An *In Situ* Approach for Approximating Complex Computer Simulations and Identifying Important Time Steps

Kary Myers, Statistical Sciences Group
Los Alamos National Laboratory

Joint work with Earl Lawrence, Mike Fugate, Claire Bowen, Larry Ticknor, Joanne Wendelberger, Jon Woodring, and Jim Ahrens

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Join us for the third Conference on Data Analysis, bringing together scientists, statisticians, and data analysts from across the Department of Energy national laboratories along with their academic and industrial collaborators.

Banquet Speaker: Rayid Ghani, Program Director, Data Science for Social Good, University of Chicago.

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- Cyber Security
- Subsurface Modeling
- Data Analysis at Exascale
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Visit cnls.lanl.gov/coda for more information and to register.
Important announcement #2: Statistics and Beer Day

A new holiday to celebrate how the field of statistics has improved the world by focusing on how it has improved beer.

**When?** June 13, William Sealy Gosset’s birthday.

**Who?** You might remember him by his pseudonym Student, as in Student’s *t*-distribution.

**Why?** Gosset worked for Guinness Brewery where he developed and applied statistical methods to improve the beer.

**How?** Have a few pints with statisticians and other normal people. Start with a Guinness.
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An *In Situ* Approach for Approximating Complex Computer Simulations and Identifying Important Time Steps!

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What’s a complex computer simulation?

Running a numerical model of a system, typically on a supercomputer. Often used when physical experiments aren’t practical.

Modeling Climate

Modeling the Universe

Model for Prediction across Scales

Millennium-XXL Project

Los Alamos National Laboratory

Max-Planck-Institute for Astrophysics
Coming soon: Exascale computing

A billion billion (1,000,000,000,000,000,000,000) calculations every second. This means more science, but only if we can extract useful information.
One idea: Only save a subset of simulation time steps

A 1-d example. (I’ll talk about the simulation behind this example later.)
One idea: Only save a subset of simulation time steps

Standard practice: Save evenly spaced time steps.
One idea: Only save a subset of simulation time steps

Our approach: An *in situ* analysis to select “important” time steps in an online fashion. We do this by cheaply computing and comparing linear fits.
Our *in situ* approach: Compare linear fits

Cheap to compute and update within the simulation as it’s running.

Compare 3 lines in 2 temporal regions of interest:

- **curr**: Time steps currently characterized by a linear fit; only sufficient statistics are stored.
- **buff**: \(B\) time steps most recently computed by the simulation; stored in the buffer.
Our *in situ* approach: Compare linear fits

Cheap to compute and update within the simulation as it’s running.

Consider 2 hypotheses:

$H_0$: **One line** fits best.

$H_1$: **Two lines** ($\text{curr} + \text{buff}$) fit best.

Use a modified *F*-statistic at some $\alpha$ level to decide when to reject $H_0$. 
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$. 

Fit a line to the time steps in *curr*:

- past
- *curr*
- *curr U buff*
- buff, fail to reject $H_0$
- buff, reject $H_0$

Simulation Time Step

$t = 0005$
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$.

Save only the line (not the time steps)

- past
- curr
- curr U buff
- buff, fail to reject $H_0$
- buff, reject $H_0$
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$.

Acquire the next $B$ time steps; fit and compare 3 lines

- past
- curr
- curr U buff
- buff, fail to reject $H_0$
- buff, reject $H_0$

Simulation Time Step
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$.

Fail to reject single line fit

- past
- curr
- curr U buff
- buff, fail to reject $H_0$
- buff, reject $H_0$

$t = 0010$

Simulation Time Step
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$.

Add new time step to buff, move oldest one to curr, update the 3 lines

And throw it away!
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$.  

---

**Fail to reject single line fit**

- **past**
- **curr**
- **curr U buff**
- **buff, fail to reject $H_0$**
- **buff, reject $H_0$**

$t = 0011$

**Simulation Time Step**

0 5 10 15 20 25 30 35
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$.

Fail to reject single line fit

- past
- curr
- curr U buff
- buff, fail to reject $H_0$
- buff, reject $H_0$
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$.

Fail to reject single line fit

- past
- curr
- curr U buff
- buff, fail to reject $H_0$
- buff, reject $H_0$

$t = 0013$

Simulation Time Step

0 5 10 15 20 25 30 35
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$. 

Reject single line fit

- past
- curr
- curr U buff
- buff, fail to reject $H_0$
- buff, reject $H_0$

Simulation Time Step

$t = 0.014$
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$.

\[
past \leftarrow past \cup curr, \text{ write things to disk}
\]
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$. 

![Diagram showing a line graph with data points and labels indicating past, current, and buffer states. The graph shows a sequence of time steps from 0 to 35, with a simulation time step at t = 0.014.](image-url)
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$.
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$. 

Fail to reject single line fit

- past
- curr
- curr U buff
- buff, fail to reject $H_0$
- buff, reject $H_0$

$t = 0020$

Simulation Time Step

0 5 10 15 20 25 30 35
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$. 

Fail to reject single line fit

- past
- curr
- curr U buff
- buff, fail to reject $H_0$
- buff, reject $H_0$

Simulation Time Step

$t = 0021$
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$.

Fail to reject single line fit

- past
- curr
- curr U buff
- buff, fail to reject $H_0$
- buff, reject $H_0$

$t = 0022$

Simulation Time Step

0 5 10 15 20 25 30 35
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$. 

Fail to reject single line fit

- **past**
- **curr**
- **curr U buff**
- **buff, fail to reject $H_0$**
- **buff, reject $H_0$**

$t = 0.023$

Simulation Time Step

0 5 10 15 20 25 30 35
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$.

Fail to reject single line fit

- past
- curr
- curr U buff
- buff, fail to reject $H_0$
- buff, reject $H_0$
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$.

![Graph showing linear fits and data points](image-url)
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$. 

---

**Fail to reject single line fit**

- **past**
- **curr**
- **curr U buff**
- **buff, fail to reject $H_0$**
- **buff, reject $H_0$**

Simulation Time Step

$t = 0.026$
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$.

Reject single line fit

- past
- curr
- curr U buff
- buff, fail to reject $H_0$
- buff, reject $H_0$

Simulation Time Step

$t = 0.027$
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$. 

\[
past \leftarrow past \cup curr, curr \leftarrow buff
\]

- past
- curr
- curr U buff
- buff, fail to reject $H_0$
- buff, reject $H_0$

Simulation Time Step

$t = 0027$
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$. 

![Graph showing piecewise linear data with buffer size $B = 5$. The graph illustrates past, current, and buffer data, with indications for rejecting or failing to reject the null hypothesis ($H_0$).]
Our *in situ* approach: Compare linear fits

A toy example: Piecewise linear data with noise. Buffer size $B = 5$. 

![Graph showing in situ approach with linear fits and buffer sizes.](Slide 35)
Our *in situ* approach: Compare linear fits

We capture each of the 3 lines with a set of **sufficient statistics**:

\[
T_0, \sum t_i, \sum t_i^2, \sum y_i, \sum y_i^2, \sum t_i y_i
\]

- Number of time steps in the line
- Time
- Response

Simulation Time Step
Our *in situ* approach: Compare linear fits

We capture each of the 3 lines with a set of **sufficient statistics**:

$$T_0, \sum t_i, \sum t_i^2, \sum y_i, \sum y_i^2, \sum t_i y_i$$

- Update these in constant time, $O(1)$, as the simulation progresses.

- Use to compute the **modified F-statistic** for our hypothesis test.

- Use to construct a linear approximation of the entire simulation with known error.
Our modified $F$-statistic

Here's the standard formulation:

$$F = \frac{RSS_1 - RSS_2}{\frac{p_2 - p_1}{RSS_2} \frac{T_{curr + buff} - p_2}{}}$$

- Number of parameters required for each model
- Total number of time steps currently under consideration
Our modified $F$-statistic

But this can reject $H_0$ when both curr and buff have extremely low RSS, which is common in these computer simulations.
Our modified $F$-statistic

So we add a “nugget” $\delta^2$, scaled by $T_{\text{curr \& buff}}$, to have the effect of adding white noise and encouraging less (or smarter) rejection.

$$F = \left( \frac{RSS_{S_1} - RSS_{S_2}}{p_2 - p_1} \right) \left( \frac{RSS_{S_2}}{T_{\text{curr \& buff}} - p_2} \right) + T_{\text{curr \& buff}} \times \delta^2$$

Now we have 3 “tuning parameters”: $\alpha$, nugget $\delta^2$, and buffer size $B$. I’ll come back to this later. But first: A demo!
Demo: Is there water on the moon? NASA finds out!

2009 LCROSS Mission: Lunar CRater Observation and Sensing Satellite

www.popularmechanics.com
But before NASA crashed the Moon…

Scientists used RAGE simulations to bound the expected results.  
Korycansky et al. 2009
But before NASA crashed the Moon…

Scientists used RAGE simulations to bound the expected results.  
*Korycansky et al. 2009*

- **RAGE:** A massively parallel Eulerian code used to solve 1D, 2D, or 3D hydrodynamics problems.  
  *Gittings et al. 2008*

- 2000 time steps, ~10 variables in 2D.

- Not a billion billion calculations per second, but a useful testbed.

Pressure
Demonstration with LCROSS simulation

First we’ll track a pixel of the pressure variable.
Demonstration with LCROSS simulation (single pixel)

First we’ll track a pixel of the pressure variable.
Demonstration with LCROSS simulation (single pixel)

Standard practice: 25 evenly spaced partitions.

Assuming linear interpolation.

Total RSS: 1140.15
Demonstration with LCROSS simulation (single pixel)

Our approach: 25 partitions selected with $\alpha = 0.001$, $\delta^2 = 0.001$, $B = 5$.

Total RSS: 6.40
But how to choose those tuning parameters?

We’ve got $\alpha$, nugget $\delta^2$, and buffer size $B$.

- $B$ we have little control over.
- We can explore $\alpha$ and $\delta^2$ in terms of their impact on the number of partitions and the total RSS.

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$\delta^2$</th>
<th>Number of partitions</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1 -</td>
<td>1e$^{-10}$</td>
<td>221 210 191 166 145 129 111 84 48 27 13</td>
</tr>
<tr>
<td>0.01</td>
<td>1e$^{-09}$</td>
<td>203 190 173 148 131 115 94 62 40 17 11</td>
</tr>
<tr>
<td>0.001</td>
<td>1e$^{-08}$</td>
<td>173 167 150 130 116 96 73 47 25 16 9</td>
</tr>
<tr>
<td>1e$^{-07}$</td>
<td>1e$^{-07}$</td>
<td>120 115 105 84 73 62 42 28 18 11 9</td>
</tr>
<tr>
<td>1e$^{-06}$</td>
<td>1e$^{-06}$</td>
<td>60  64  46  38  35  31  29  15  12  11  9</td>
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<tr>
<td>1e$^{-04}$</td>
<td>1e$^{-04}$</td>
<td>20  18  18  17  15  14  11  11  3  5</td>
</tr>
<tr>
<td>1e$^{-03}$</td>
<td>1e$^{-03}$</td>
<td>11  10  10  10  9  10  7  7  3  3</td>
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<tr>
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<td>10  10  10  10  9  9  7  7  3  3</td>
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<tr>
<td>1e$^{-01}$</td>
<td>1e$^{-01}$</td>
<td>10  10  10  10  9  9  4  7  3  3</td>
</tr>
</tbody>
</table>
But how to choose those tuning parameters?

We’ve got $\alpha$, nugget $\delta^2$, and buffer size $B$.

- $B$ we have little control over.
- We can explore $\alpha$ and $\delta^2$ in terms of their impact on the number of partitions and the total RSS.

![Diagram](image.png)
Start by understanding the $\delta^2 = 0$ case

You might think we could just turn the $\alpha$ knob to reject less often.

<table>
<thead>
<tr>
<th>$\delta^2$</th>
<th>0.1</th>
<th>0.01</th>
<th>0.001</th>
<th>$1 \times 10^{-4}$</th>
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<th>$1 \times 10^{-6}$</th>
<th>$1 \times 10^{-7}$</th>
<th>$1 \times 10^{-8}$</th>
<th>$1 \times 10^{-9}$</th>
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<td>191</td>
<td>166</td>
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<td>129</td>
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</tbody>
</table>
What can we accomplish by adjusting $\alpha$ alone?

With $\delta^2 = 0$, the hypothesis test gets fooled when $\text{curr}$ and $\text{buff}$ both have extremely low error.
What can we accomplish by adjusting $\alpha$ alone?

With $\delta^2 = 0$, the hypothesis test gets fooled when $\text{curr}$ and $\text{buff}$ both have extremely low error.
What can we accomplish by adjusting $\alpha$ alone?

With $\delta^2 = 0$, the hypothesis test gets fooled when `curr` and `buff` both have extremely low error.
What can we accomplish by adjusting $\alpha$ alone?

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With $\delta^2 = 0$, the hypothesis test gets fooled when $\text{curr}$ and $\text{buff}$ both have extremely low error.

![Graph showing simulation time step vs. log(pressure)](image)
What can we accomplish by adjusting $\alpha$ alone?

With $\delta^2 = 0$, the hypothesis test gets fooled when \textit{curr} and \textit{buff} both have extremely low error.
What can we accomplish by adjusting $\alpha$ alone?

With $\delta^2 = 0$, the hypothesis test gets fooled when \texttt{curr} and \texttt{buff} both have extremely low error.
What can we accomplish by adjusting $\alpha$ alone?

With $\delta^2 = 0$, the hypothesis test gets fooled when `curr` and `buff` both have extremely low error.
Q: What’s going wrong? A: What isn’t going wrong?

These deterministic computer codes violate pretty much every statistical assumption we typically like to make:

- Samples aren’t i.i.d. but rather come from a smooth process.
- Error isn’t Gaussian.
- Variances of `curr` and `buff` aren’t necessarily equal.
Take a look at a positive $\delta^2$ case

<table>
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<td>9</td>
<td>9</td>
</tr>
<tr>
<td>$0.1$</td>
<td>0</td>
<td>7</td>
<td>7</td>
<td>7</td>
<td>7</td>
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<td>7</td>
<td>7</td>
<td>7</td>
<td>7</td>
</tr>
</tbody>
</table>
What does a positive $\sigma^2$ buy us?

It’s like adding white noise with variance $\sigma^2$, providing a global effect on the kinds of changes that can be ignored.
What does a positive $\delta^2$ buy us?

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It’s like adding white noise with variance $\delta^2$, providing a global effect on the kinds of changes that can be ignored.
Ok, but still: How to choose those tuning parameters?

Here’s what we’ve learned:

- $\alpha$ governs local choices about partitioning `curr` and `buff`. Increasing $\alpha$ fills in areas that already have partitions, making the fit more detailed.

- $\delta^2$ provides a global effect about the kinds of changes to ignore.

- For now we recommend doing a few “scanning” runs of the simulation to build small versions of tables like these.
We argue: It’s worth it to do a few scanning runs

Standard practice: 80 partitions, total RSS 280.43.
We argue: It’s worth it to do a few extra runs

**Standard practice:** 80 partitions, total RSS 280.43.

**Our approach:** 84 partitions, total RSS 1.30.
We argue: It’s worth it to do a few extra runs

**Standard practice:** 80 partitions, total RSS 280.43.
**Our approach:** 11 partitions, total RSS 281.61.
Tradeoff between number of partitions and total RSS

Ultimately would like to find an AIC-like criterion to balance this.

<table>
<thead>
<tr>
<th>Number of partitions</th>
<th>Total RSS (rounded)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1 -</td>
<td>34 34 34 34 0 0 34 1 32 14</td>
</tr>
<tr>
<td>0.01 -</td>
<td>0 0 0 0 0 0 1 1 1 8 419</td>
</tr>
<tr>
<td>0.001 -</td>
<td>1 1 1 1 1 1 1 2 1 1 6 11 534</td>
</tr>
<tr>
<td>$10^{-4}$ -</td>
<td>1 1 1 1 1 1 2 4 11 12 282 154</td>
</tr>
<tr>
<td>$10^{-5}$ -</td>
<td>11 11 11 11 11 13 9 44 45 40 154</td>
</tr>
<tr>
<td>$10^{-6}$ -</td>
<td>9 9 9 9 9 9 9 9 15 39 307 940</td>
</tr>
<tr>
<td>$10^{-7}$ -</td>
<td>36 36 36 36 36 36 38 38 2709 1027</td>
</tr>
<tr>
<td>$10^{-8}$ -</td>
<td>1205 1205 1205 1205 1205 1205 1208 1208 2678 2014</td>
</tr>
<tr>
<td>$10^{-9}$ -</td>
<td>1205 1205 1205 1205 1205 1205 1205 1205 1193 2615 1980</td>
</tr>
<tr>
<td>$10^{-10}$ -</td>
<td>1205 1205 1205 1205 1205 1205 1205 1205 1205 2078 1194 2584 1980</td>
</tr>
</tbody>
</table>
Incorporating spatial characteristics of the simulation

A simple initial approach with the LCROSS simulation:

- Split the simulation frames into blocks.
- For each block and each time step, compute the mean over pixels.
- Apply the method to the trace of each block mean.
Incorporating spatial characteristics of the simulation

Applying our approach to pixel means for different regions of the simulation with $\alpha = 0.001$, $\sigma^2 = 0.001$, $B = 5$.

Atmosphere blocks

Doomed rocket stage lands in this block.

Pressure
Incorporating spatial characteristics of the simulation

Applying our approach to pixel means for different regions of the simulation with $\alpha = 0.001$, $\delta^2 = 0.001$, $B = 5$.

Doomed rocket stage lands in this block.

Atmosphere blocks
Lots of potential next directions

To name just a few:

- Using our partitioning approach to define spatial regions as the simulation evolves.
- Identifying a mathematical criterion to guide selection of $\alpha$ and $\delta^2$.
- Incorporating other types of fits that can be cheaply computed and updated.
- Handling multivariate trajectories.
But for now…

…our in situ approach is cheap to compute and update, and it provides:

- Substantial memory savings over storing the full output of the simulation.
- Improved fidelity to the simulation over selecting evenly spaced partitions.
- Ability to reconstruct a linear approximation of the simulation with known error.
The end

More details: arxiv.org/abs/1409.0909
Or: The end!

More details: arxiv.org/abs/1409.0909

Also: Statistics and Beer Day
June 13
Some math

In a typical simulation setting, a scalar response $y_i$ will be an unknown deterministic function of time $t_i$:

$$y_i = \mathcal{F}(t_i), \ i = 1, \ldots, T$$

where $T$ is the total number of time steps in the simulation. Our goal is to approximate this function and locate interesting changes:

$$y_i = f(t_i) + \epsilon_i, \ i = 1, \ldots, T$$

Let $P_0, P_1, \ldots, P_m$ be a set of breakpoints of the sequence 1, ..., $T$, with $P_0 = 0$ and $P_m = T$. The function $f$ can be written as a sum over the partitions defined by the breakpoints:

$$f(t_i) = \sum_{j=1}^{m} (\beta_{j,0} + \beta_{j,1} t_i) I\{P_{j-1} < i \leq P_j\}$$

To fit the model, we need to estimate the number of partitions, the breakpoints, and the regression coefficients.
Sufficient statistics

\[\theta = \sum t_i\]
\[\Theta = \sum t_i^2\]
\[\psi = \sum y_i\]
\[\Psi = \sum y_i^2\]
\[\tau = \sum t_i y_i\]
\[T_\bullet\]

Compute the residual sum of squares (RSS) and the slope and intercept:

\[RSS = \Psi - \frac{1}{T_\bullet} \psi^2 - \frac{(\tau - \theta \psi / T_\bullet)^2}{\Theta - \theta^2 / T_\bullet}\]
\[\hat{\beta}_0 = \frac{1}{T_\bullet} (\psi - \hat{\beta}_1 \theta)\]
\[\hat{\beta}_1 = \frac{\tau - \theta \psi / T_\bullet}{\Theta - \theta^2 / T_\bullet}\]
RAGE uses adaptive mesh refinement (AMR)

- Considers **spatial variation** in each variable to choose cell size.
- Makes decisions to split / merge cells at each time step.
- **Constrains splits and merges** so adjacent cells are within 1 level of each other.

Gittings et al. 2008
Other examples of pixel trajectories

Pixel 100

Pixel 2

Pixel 42
We describe capturing the lines with sufficient statistics

But in practice, these sums can get too large to be computationally stable.

\[ T, \sum t_i, \sum t_i^2, \sum y_i, \sum y_i^2, \sum t_i y_i \]

An alternative: incremental QR decomposition:


This is implemented in the R package `biglm`.
Adjusting $\alpha$ alone doesn’t make the decisions we want

60 partitions via $\alpha = 1 \times 10^{-5}, \delta^2 = 0$. 

![Graph showing log(pressure) vs Simulation Time Step]

Total RSS: 11.05
Adjusting $\alpha$ alone doesn’t make the decisions we want

62 partitions via $\alpha = 1 \times 10^{-4}$, $\delta^2 = 1 \times 10^{-6}$.

Total RSS: 1.51
Adjusting $\alpha$ alone doesn’t make the decisions we want

11 partitions via $\alpha = 1 \times 10^{-8}$, $\delta^2 = 0$.

Total RSS: 1205.31
Adjusting $\alpha$ alone doesn’t make the decisions we want

11 partitions via $\alpha = 1 \times 10^{-7}$, $\delta^2 = 1 \times 10^{-4}$.

Total RSS: 38.33