

# A shiny update to an old experiment game

Robert B. Gramacy  
Department of Statistics  
Virginia Tech\*

## Abstract

A full appreciation of aspects of experimental design, modeling, and decision making in applied settings takes time, in two senses. That learning requires patience and diligence is the first, obvious, sense. The second one is that applied work, and experimentation, often play out over long time scales, during which theories are revised, model and inferential techniques are improved, and knowledge is updated. Here I present a game, borrowing liberally from one first played over forty years ago, that attempts to synergize these aspects of learning time. The goal is to reinforce a cascade of topics in modern response surface methods, sequential design and optimization, in a stimulating, competitive and realistic environment. Interface, rules, and evaluation are described, along with a “case study” involving a cohort of students at Virginia Tech.

**Key words:** response surface, computer experiment, experimental design, Bayesian optimization, input sensitivity, teaching game

## 1 The setting

In-class games are a common way to encourage learning—to interject some fun and build intuition in an seemingly esoteric, or tedious technical landscape. A good game could be fundamental to retaining students, say in introductory statistics. One fine example uses chocolate chip cookies to illustrate aspects of sampling distributions (Lee, 2007). The long arc of an out-of-class game played over an entire semester is attempted rather less frequently. However for some topics, like experimental design and response surface optimization, that setting is quite natural: real-life applications play out on longer temporal scales, and in an inherently dynamic landscape. In this article I present such a game, which was played during

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\*Contact: [rbg@vt.edu](mailto:rbg@vt.edu) or Hutcheson Hall (MCO439), 250 Drillfield Drive, Blacksburg, VA 24061

a graduate course I recently gave at Virginia Tech. The game is an update of one first played over forty years ago (Mead and Freeman, 1973).

Mead and Freeman’s game was ahead of its time. Today it is all but forgotten. Although it is cited prominently in Box and Draper (1987), which is how I found it, that is one of just eight references in the literature. Perhaps this is because, for many decades (70s-90s, say) the setup of the game, requiring a custom computing environment with student access, was hard to replicate. Today, with R/CRAN (R Core Team, 2017) implementation and `shiny` (Chang et al., 2017) web interfaces, barriers have come way down.

The original game involves *blackbox* evaluation of agricultural yield as a function of six nutrient levels, borrowed from Nelder (1966) and reproduced in R as follows.

```
yield <- function(N, P, K, Na, Ca, Mg)
{
  l1 <- 0.015 + 0.0005*N + 0.001*P + 1/((N+5)*(P+2)) + 0.001*K + 0.1/(K+2)
  l2 <- 0.001*((2 + K + 0.5*Na)/(Ca+1)) + 0.004*((Ca+1)/(2 + K + 0.5*Na))
  l3 <- 0.02/(Mg+1)
  return(1/(l1 + l2 + l3))
}
```

Although my updated game has kept this `yield` form in its inaugural run, swapping in code for a new blackbox is a trivial matter. Section 4 discusses some potential alternatives.

The original game involved observations of `yield` with additive (Gaussian) block and plot-within-block effects. Players could obtain noisy `yield` evaluations, with the ultimate goal of maximizing, across up to five computer sessions (simulating crop years). Multiple experiments could be undertaken in a single session; however strategies could only be revised “between years”. My updated version retains this spirit of play, but differs on many specifics, as detailed in Section 2.

Adaptations in the new game are motivated by technology, and a desire to teach a more modern statistical toolkit. Classical response surface methods, and design, emphasize low degree (first- and second-order) linear modeling. The resulting steepest ascent and ridge

analyses (see, e.g., Box and Draper, 1987; Myers et al., 2016) enjoy a high degree of analytical tractability. Many relevant calculations can either be performed by hand, or with a graphing calculator. Yet such tools represent the tip of the iceberg in modern application domains like information technology. They seem particularly crude in situations where physical experimentation is coupled with computer simulation experiments, a setup originating in physics and engineering, but becoming increasingly commonplace in the other applied sciences. Modern response surface methods borrow heavily from geostatistics and machine learning with Gaussian processes, deep neural networks, and regression and classification trees. Sequential design strategies like expected improvement (Jones et al., 1998) promise a more modular approach to (so-called Bayesian) optimization, allowing fancy models to be swapped in and out, and a degree of human-free automation with light coding.

Exploring a diverse, state-of-the-art, toolkit benefits from sandboxing aspects of game play, but moreover the superlative nature of the goal—of optimizing **yield**—perhaps suggests that an element of competition may further enhance the learning arena. Section 3 covers player benchmarking, timing of methodology with lecture material, and an assessment strategy designed to encourage regular engagement and the deployment of a wealth of tools. Some results from a real run of the game at Virginia Tech are provided. Section 4 concludes with lessons learned and ideas for future variations. The online supplement includes a full suite of supporting codes and other teaching materials.

## 2 Game design

The core of game play is facilitated by an R **shiny** app, shown in Figure 1, which serves as both a multi-player portal and an interface to the back-end database of player(s) records. An R**markdown** document, `yield.Rmd`, provided with the supplementary material, compiles a full set of instructions on how to use the app, the rules of the game, and some suggestions about

strategy. An HTML rendering of that document is provided at <http://bobby.gramacy.com/teaching/rsm/yield.html>. The salient details follow.

## 2.1 Using the shiny app

Since all game players use the same app, interaction begins with a “logging in” phase. In advance of opening the game, I asked each player to provide me with their initials (2–4 characters) and a four-digit secret PIN, the combination of which comprises the login token. Logging in involves providing “url?token” in the browser search bar. In Figure 1 the URL points to a local **shiny** server, and the token is “rbg4036”, a combination of my initials (I played the game too) and my office number, 403G.

Once logged in, the player is presented with three blocks of game content. A greeting block provides details on spent and total budget for experimental runs. How the budget works, costs of runs, etc., is discussed in detail in Section 2.2. As long as the player has not fully spent, or over-spent, their budget, new runs may be performed, via the second block on the page. Here, the player enters the coordinates of the next run. Until all fields are populated with valid (positive, non-empty) values, helpful error messages appear on the right. The last input, which is a slider, indicates the number of replicates desired—again discussed in more detail shortly. Once all entries are valid, the error messages are replaced by a “Run” button and a warning that there are no do-overs.

Performing a run causes the table in the final block of the page to be updated, with the inputs and outputs of the new run appearing at the top of the table. All together, the table has 18 columns, recording the run week, 7 inputs, and up to ten outputs. The primary purpose of the table is to provide visual confirmation that the run has been successfully stored in the player’s database file. Buttons are provided to aid in browsing, however this is not intended as the main data-access vehicle. A “Download” button at the bottom creates a text file which can be saved via browser support—usually into the `~/Downloads` directory.

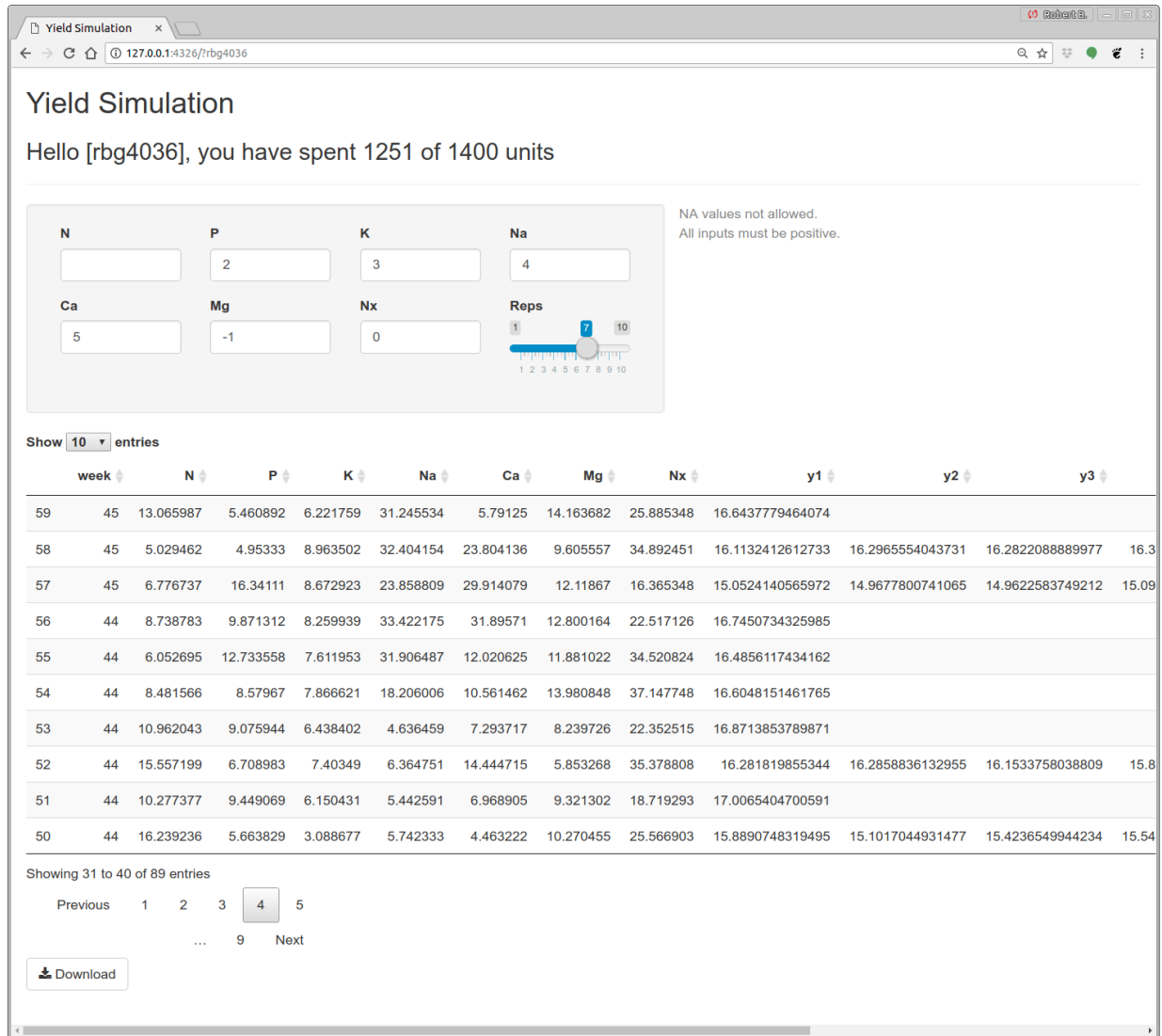


Figure 1: An interactive **yield** simulation session. User **rbg4036** may inspect the run budget, perform new runs (if budget remains), browse historical runs, or download a text file.

Empty output fields are converted to **NAs** in the downloaded file.

Under the hood, the app maintains the player database as files quite similar to those offered for downloading. If the app is being hosted on a standalone node running a **shiny** server, those files may be stored locally in the app's working directory. However, if the game is hosted in the cloud, say on **shinyapps.io**, the database can only temporarily be stored locally, while that instance is active. Ensuring that each of multiple running instances share

the same game database, and guaranteeing its integrity after an instance times out due to inactivity (which causes the local running directory to be purged), requires that the files be stored elsewhere, in a single persistently available location in the cloud. I hosted my game at <http://gramacylab.shinyapps.io/yield>, with database files at [www.dropbox.com](http://www.dropbox.com) accessed through the `rdrop2` (Ram and Yochum, 2017) API. When a new instance is created, startup code triggers `rdrop2` calls to `drop_get` files into the local working directory,<sup>1</sup> and subsequently `drop_upload` to sync those with new runs.

## 2.2 Rules, startup and twists

Many of the rules of the game are enforced by the interface. The most important exception is to do with players sharing data files and/or login tokens, which is not allowed. Players are encouraged to collaborate on strategy, and the development of relevant mathematical calculations, but they may not share code or data. All players start with a database containing an identical design of seven input settings, each with five replicate responses whose noise structure is explained momentarily. Students were introduced to the game in the fifth week (game week zero), and could perform their first runs in the sixth week of a 15-week semester. Including Thanksgiving and a final exams tallies thirteen weeks of game play.

In each week, including week zero, students accrued 100 playing units to spend on runs, with full roll-over from previous weeks. The cost structure for runs favors replicates. Obtaining a single run (i.e., the first replicate) costs ten units. Replicates two through four cost an additional three units each; five through seven cost two, and eight through ten cost one each. As long as a player's account is in the black (i.e., positive balance), s/he can perform a new run with as many replicates as desired. If performing that run causes the balance to be zero, or negative, future runs will not be allowed (the run box on the app disappears)

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<sup>1</sup>All of the player files are downloaded as part of the instance initialization, which can unfortunately be time consuming. However, the instance is then ready to serve multiple players, if needed.

until the following week, after 100 new units are added.

Replication is important for two game “twists” designed to encourage players to think about signal-to-noise trade-offs, and to nudge them to spend units regularly, rather than save them all until the end of the semester. The first is that players are told that the variance of the additive noise on `yield` is changing weekly, following a smooth process in time, and that they will need to provide an estimate of that variance over time for their final report. They are further warned that the variance may be increasing, effectively devaluing unused units. In fact the variance in week  $w$  followed a simple sinusoidal structure

$$\sigma^2(w) = 0.1 + 0.05(\cos(2\pi(w - w_s)/10) + 1) \quad \text{for starting week } w_s,$$

which peaks in the first and tenth week. The second wrinkle is a seventh input, `Nx`, which is unrelated to the response. Students are not told that one of the inputs is useless, however the final writeup instructions ask for sensitivity analyses for the inputs, including main, partial dependence, and total effects.

### 3 Timing, outcomes and evaluation

Starting in the fifth week of the semester allows for ramp-up on methodological training, giving students the chance to learn fundamentals like steepest ascent and ridge analyses (e.g., Myers et al., 2016, Chapters 5–6) before entering the game as players. Using R code provided in class, most students were able perform runs in the first two weeks that improved upon `yields` from week zero. In subsequent weeks, new methodology was introduced which students were expected to try in the game. Details on how game play tracks course material, cookie crumbs to “catch up” stragglers, and windows into game progress are provided below.

### 3.1 Subject progression and homeworks

Homeworks are assigned roughly every two weeks and each one, from the third onward, contains a problem on the game. Problem statements and solutions are provided with the supplementary material. The third homework is the the most prescriptive about what to do in the game. It instructs the student to fit a first-order model to the initial data set ( $7 \times 5$  runs) and determine which of the seven main effects are useful for describing variation in **yield**. In my own solution, only the first three are relevant, e.g., after a backwards **step**-wise selection procedure with BIC. Then, after reducing to a first order model having only those three components, they are asked to search for interactions. I found one.

With best fitted model in hand, students are asked to characterize a path of steepest ascent, and to obtain **yield** responses along that path. This requires determining values for the remaining (in my case four) inputs. No guidance is given here; I used a Latin hypercube sample, paired with six settings of the three active variables a short ways along the path of steepest ascent. Next, students are given several options about how to proceed, including a second-order ridge analysis, more exploration with space-filling designs, or more steepest ascent. In my own solution I did a bit of all three, and the result was a second-order fit to the data that had many relevant main effects, interactions, etc.

After the homework deadline, I released my solution so students could see what I did, and use it to “catch up” with other players during subsequent weeks. Then we transitioned to modern material involving Gaussian processes (GPs), presented from machine learning (Rasmussen and Williams, 2006) and computer surrogate modeling (Santner et al., 2003) perspectives. Both communities evangelize the potential for fitted GP predictive surfaces to guide searches for global optima in blackbox functions. Machine learning researchers call this Bayesian optimization, whereas computer modelers call it surrogate-assisted optimization (however increasingly they are adopting the machine learning terminology). The simplest variation involves optimizing the fitted GP predictive mean equations (Booker et al., 1999),



in lieu of working directly with locally winnowed input–output data pairs. The method of expected improvement (EI, Jones et al., 1998) and integrated variations (e.g., IECI, Gramacy and Lee, 2011) are subsequently introduced to better balance exploration and exploitation by incorporating degrees of predictive variability (local to global), a hallmark of statistical decision-making. These three approaches are reinforced in three questions spanning three subsequent homeworks. Solutions are provided (after the due dates) as plug-n-play R scripts leveraging mature `laGP` subroutines (Gramacy, 2016) converting a database file into a suggested new run without any additional human interaction.

### 3.2 Leaderboard

In hopes that friendly competition would spur creativity, I provided leaderboard-style views into players’ performance relative to one another, updated in real time. An `Rmarkdown` script, pulling from the same `rdrop2` API and hosted on `shinyapps.io`, compiled four views into player progress. Two of those views, snapped during the final week of game play, are provided

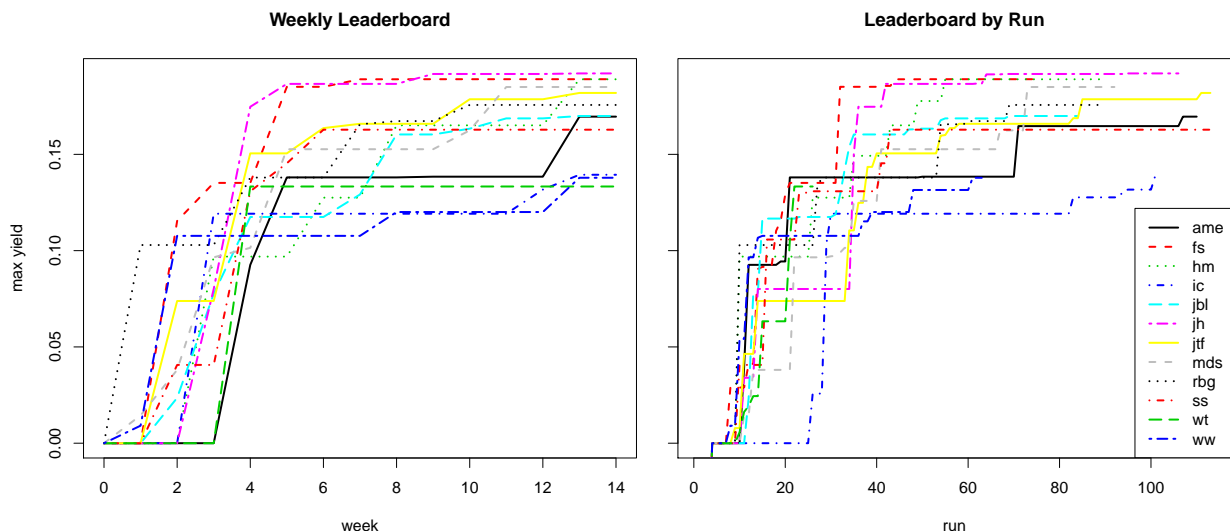


Figure 2: Two de-noised views into the real-time leaderboard during the final week of game play: best yield buy week (*left*), and by run (*right*).

in Figure 2. On the  $x$ -axis is the week of game play (*left* panel) or the unique run number (*right*), and on the  $y$ -axis is a normalized `yield` response value. Each player has a line in the plot, with color and type indicated by their initials (masking the pin). The responses shown have been de-noised in order to view pure progress, making normalization essential otherwise players would know the true mean value of their best noisy response. The two other views provided by the `Rmarkdown` script show “raw” versions of these same plots, on the original scale—these are not shown here.

Observe from the panel that about half of the progress is made in the first five weeks, spanning around forty runs. Students “jh” and “fs” made rapid progress. By contrast, “hm” ends up at the same place in the end, but with more steady increments. The leaderboard would seem to partition students into three classes, comprising of the top five, middle four, and lower four. Apparently, students “wt” and “ww” gave up early. My own strategy placed me fifth by these measures. I favored replication over unique runs in hopes of obtaining better main effects, sensitivity indices, and estimates of variance over time.

## 4 Discussion

I have described a statistical optimization game updating a previous one in two senses. The first sense is that the game uses modern tools for implementation. Supplementary materials provide R code with support for a `shiny` app interface, cloud storage for instance-based hosting like `shinyapps.io`, and real-time views into progress via a leaderboard. Although the original version of the game was innovative, when introduced it was essentially unusable by others at the time owing to the nature of computing environments available in the early 1970s. The second update has to do with modern response surface methods. My re-casting of the game, and the homework problems from class which support it, emphasize a machine learning and computer surrogate modeling “hands-free” toolkit from the 21st century.

Upon reflection, the game perhaps could be revised to better emphasize these more modern tools. Students who made early progress on the leaderboard became impatient with subsequent lack of positive feedback from further runs. They had been “unlucky” in finding right answer “too early” to benefit from the modern tools. In future play I may opt for a multi-modal `yield` surface in order to keep them engaged, and to demonstrate the explorative value that comes from EI and IECI-like heuristics appearing later in the syllabus. Another potentially exciting variation may entertain a real `yield` simulation, a promising example being the so-called assemble-to-order (ATO, Xie et al., 2012) solver. This eight-dimensional example is challenging because it has a spatially dependent noise structure.

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