *
CAG
Arg
CGA
CGC
CGG
CGT*
AGA
AGG
Ser_1
TCA
TCC *
TCG
TCT
Thr
ACA
ACC *
ACG
ACT
Val
GTA
GTC *
GTG
GTT
Tyr
TAC *
TAT
Ser_2
AGC *
AGT
Propotion
0.0
0.2
0.4
0.6
0.8
1.0
−3
−2
−1
0
1
2
Production Rate (log10)

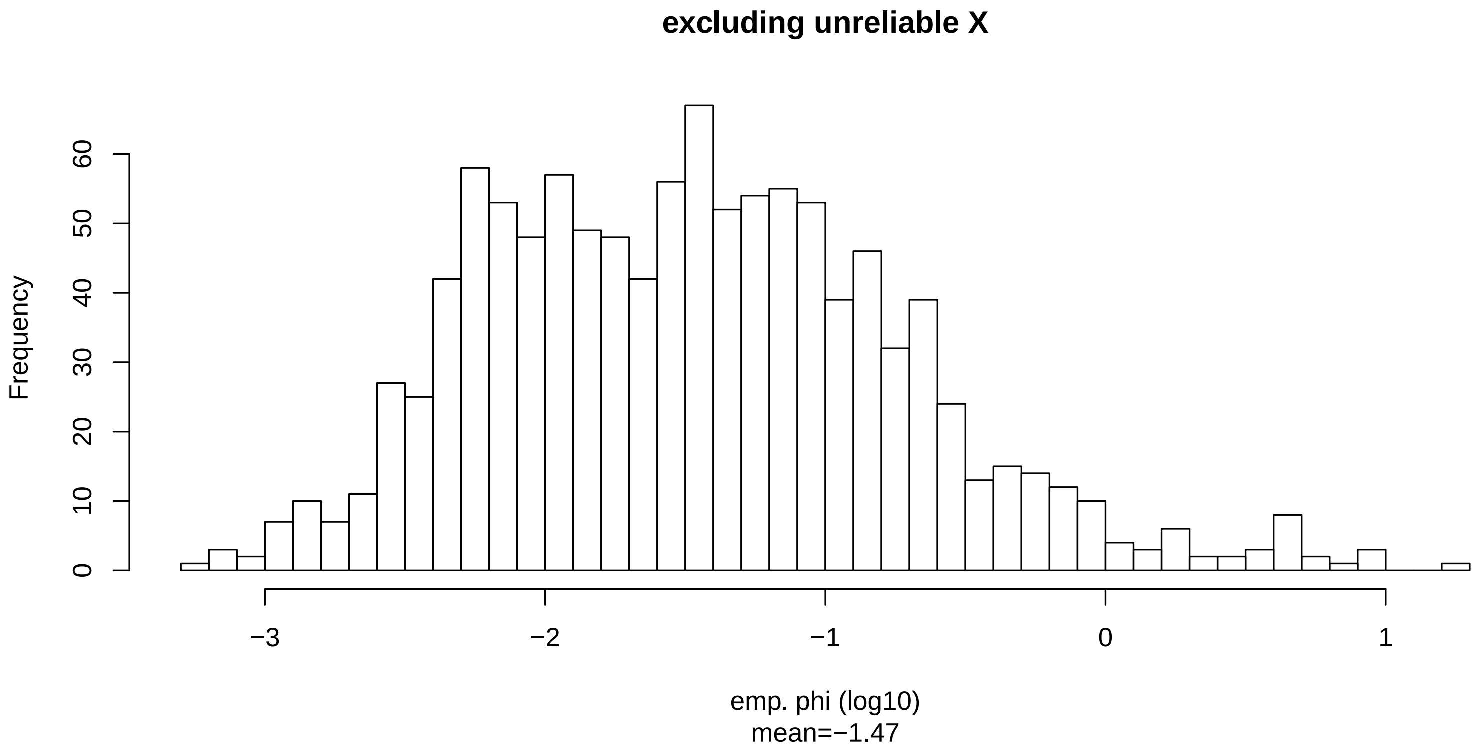
AA parameter trace 1105

Wed Nov 5 16:04:14 2014



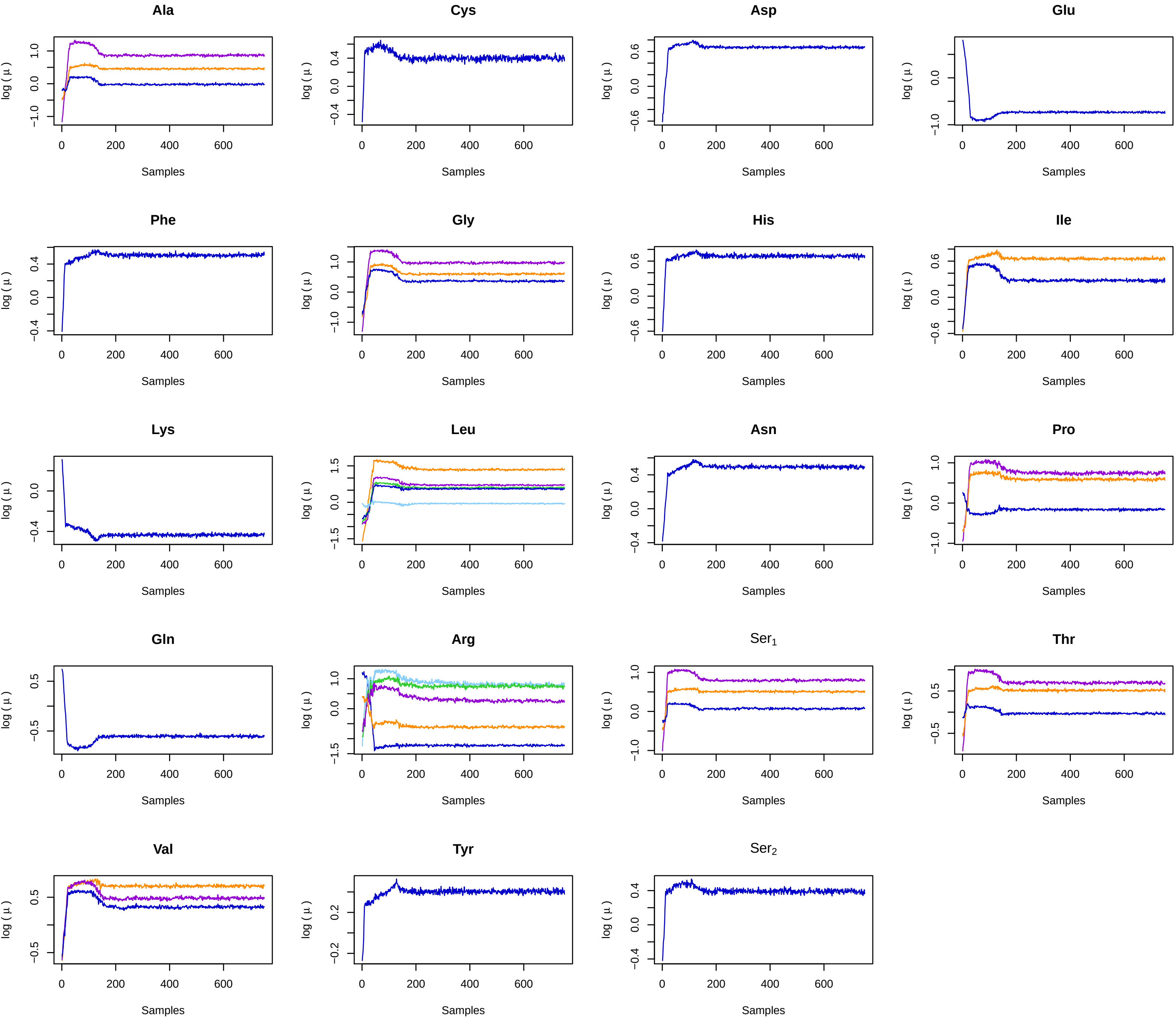

Trace E[ϕ]
E[ϕ]
0.0
1.0
2.0
3.0
0
200
400
600
Iteration

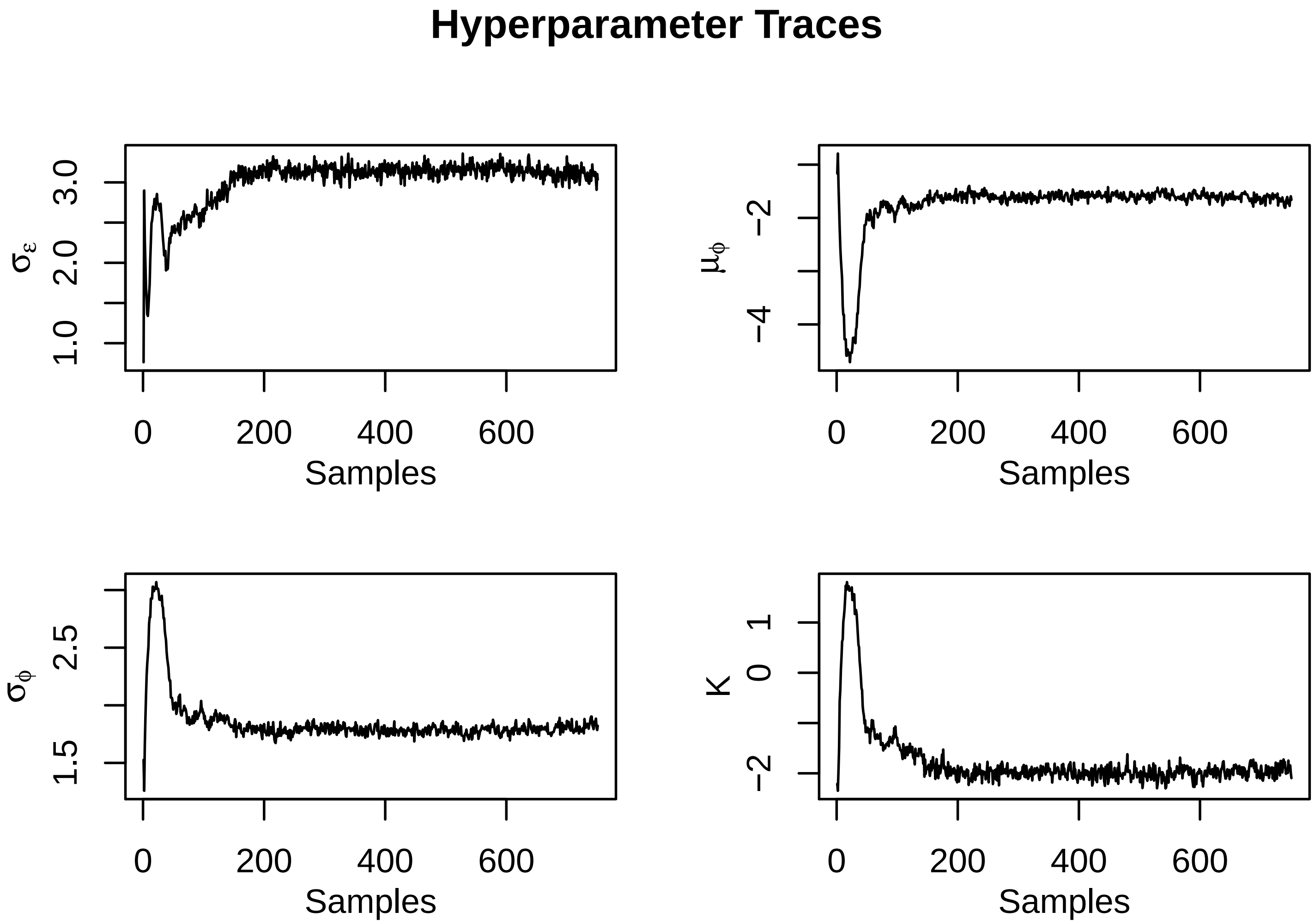

1105 X obs.
Frequency
0
20
40
60
80
−2
−1
0
1
2
estim. phi (log10)
mean=−0.448

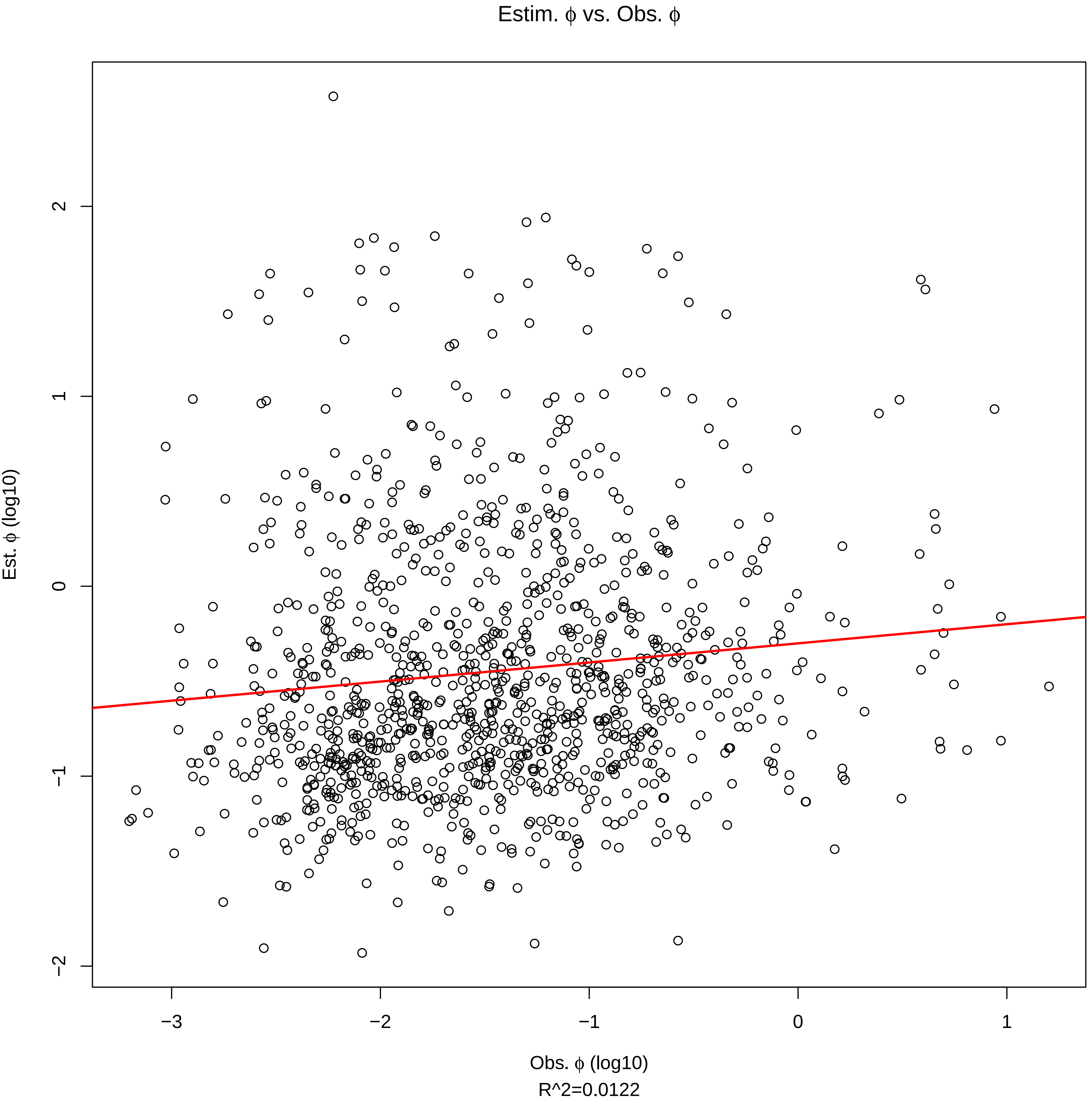

excluding unreliable X
Frequency
0
10
20
30
40
50
60
−3
−2
−1
0
1
emp. phi (log10)
mean=−1.47

AA parameter trace 1105

Wed Nov 5 16:04:13 2014



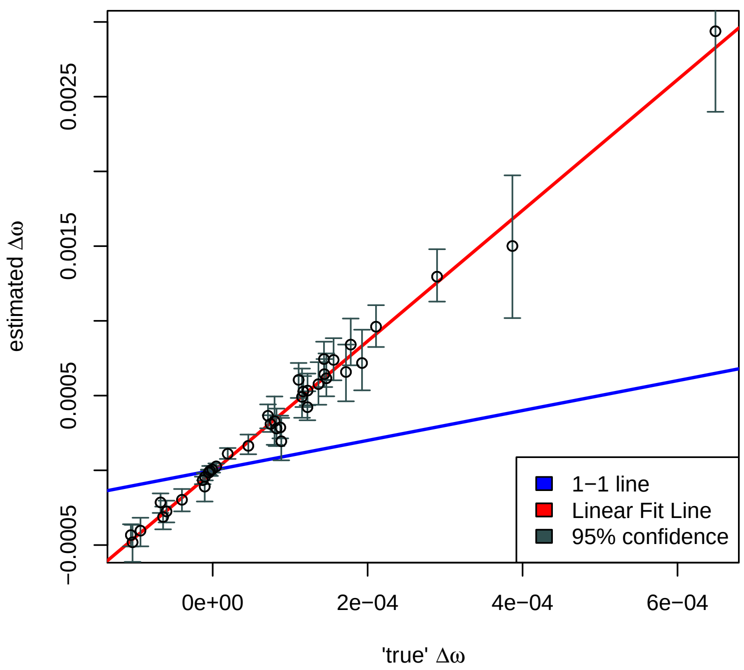

Hyperparameter Traces
σ_ε
1.0
2.0
3.0
0
200
400
600
Samples
μ_ϕ
−4
−2
0
200
400
600
Samples
σ_ϕ
1.5
2.5
0
200
400
600
Samples
K
−2
0
1
0
200
400
600
Samples



Estim. ϕ vs. Obs. ϕ
Est. ϕ (log10)
2
1
0
−1
−2
−3
−2
−1
0
1
Obs. ϕ (log10)
R^2=0.0122

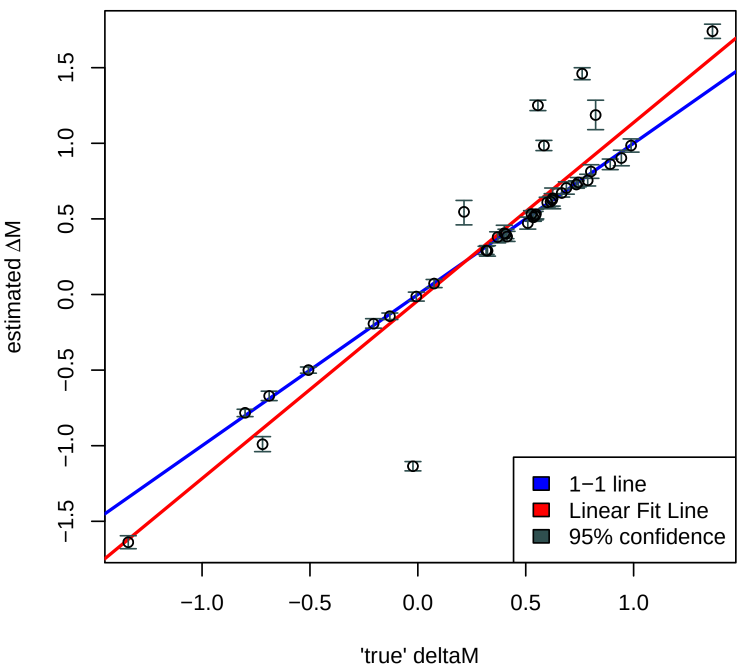
Note how different the $\Delta\omega$ values are between Preston's yeast genome and the REU students' yeast genome.

REU YeastΔω



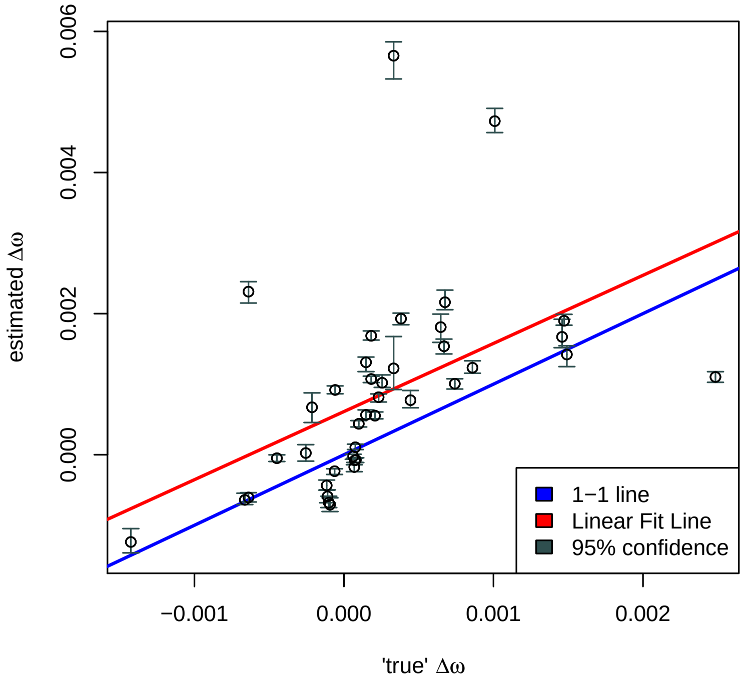
R^2=0.987

REU YeastΔM



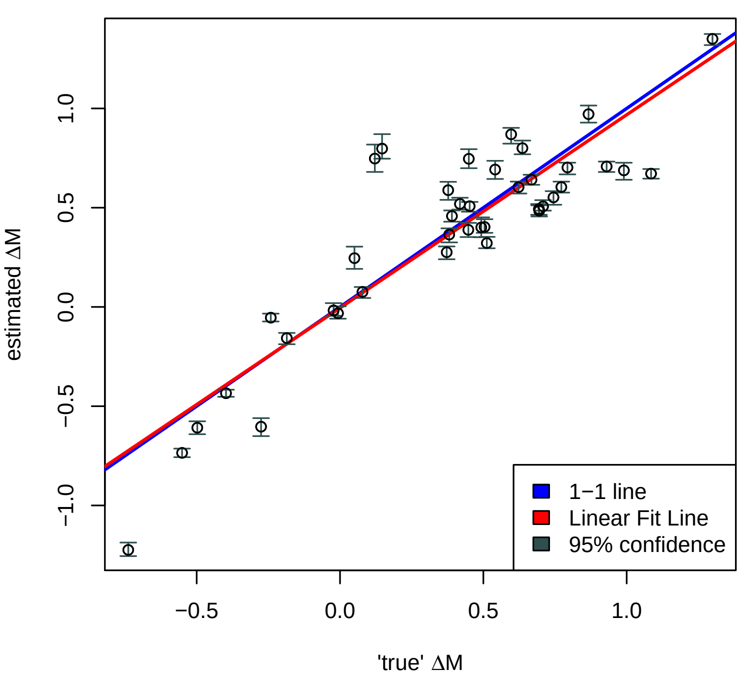
R^2=0.868

Preston's YeastΔω



R^2=0.237

Preston's YeastΔM

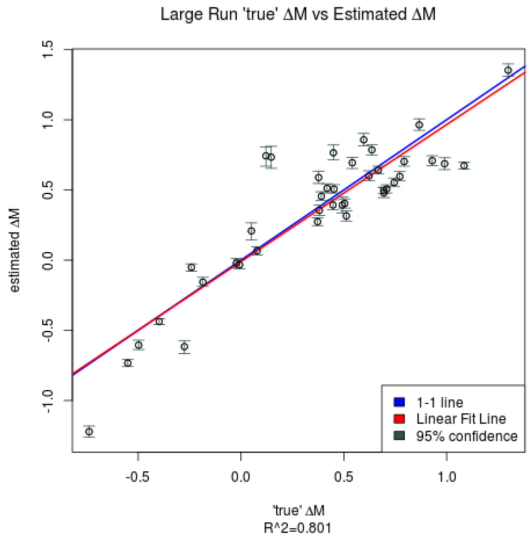


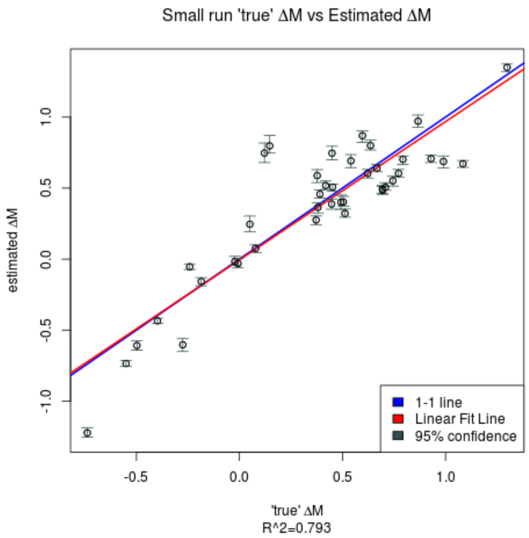
R^2=0.793

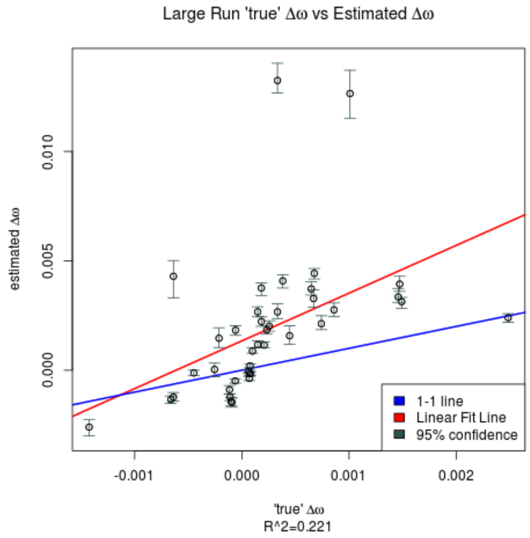
2.1.1 Longer Run?

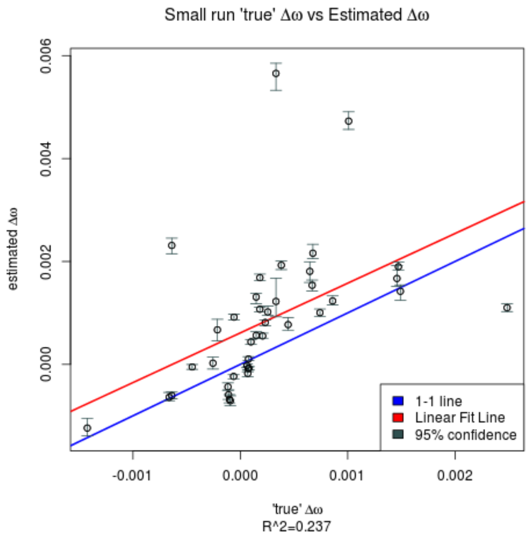
A longer run creates some interesting results. I did a run that used 7500 samples instead of 750 (which, since I'm thinning by 10, it's actually 75,000 proposals).

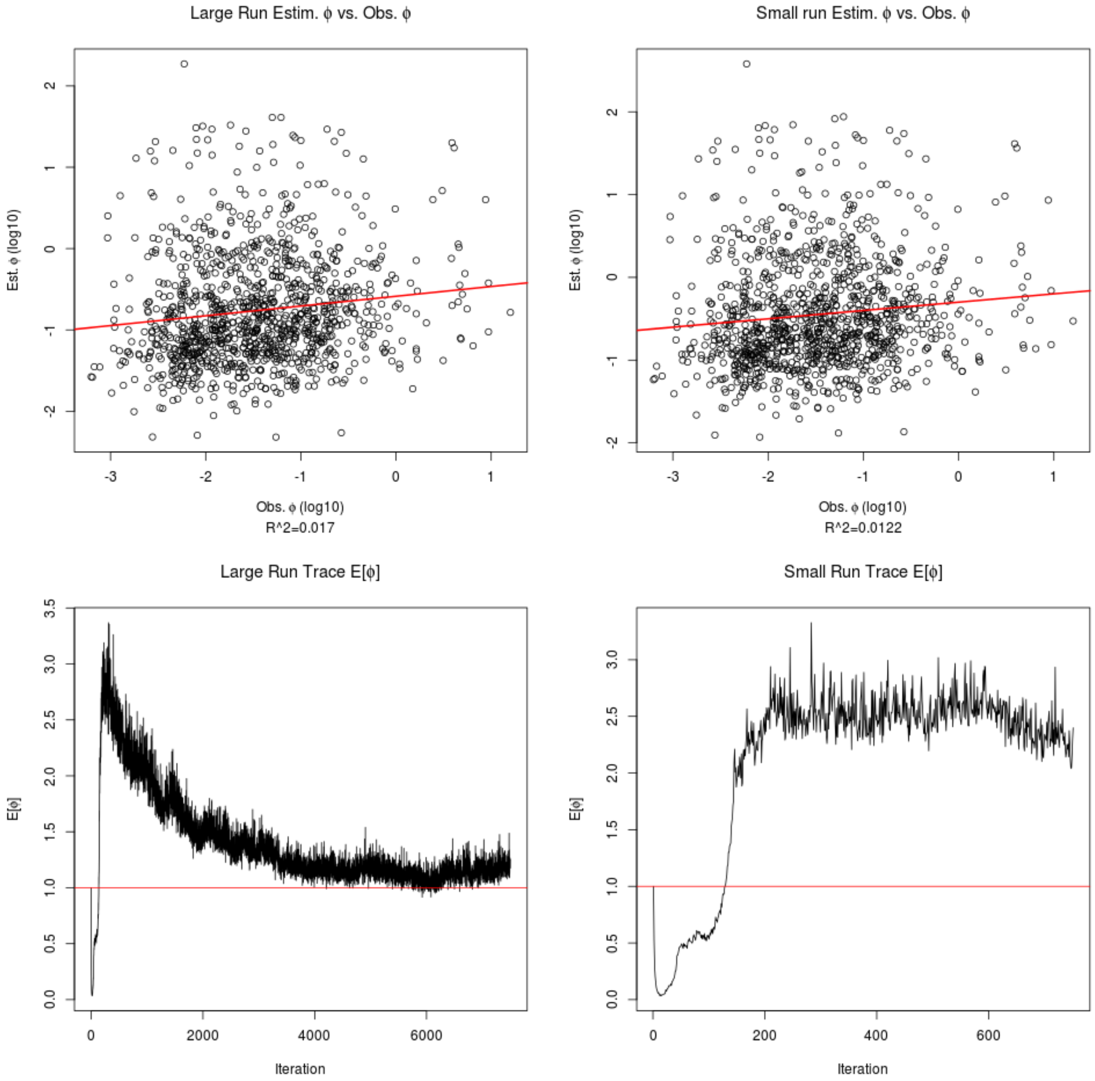
Here's the results (Large run is on the left, small run is on the right)











The most relevant thing in my opinion is the E(ϕ) graphs. E(ϕ) should hover around 1. in the small run, it leapt up to 3, and I was concerned this was an inherent problem in the code. But

2.2 Visualization

2.2.1 'true' values vs simulated values

Changes have been added to visualize.r, based on other plotting functions.

I've added confidence intervals (the scale of the interval can bet set in visualize.r). Cedric didn't have any functions to do so, but I was able to apply the "plotrix" package. I've also installed that package to "/home/lbrown/cubfits/Dependencies/plotrix". Everyone else should have permissions on that directory, in case someone wants to use my edited visualize.r function.

2.3 Parallelize the Code

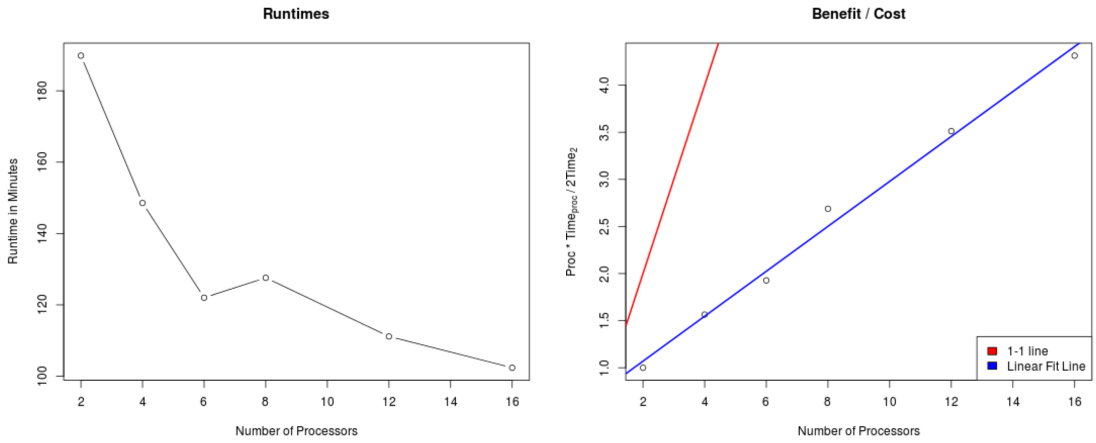
2.3.1 getOption(“mc.cores”)

How to set the number of cores for an mclapply call? mclapply's default number of cores is getOption(“mc.cores”,2L);

getOption(“(option)”, (value)) returns the value previously set to that (option), or otherwise it returns (value). mc.cores is not set by default. So first, set option(“mc.cores”=Number_of_Cores Then mclapply should correctly get the number of cores.

2.3.2 Timing

As expected, we get diminshing returns on adding additional processors



2.4 Add (a1-a2) as a parameter

In the code, when the posterior probability of a codon is calculated, instead of calculating

$$\Pr(c_i|\phi, i) = \frac{\exp[\mathrm{M}_i + \omega_i(a_1 - a_2)y_1 + \omega_i a_2 y_1 i]}{\sum_{u=1}^{m} \exp[\mathrm{M}_i + \omega_i(a_1 - a_2)y_1 + \omega_i a_2 y_1 i]}$$

Wei Chen calculates

$$\Pr(c_i|\phi, i) = \frac{\exp[\mathrm{M}_i - \omega_i \phi i]}{\sum_{u=1}^{m} \exp[\mathrm{M}_i - \omega_i \phi i]}$$

This was done for a number of reasons. The y_1 term is just the aggregate of the effective population, ϕ, and a scaling term $-q$. Also, the assumption was that $a_1 \approx a_2 =$ 4ATP. To better account for the parameters of the model, we're going to add another parameter called $\Delta a_{12} = (a_1 - a_2)$, and use

$$\Pr(c_i|\phi, i) = \frac{\exp[\ln - \omega_i(\Delta a_{12})\phi - 4\omega_i\phi i]}{\exp[\ln \sum_{u=1}^{m} \exp[\ln - \omega_i(\Delta a_{12})\phi - 4\omega_i\phi i]}$$

The math part of the change takes place in my.logdmultinomCodOne.r, adding an extra row to xm and multiplying $\omega\phi\Delta a_{12}$, which is baa[2]*tmp.phi*(new parameter)

2.5 Move to Newton

Newton uses R 3.0.1, all my dependencies were build under 3.1.1. Newton HAS R 3.1.0, but not 3.1.1.

2.6 Wrong Names

It's not just a problem in the chain$b.Mat data. It's in the my.fitmultinomOne.r

2.7 Wei Chen's Yeast / Real Yeast Genome

2.8 Generate my own simulated yeast, using a reverse engineered cubfits

3 Goals for next Month

1. Future Goal