Constructing Experimental Solutions to Inverse Problems with Mathematica – Joel Schwartz

Purpose
This activity introduces the field of inverse problems, specifically those where a single input constraint produces a potentially infinite number of two-parameter solutions. Experimentation, statistics, and computational methods are combined to demonstrate one methodology for handling such situations. Instructor familiarity with the Mathematica environment, though not mandatory, is recommended.

Overview
A background talk on the topics of inverse problems and relevant mathematics will begin the activity. Students will then be presented with a scenario that initially appears unsolvable, suggested here to be finding the amounts of two colors of M&Ms which are inside a container. After a class survey of guesses as to the amounts, a discussion of how to approach this problem will follow. Next students will perform various experiments, such as weighing the container, weighing a single M&M, and sampling M&Ms from the container (or other source.) With the information obtained, students will use a Mathematica template to create plots of possible solutions to the problem, plus see how certain adjustments affect the results. The activity will proceed with an unveiling of the true color amounts, concluding with a class discussion on the accuracy and utility of the methods used.

Student Outcomes
Students will be able to:

- State what an inverse problem is and why it is difficult to solve exactly.
- Describe the relevant mathematics (contours, chi-square values, normal distribution, etc.)
- Describe the approach for trying to solve the M&M color scenario.
- Use scales to estimate the weight of both the container and individual M&Ms.
- Take samples from the container (or other source) to estimate the M&M color proportion.
- Transfer their information into a Mathematica template and run its procedures.
- Analyze the effect constraint changes have on the possible solutions.
- Evaluate their methods and results before & after learning the actual M&M color amounts.

Standards Addressed
NGSS Standards:

- HS-ETS1-2 (complex problems into more manageable problems)
- HS-ETS1-4 (computer simulation to model solutions to complex problems)

CCSS Standards:

- A-REI-10 (two-variable equation solutions form curves in coordinate plane)
- S-MD-7 (analyze decisions using probability concepts

Time
Two to three 45-minute class periods, depending on student ability.

Level
High School- general science/math (techniques apply to many different fields.)

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Materials and Tools

Wolfram Mathematica software:
http://www.wolfram.com/mathematica/

"Inverse Problem Template" notebook (Joel Schwartz, Northwestern University):
(Contains commentary notes)

IPA Supplemental worksheet for template notebook

"Inverse Problems" PowerPoint file (Joel Schwartz, Northwestern University):

Laptops/computers (with *Mathematica* installed; enough for pairs/small groups)

M&Ms (ideally in the 250-500 range, plus possible extras for experiments)

2 identical containers/jars (preferably opaque)

Scales for weighing objects

Preparation

Decide on what the color categories of M&Ms will be. For example, it may be good to use "red" and "non-red" as the investigation types, since these ensure all the candy will be usable. If desired, count and record the total amount in each category (not doing this also has benefits), then place all the M&Ms into one of the containers (the other should be left empty.) Keep another supply of M&Ms available for experiments if the container is not going to be sampled from during the activity. If possible, have multiple scales available to avoid bottlenecks when conducting experiments. Also, ensure Mathematica is installed and accessible on all laptops/computers which will be used during the activity. Instructors are advised to look over the template notebook ahead of time, so they are familiar with the variable names and how it functions. If unfamiliar with inverse problems and/or the associated mathematics, instructors should review these concepts and accompanying PowerPoint file as well.

Prerequisites

Basic understanding of functions involving more than one variable, as well as minor familiarity with probability and statistics (such as what a probability represents, what "means" and "uncertainties" are, etc.) These topics can be briefly reviewed at the beginning of the activity as necessary. Previous use of Mathematica is ideal, but certainly not required.

Background

Suppose that a friend of ours is currently working two jobs. If we know that she collected $500 on one paycheck and $400 on the other, then it is not difficult to reason that she earned $900 in total. However, if on her next payday we know that she collected $1200 in total, then how much did she earn on each paycheck individually? Think about this for a minute, and you will likely conclude that this situation is much more complicated. Any set of amounts which sum to $1200 is valid, and thus there are a wide variety of possible solutions to the question. Scenarios like this and similar are known as "inverse problems" in the scientific fields, since they involve thinking about a situation in an opposite manner than is normally done.

Although difficult to give specific solutions to, inverse problems are by no means impossible to handle. In fact, they are often some of the most well-studied problems due to their importance in science and mathematics. This activity will explore one particular method for tackling inverse problems with two-parameter solutions, like in our friend's paycheck example above. We will use scientific experimentation, statistical reasoning, and computer programming to turn a very extensive problem into something much more focused. At the end, we will examine the quality of our inferences and gauge the usefulness our methods have for application elsewhere in the world.

As the activity progresses, keep in mind and think over the following questions :

- Have you ever encountered an inverse problem before in real life?
- What additional information would help you solve a particular inverse problem?
- Is all extra information good, or is some more useful than others?
- How does each aspect of our approach aid in trying to find the solution?
- Where & how can we incorporate such scientific reasoning in our everyday lives?

Remember that nothing worthwhile comes easy, and the same is true for cracking inverse problems: they are difficult precisely because they are rewarding. Happy science adventuring!

Teaching Notes

Depending on the type and ability of class being taught, the background discussion on inverse problems and mathematical framework may need more or less emphasis. The included PowerPoint presentation gives an overview of these topics, and was used during the preliminary teaching of this activity. The graphs/plots displayed were all created using Mathematica (many with an earlier version of the template notebook used here.) It may be referred to as a reference, or shown directly as part of the introduction.

Basically, inverse problems are those where data are used to infer the values of given model parameters, such as measurements of localized motion from seismic waves being used to infer the variable density of the Earth. This activity simplifies the idea to situations where single numbers place constraints on a general combination of two other parameters (for example, total class enrollment constrains the sum of women and men in attendance.) These equations can be expressed graphically as contour lines, akin to lines of constant elevation on a topographical map. By incorporating the uncertainty on the constraint value, Chi-square statistics can be used to broaden the contour line into a region of acceptable solutions (Chi-square is related to the normal distribution, in that it measures deviations from the mean value in units of standard deviations.) Combining multiple distinct constraints will then limit the acceptable solutions, since only those regions mutually overlapped are the most probable.

Once a suitable background talk has been completed, have students obtain laptops/computers, then open the Mathematica "Inverse Problem Template" notebook while passing out the supplemental worksheet. Commentary is provided in the template notebook for reference, and should be pointed out to the students. Briefly state the role of the template notebook to create several Chi-square plots from the data provided, and indicate that the supplemental worksheet has an identical set of input variables on which to write down information. The plots they will be creating are analogous to the ones shown in the PowerPoint presentation, so having students recognize this connection early on is helpful.

The main activity scenario can now be described. Show the filled container and state that it has an unknown number of M&Ms inside. Stipulate further that these M&Ms can be broken down into two categories, using the category types selected before the lesson began. The question for the students to resolve: how many of each M&M type are held within the container? Take a survey here of each student's preferred guess before supplying any additional information. There will likely be a wide range of amounts suggested, and ideally students will identify this as an exemplary inverse problem. Explain here, however, that they will now attempt to solve this scenario, using the following principles:

- Weighing the container on a scale is an indirect way of counting the total number of M&Ms inside. Thus, one equation is $M_{total} = [(n_x + n_y) \cdot m_{one} + M_{empty}]$.
- Sampling M&Ms from the container (or other source, if similar in composition) is a way of gauging the ratio between the color types. Thus, a second equation is $R_{color} = (n_x / n_y)$.

Here M_{total} is the total mass of the container plus M&Ms, n_x and n_y are the number of each M&M color type, m_{one} is the mass of a single M&M, M_{empty} is the mass of the empty container, and R_{color} is the ratio between the color types.

At this point, students should begin filling out the supplemental worksheet, as this will assist them later when transitioning to Mathematica. The **parameterX** and **parameterY** variables should be the names of the two color categories, while **lowX**, **highX**, **lowY**, and **highY** are the numerical limits each category is considered to be within. It is suggested that the lower limits be set above 0, as this will avoid "divide-by-zero" errors when running the Mathematica code. The upper limits should be set appreciably higher than the true container values, so that the actual solution region is included on the plots. The **constraintONE** and **constraintTWO** variables should be the names of the attributes students will measure shortly, here "Single M&M Mass (g)" and "Color Ratio" respectively. The **equationONE[X_,Y_]** and **equationTWO[X_,Y_]** lines are

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the equations which relate the parameters to the constraints; they should be written respectively <u>exactly</u> as follows:

- $(M_{total} - M_{empty})$ / (X+Y) *[The masses are placeholders for the measured values.]*
- X / Y *[Remember which order the ratio is defined as.]*

Students are now left to fill in the remaining worksheet variables by performing some experiments (all masses should be taken in grams.) The class should first weigh the filled and empty containers, and the values should be substituted into the 1st constraint equation as indicated above. Students will then independently measure the mass of a single M&M, as well as calculate the color ratio of a small sample of M&Ms from the container (or other source.) In both cases the value <u>and</u> uncertainty should be recorded, and the manner for doing this is left to the instructor's discretion. Students new to statistics can simply state a "gut feeling" uncertainty for their single measurement/sample; those well-versed can take multiple measurements/samples to calculate means and standard deviations. In any case, the outcomes should be noted on the worksheet for **valueONE**, **uncertaintyONE**, **valueTWO**, and **uncertaintyTWO** as appropriate.

Once students obtain all their information, it should be transferred into the Mathematica template notebook. Stress that <u>attention should be paid to format when entering the information</u>, as the software requires specific syntax in order to run correctly. These formats are reflected on the supplemental worksheet, but some aspects to remember:

- The default values are placeholders and should be overwritten.
- Nothing should be entered/changed to the left of the equal sign for any variable/equation.
- Strings (here for written names) should be surrounded by quotation marks.
- Numbers should not have units attached (Mathematica will assume those are new variables.)
- As coded, the constraint equations use capital, not lowercase, X and Y letters.
- The trailing semicolon is used on each variable/equation to suppress extraneous output.

When all data has been transferred, students should use the "Evaluate Notebook" command under "Evaluation" in the menu bar. This will execute all commands in the notebook, including those which are in the hidden cells. Improper syntax will cause Mathematica to output orange error messages, and these cases can be handled accordingly.

Correct use of the template will result in three different Chi-square plots being produced at the bottom of the notebook. These graphs display potential amounts for each M&M color type when considering (respectively) the 1st constraint only, 2nd constraint only, and both constraints together. Dark regions correspond to more likely combinations, while light regions are less likely. The contours on each plot represent deviations of 0.5, 1, 1.5, 2, 2.5, and 3 standard deviations from the constraint values. (Hovering over these contours displays the square of these numbers, due to the definition of the Chi-square statistic.) Students should note the features of their graphs, such as the contour line shape, spread between contour lines, and regions of best-fit. By right-clicking on a plot and selecting "Get Coordinates" from the drop-down list, more precise values of X and Y can be obtained. Ask students to find a pair of M&M color amounts that the statistics suggest to be very likely inside the container.

The supplemental worksheet contains additional questions about altering the information supplied to the template, and students should test out those ideas next. Remind them that after updating the desired variables, they should use "Evaluate Notebook" to reconstruct a new set of plots. Students should analyze the impact these changes have on the graphs and solution to the problem; allow adequate time for this portion of the lesson since it is probably unfamiliar. Towards the end of the activity, find the true amount of each color type by separating and counting the M&Ms inside the container. This can be done by students who are ahead in the lesson, or the entire class by dividing the M&Ms amongst everyone. Finish with a class discussion that includes:

- Students comparing their results to the true color amounts.
- The accuracy and utility of the chi-square method (here, and for general inverse problems.)
- The thought questions posed to students in the "Background" section above.

The timing breakdown for the lesson might look as follows:

- $\leq$ 1 class period for background discussion
- $\approx$ ½ class period for describing M&M scenario, related equations, and template notebook
- ½ class period for conducting experiments and recording information
- ½ class period for analyzing Chi-square plots (and modifications) in Mathematica
- $\approx$ ½ class period for concluding discussion

Assessment

- Ask level-appropriate questions & survey for understanding about mathematical foundation of inverse problems.
- Observe students' experimental techniques & ask for explanations on why they chose particular constraint values and uncertainties.
- Observe that students are able to properly transfer the necessary information into Mathematica to generate the statistical plots.
- Ask questions (including those on supplemental worksheet) concerning the validity of the results obtained through this procedure.

Additional Information

This activity has been presented in the context of finding M&M color amounts inside a container, but the template notebook for Mathematica has been written to accept general input of a similar nature. Thus, instructors wishing to apply the technique to any other two-parameter inverse problem are free to do so (just modify the names, ranges, and equations as appropriate.) Also, the Mathematica template code is fairly straightforward overall, so the entire procedure could be written up for another platform without much difficulty. Mathematica was chosen for its math focus and favorable plotting features.

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