

A/B Testing and Beyond

Designed Experiments for Data Scientists



Week 5

Tuesday October 2nd, 2018



Outline

- Recap
- Primer on linear regression
- Experiments with Multiple Conditions
 - Comparing means
 - Comparing proportions
 - The multiple comparison problem
- Multi-armed Bandit Experiments



RECAP



Recap

- Experiments with Two Conditions
 - Evaluating Assumptions
 - Welch's t -test
 - Randomization tests
 - Another way of comparing proportions: χ^2 -tests
 - A discussion of “peeking”



LINEAR REGRESSION – A PRIMER



Linear Regression

- This is a form of statistical modeling that is appropriate when interest lies in relating a response variable (Y) to one or more explanatory variables (x_1, x_2, \dots, x_p).
- The idea is that Y is influenced in some manner by $\{x_1, x_2, \dots, x_p\}$ according to an unknown function:

$$Y = f(x_1, x_2, \dots, x_p)$$



Linear Regression

- The goal of statistical modeling in general (and linear regression in particular) is to approximate the function $f(\cdot)$

- The linear regression model relates Y to $\{x_1, x_2, \dots, x_p\}$ via

$$Y = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p + \epsilon$$

where

- Y is the response variable
- The x_j 's are explanatory variables we treat as fixed
- The β 's are unknown parameters quantifying the influence of a particular x_j on Y



Linear Regression

- And ϵ is the **random error term** that accounts for the fact that

$$f(x_1, x_2, \dots, x_p) \neq \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p$$

and we assume $\epsilon \sim N(0, \sigma^2)$

- This distributional assumption has several consequences. In particular, it implies

$$Y \sim N(\mu = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p, \sigma^2)$$

which means that we expect, for specific values of the x 's, the response to be equal to

$$\mu = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p$$



Linear Regression

Based on this distributional result

$$E[Y | x_1 = x_2 = \dots = x_p = 0] = \beta_0$$

And so β_0 is interpreted as the **intercept** of the model:

- The expected response when all of the explanatory variables are equal to zero.



Linear Regression

Also notice that

$$\begin{aligned} & E[Y|x_j = x + 1] - E[Y|x_j = x] \\ &= (\beta_0 + \beta_1 x_1 + \cdots + \beta_j(x + 1) + \cdots + \beta_p x_p) \\ &\quad - (\beta_0 + \beta_1 x_1 + \cdots + \beta_j x + \cdots + \beta_p x_p) \\ &= (\beta_0 + \beta_1 x_1 + \cdots + \beta_j x + \beta_j + \cdots + \beta_p x_p) \\ &\quad - (\beta_0 + \beta_1 x_1 + \cdots + \beta_j x + \cdots + \beta_p x_p) \\ &= \beta_j \end{aligned}$$

And so β_j is interpreted as the expected change in response associated with a unit increase in x_j , while holding all other explanatory variables fixed



Linear Regression

To actually use the linear regression model we must **estimate** the β 's.

This is typically done with **least squares estimation** where the goal is to find values of $(\beta_0, \beta_1, \dots, \beta_p)$ that minimize the model's error, ϵ .

For observed data $(y_i, x_{i1}, x_{i2}, \dots, x_{ip})$, $i = 1, 2, \dots, n$ we wish to minimize

$$\sum_{i=1}^n \epsilon_i^2 = \sum_{i=1}^n \left(y_i - (\beta_0 + \beta_1 x_{i1} + \dots + \beta_p x_{ip}) \right)^2$$



Linear Regression

The linear regression model can be expressed in vector-matrix notation as follows

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$
$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$



Linear Regression

Using this formulation it can be shown that the least squares estimate of $\boldsymbol{\beta}$ and hence of the individual β 's is given by

$$\hat{\boldsymbol{\beta}} = (X^T X)^{-1} X^T \mathbf{y}$$

$$= \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \vdots \\ \hat{\beta}_p \end{bmatrix}$$



Linear Regression

With the regression coefficients estimated we define the **fitted values** to be

$$\hat{\mu}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \cdots + \hat{\beta}_p x_{ip}$$

which are interpreted as an estimate of the expected response for specific values of the x 's

Next we define the **residuals** to be

$$e_i = y_i - \hat{\mu}_i$$

which represent the difference between observed values of the response and what the model predicts the response to be.



Linear Regression

It can be shown that the least squares estimate of σ^2 is

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^n e_i^2}{n - p - 1} = \frac{\sum_{i=1}^n (y_i - \hat{\mu}_i)^2}{n - p - 1}$$

- This estimate is sometimes referred to as the **mean squared error** (MSE) of the model
- This is because $\hat{\sigma}$ quantifies the typical distance (error) between an observed response value and the value predicted by the model



Linear Regression

Having estimated $\beta_0, \beta_1, \dots, \beta_p$ and σ^2 the fitted linear regression model can be used for **inference** and **prediction**

Of particular importance are hypothesis tests of the form

$$H_0: \beta_j = 0 \text{ vs. } H_A: \beta_j \neq 0$$

for some $j = 1, 2, \dots, p$

And confidence and prediction intervals for predicted values of Y



EXPERIMENTS WITH MULTIPLE CONDITIONS



Comparing Multiple Conditions

- We now consider the design and analysis of an experiment consisting of multiple experimental conditions i.e., an A/B/n Test
- Like an A/B test, the goal is to decide which condition is optimal with respect to some metric of interest – but now we have several conditions

CLICK ME

CLICK ME

CLICK ME

CLICK ME

- Given several options, which one is best?



Comparing Multiple Conditions

Designing a multi-condition test:

- Choose your response variable (y)
- Choose a metric θ that summarizes the response
- Choose a design factor and m levels to experiment with
- Choose n_1, n_2, \dots, n_m – the number of units to assign to each condition



Comparing Multiple Conditions

Data Collection:

- Randomly assign n_j units to condition $j = 1, 2, \dots, m$
- Measure the response (y) on each unit and summarize the measurements with the metric of interest θ in each of the conditions and hence obtain

$$\hat{\theta}_1, \hat{\theta}_2, \dots, \hat{\theta}_m$$

Goal:

- Identify the optimal condition



Comparing Multiple Conditions

In order to identify the optimal condition, we simply need to do a series of **pairwise comparisons** using two-sample tests

- t -tests, Z -tests, and χ^2 -tests may be used for this purpose

However, while identifying the optimal condition is the ultimate goal, it is prudent to first **decide whether a difference exists, at all**, between the conditions



Comparing Multiple Conditions

To answer this question formally, we may test a hypothesis of the form

$$H_0: \theta_1 = \theta_2 = \cdots = \theta_m \text{ vs. } H_A: \theta_j \neq \theta_k$$

for some $j \neq k$

Next we discuss how to test this hypothesis in the cases that the metric of interest is either a

- Mean, or a
- Proportion (rate)



Comparing Multiple Means

The Linear Regression F -test

Here interest lies in testing the hypothesis

$$H_0: \mu_1 = \mu_2 = \cdots = \mu_m \text{ vs. } H_A: \mu_j \neq \mu_k$$

for some $j \neq k$.

This may be done with the F -test associated with an appropriately defined linear regression model.

Specifically, we adopt the following model:

$$Y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_{m-1} x_{i,m-1} + \epsilon_i$$



Comparing Multiple Means

The Linear Regression F -test

In this model

- $Y_i \sim N(\mu_j, \sigma^2)$ represents the response observation for unit $i = 1, 2, \dots, N = \sum_{j=1}^m n_j$.
- Each x_{ij} is a dummy (indicator) variable taking on the value 1 if unit i is in condition j , and 0 otherwise
- $\epsilon_i \sim N(0, \sigma^2)$ represents the random error term for unit i
- The β 's are unknown regression parameters



Comparing Multiple Means

The Linear Regression F -test

The parameter β_0 is interpreted as the expected response value when $x_1 = x_2 = \cdots = x_{m-1} = 0$

In other words, β_0 is the expected response value in condition m

We can also show that $\beta_0 + \beta_j$ is the expected response value in condition $j = 1, 2, \dots, m - 1$



Comparing Multiple Means

The Linear Regression F -test

As such

$$\mu_1 = \beta_0 + \beta_1$$

$$\mu_2 = \beta_0 + \beta_2$$

$$\mu_3 = \beta_0 + \beta_3$$

$$\vdots$$

$$\mu_{m-1} = \beta_0 + \beta_{m-1}$$

$$\mu_m = \beta_0$$

and

$$\mu_1 = \mu_2 = \cdots = \mu_m$$

if and only if

$$\beta_1 = \beta_2 = \cdots = \beta_{m-1} = 0$$



Comparing Multiple Means

The Linear Regression F -test

So testing

$$H_0: \mu_1 = \mu_2 = \cdots = \mu_m \text{ vs. } H_A: \mu_j \neq \mu_k$$

for some $j \neq k$

is equivalent to testing

$$H_0: \beta_1 = \beta_2 = \cdots = \beta_{m-1} = 0 \text{ vs. } H_A: \beta_j \neq 0$$

for some $j = 1, 2, \dots, m$

This latter test corresponds to the F -test for overall significance in a linear regression model



Comparing Multiple Means

Example: Candy Crush

Candy Crush is experimenting with three different versions of in-game “boosters”:

- The lollipop hammer
- The jelly fish
- The color bomb

Users are randomized to one of these three conditions ($n_1 = 121$, $n_2 = 135$, $n_3 = 117$) and they receive (for free) 5 boosters corresponding to their condition.

Let μ_j represent the average length of game play in condition $j = 1, 2, 3$.



Comparing Multiple Means

Example: Candy Crush

While interest ultimately lies in finding the booster condition that maximizes user engagement, (i.e., has the largest μ_j) we will first decide whether any difference at all exists between the conditions:

$$H_0: \mu_1 = \mu_2 = \mu_3 \text{ vs. } H_A: \mu_j \neq \mu_k$$

for some $j \neq k$

To do so, we fit an “appropriately defined linear regression model”. The results are shown on the next slide.



Comparing Multiple Means

Example: Candy Crush

Call:

```
lm(formula = time ~ factor(booster), data = candy)
```

Residuals:

Min	1Q	Median	3Q	Max
-2.84231	-0.69476	0.02617	0.65326	2.76681

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	5.01281	0.08664	57.859	<2e-16 ***
factor(booster)2	1.17528	0.11931	9.851	<2e-16 ***
factor(booster)3	4.88279	0.12357	39.515	<2e-16 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '1'

Residual standard error: 0.953 on 370 degrees of freedom

Multiple R-squared: 0.8216, Adjusted R-squared: 0.8206

F-statistic: 851.9 on 2 and 370 DF, p-value: < 2.2e-16



Comparing Multiple Means

Example: Candy Crush

From this output we see that $\hat{\beta}_0 = 5.0128$, $\hat{\beta}_1 = 1.1753$ and $\hat{\beta}_2 = 4.8828$

This means that the average length of game play in each condition is estimated to be

- $\hat{\mu}_1 = 5.0128$ minutes in the lollipop hammer condition
- $\hat{\mu}_2 = 6.1881$ minutes in the jelly fish condition
- $\hat{\mu}_3 = 9.8956$ minutes in the color bomb condition



Comparing Multiple Means

Example: Candy Crush

The p-value associated with the F -test for overall significance in a linear regression model is less than 2.2×10^{-16} which provides very strong evidence against H_0

Thus we conclude that the average length of game play is not the same for each of the boosters.

To determine which booster is optimal – the one that maximizes game play duration – we must use a series of pairwise t-tests



Comparing Multiple Proportions

χ^2 -test of Independence

Here interest lies in testing the hypothesis

$$H_0: \pi_1 = \pi_2 = \cdots = \pi_m \text{ vs. } H_A: \pi_j \neq \pi_k$$

for some $j \neq k$.

This may be done with the same χ^2 -test of independence that we discussed in the $m = 2$ case

Yes, it generalizes!



Comparing Multiple Proportions

χ^2 -test of Independence

In the case of m conditions we have a $2 \times m$ contingency table:

		Condition				
		1	2	...	m	
Conversion	Yes	$O_{1,1}$	$O_{1,2}$...	$O_{1,m}$	O_1
	No	$O_{0,1}$	$O_{0,2}$...	$O_{0,m}$	O_0
		n_1	n_2	...	n_m	$\sum_{j=1}^m n_j$

- $O_{1,j}$ and $O_{0,j}$ respectively represent the observed number of conversions and non-conversions in condition $j = 1, 2, \dots, m$
- O_1 and O_0 represent the overall number of conversions and non-conversions



Comparing Multiple Proportions

χ^2 -test of Independence

If $\pi_1 = \pi_2 = \dots = \pi_m = \pi$ then we would expect the conversion rate in each condition to be the same

Pooled estimates of $\hat{\pi}$ and $1 - \hat{\pi}$ are given by

$$\hat{\pi} = \frac{O_1}{\sum_{j=1}^m n_j} \text{ and } 1 - \hat{\pi} = \frac{O_0}{\sum_{j=1}^m n_j}$$

With these we can calculate the **expected number of observations** in each cell of the contingency table:

$$E_{1,j} = n_j \hat{\pi} \text{ and } E_{0,j} = n_j (1 - \hat{\pi})$$

for $j = 1, 2, \dots, m$



Comparing Multiple Proportions

χ^2 -test of Independence

The expected frequencies can also be summarized in a contingency table:

		Condition				
		1	2	...	m	
Conversion	Yes	$E_{1,1}$	$E_{1,2}$...	$E_{1,m}$	O_1
	No	$E_{0,1}$	$E_{0,2}$...	$E_{0,m}$	O_0
		n_1	n_2	...	n_m	$\sum_{j=1}^m n_j$

Note that the margin totals do not change.

As in the 2×2 case, the χ^2 -test formally compares what was observed and what is expected under the null hypothesis



Comparing Multiple Proportions

χ^2 -test of Independence

The **test statistic** that compares the observed count in each cell to the corresponding expected count, is defined as

$$T = \sum_{l=0}^1 \sum_{j=1}^m \frac{(O_{l,j} - E_{l,j})^2}{E_{l,j}}$$

Assuming H_0 is true, T approximately follows a $\chi^2_{(m-1)}$ distribution

- As a rule of thumb, this approximation may be very poor unless the **observed and expected cell frequencies** are all greater than 5



Comparing Multiple Proportions

Example: Nike SB

- Suppose that Nike is running an ad campaign for Nike SB, their skateboarding division
- The ad campaign involves $m = 5$ different video ads being shown in Facebook newsfeeds
- In these five video conditions there are $n_1 = 5014$, $n_2 = 4971$, $n_3 = 5030$, $n_4 = 5007$, and $n_5 = 4980$ users, respectively
- The videos in these conditions are viewed 160, 95, 141, 293, and 197 times yielding watch rates:

$$\hat{\pi}_1 = 0.03, \hat{\pi}_2 = 0.02, \hat{\pi}_3 = 0.03,$$

$$\hat{\pi}_4 = 0.06, \hat{\pi}_5 = 0.04$$



Comparing Multiple Proportions

Example: Nike SB

The observed contingency table is

		Condition					
		1	2	3	4	5	
View	Yes	160	95	141	293	197	886
	No	4854	4876	4889	4714	4783	24116
		5014	4971	5030	5007	4980	25002

And the expected contingency table is

		Condition					
		1	2	3	4	5	
View	Yes	177.68	176.16	178.25	177.43	176.48	886
	No	4836.32	4794.84	4851.75	4829.57	4803.52	24116
		5014	4971	5030	5007	4980	25002



Comparing Multiple Proportions

Example: Nike SB

- The observed value of the test statistic for this test is $t = 129.1761$ and the corresponding p-value is 5.84×10^{-27} and so there is strong evidence against H_0
- As such, we conclude that the likelihood that someone “views” a video is not the same for all of the videos
- To determine which video is optimal – the one with the highest likelihood of viewing – we must use a series of pairwise Z-tests or χ^2 -tests



The Multiple Comparison Problem

As we saw in the previous two examples, the null hypothesis of overall equality is often rejected

In these cases a family of follow-up pairwise comparisons are necessary to determine which condition(s) is (are) optimal

Statistically we know how to do this

However, when doing multiple comparisons, it is important to recognize that the overall Type I Error rate associated with this family of tests is inflated



The Multiple Comparison Problem

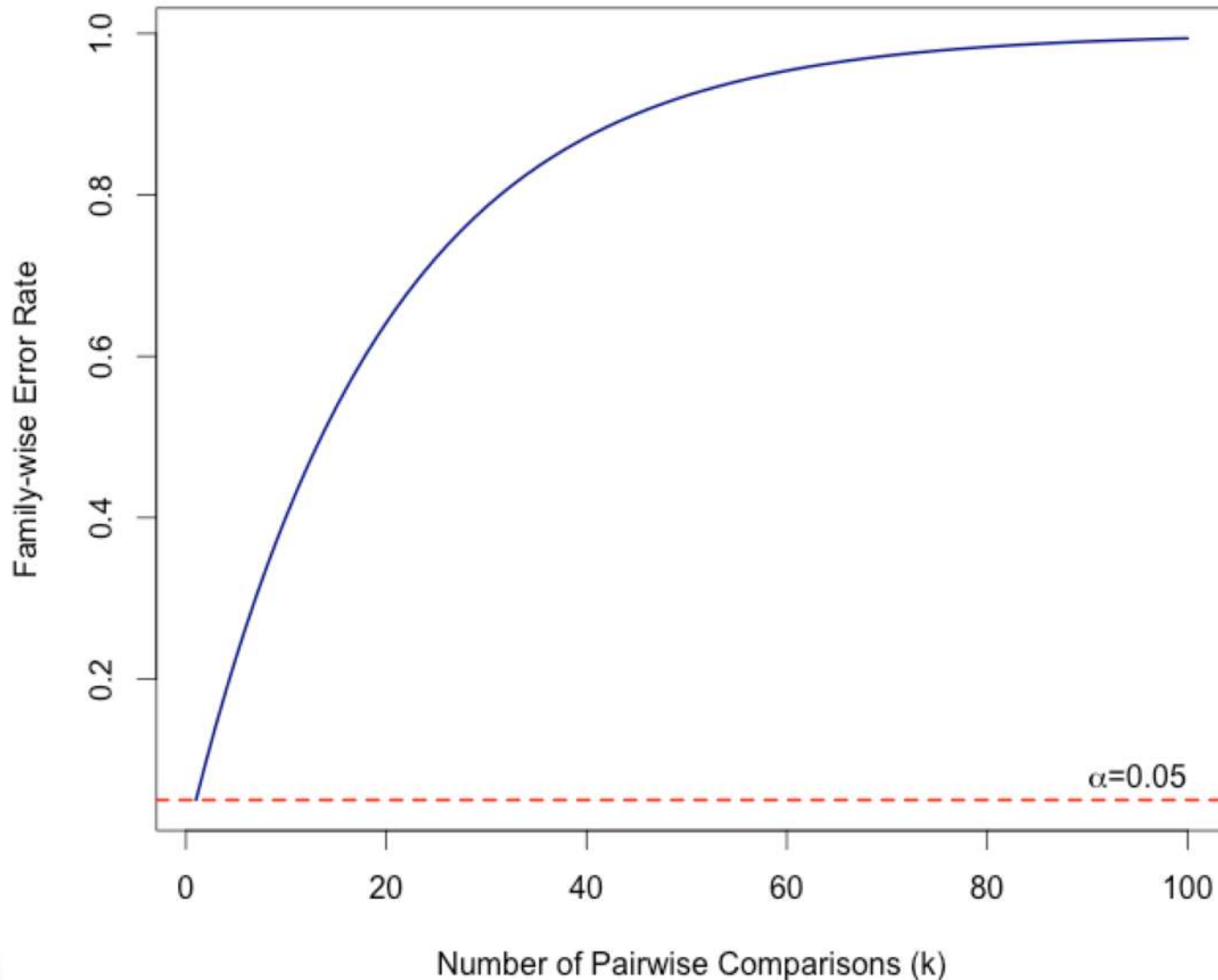
This problem – where a series of independent hypothesis tests lead to an inflated family-wise error rate – is known as the multiple comparison or multiple testing problem.

It can be shown that for a family of k hypothesis tests, each with significance level α , the family-wise error rate is

$$1 - (1 - \alpha)^k$$



The Multiple Comparison Problem



The Multiple Comparison Problem

We combat this problem with the Bonferroni correction

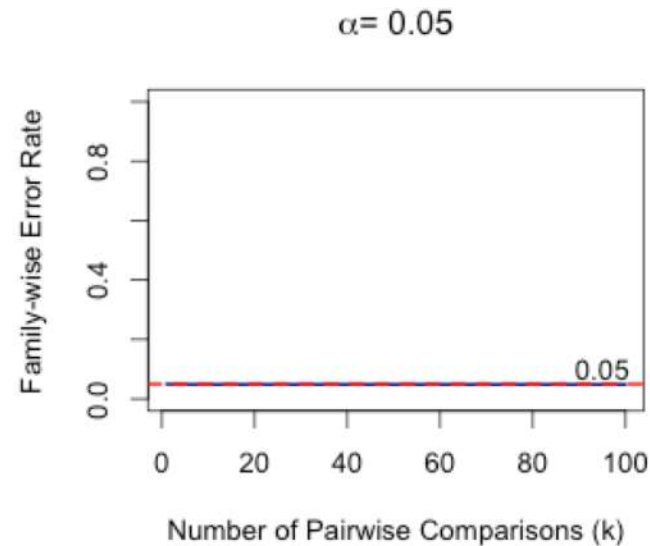
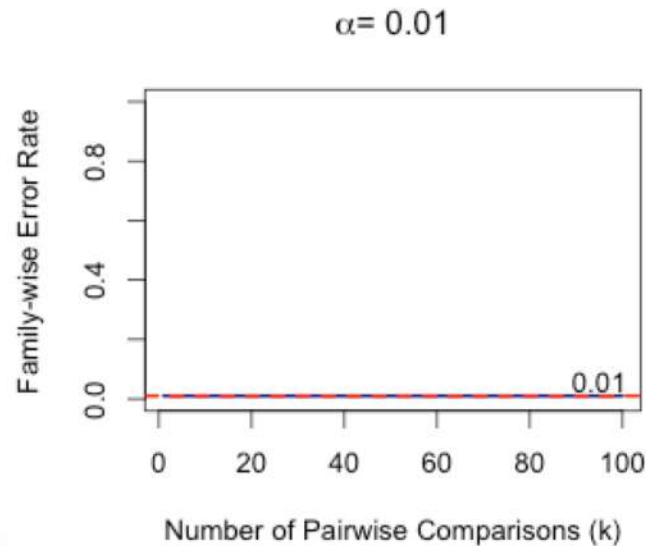
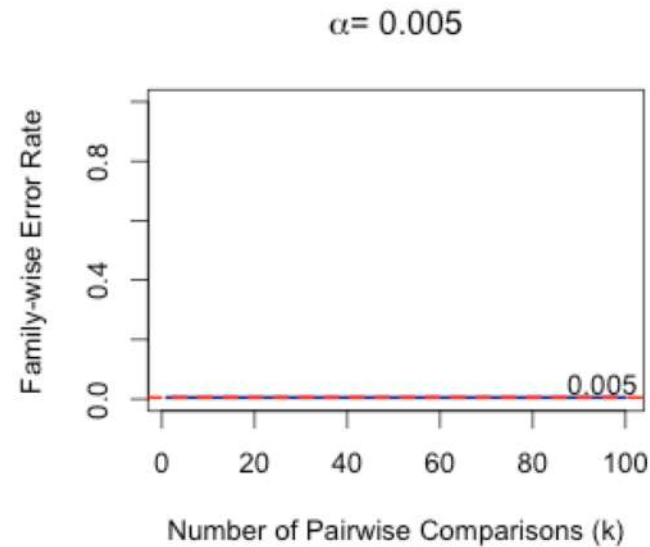
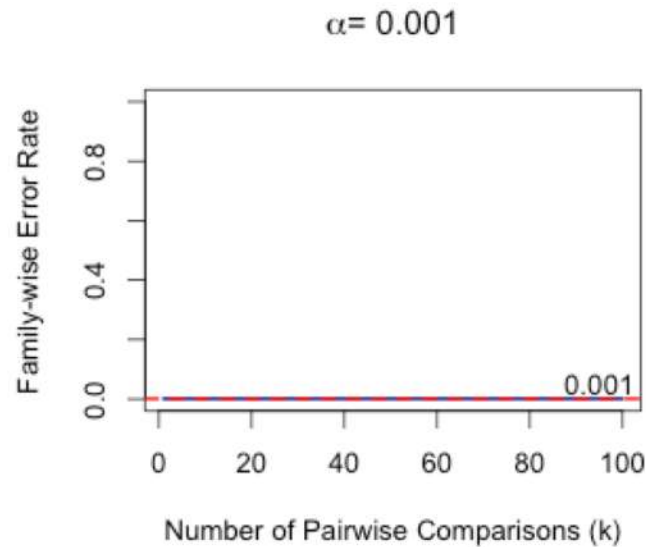
- With this correction we test each of the k hypothesis tests at a significance level α/k , if maintaining an error rate of α is of interest
- Doing so yields a family-wise error rate of

$$1 - \left(1 - \frac{\alpha}{k}\right)^k$$

which, for typical values of α is approximately equal to α



The Multiple Comparison Problem



The Multiple Comparison Problem

So what does this mean for sample size calculations and power analyses?

The sample size formulas we derived previously did not account for this multiple comparison problem

In order to do so, when performing a power analysis, use α/k and not α as the significance level in the sample size calculations



MULTI-ARMED BANDIT EXPERIMENTS



Multi-armed Bandit Experiments

- The comparison of $m \geq 2$ conditions, where the goal is to find the optimal condition, may be thought of as a multi-armed bandit problem
- A slot machine is colloquially referred to as a one-armed bandit



Multi-armed Bandit Experiments

- A row of slot machines is referred to as a multi-armed bandit



Multi-armed Bandit Experiments

- The goal, when faced with several slot machines, is to decide which one has the highest expected reward
- In other words, find the slot machine that is going to make you the most money, and repeatedly play that one
- Using notation from this course, let θ_j represent the expected reward from slot machine (a.k.a. “arm”) j for $j = 1, 2, \dots, m$
- The goal is to find the best θ_j



Multi-armed Bandit Experiments

- This is exactly what we've been doing!
- The approach we have been taking is what some might call the “classical” approach:
- Collect a certain amount of data in accordance with Type I and Type II error constraints, and once that data has been observed, conduct a hypothesis test
- Typical multi-armed bandit solutions differ from classical experiments largely with respect to the exploration-exploitation trade off

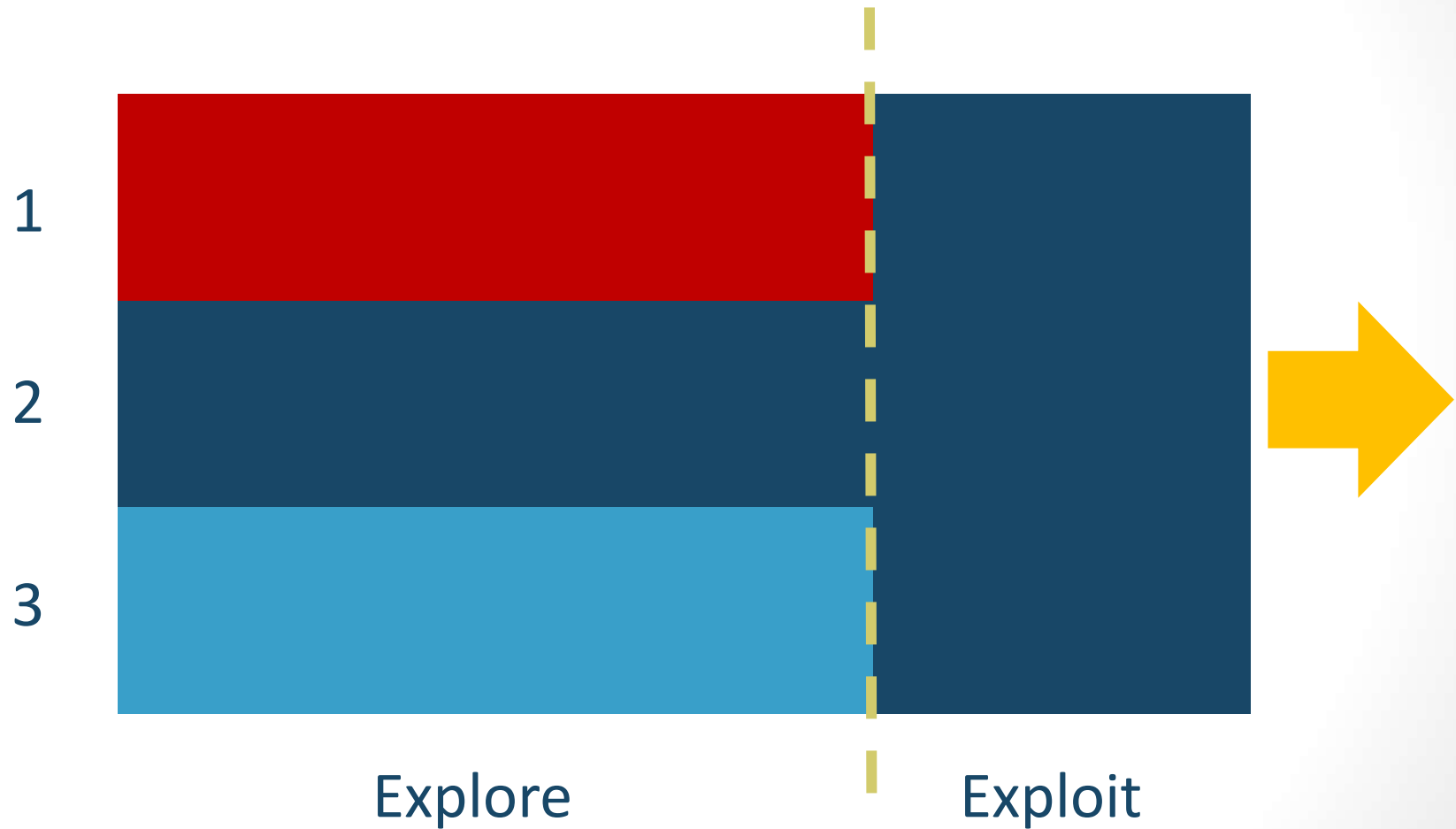


Multi-armed Bandit Experiments

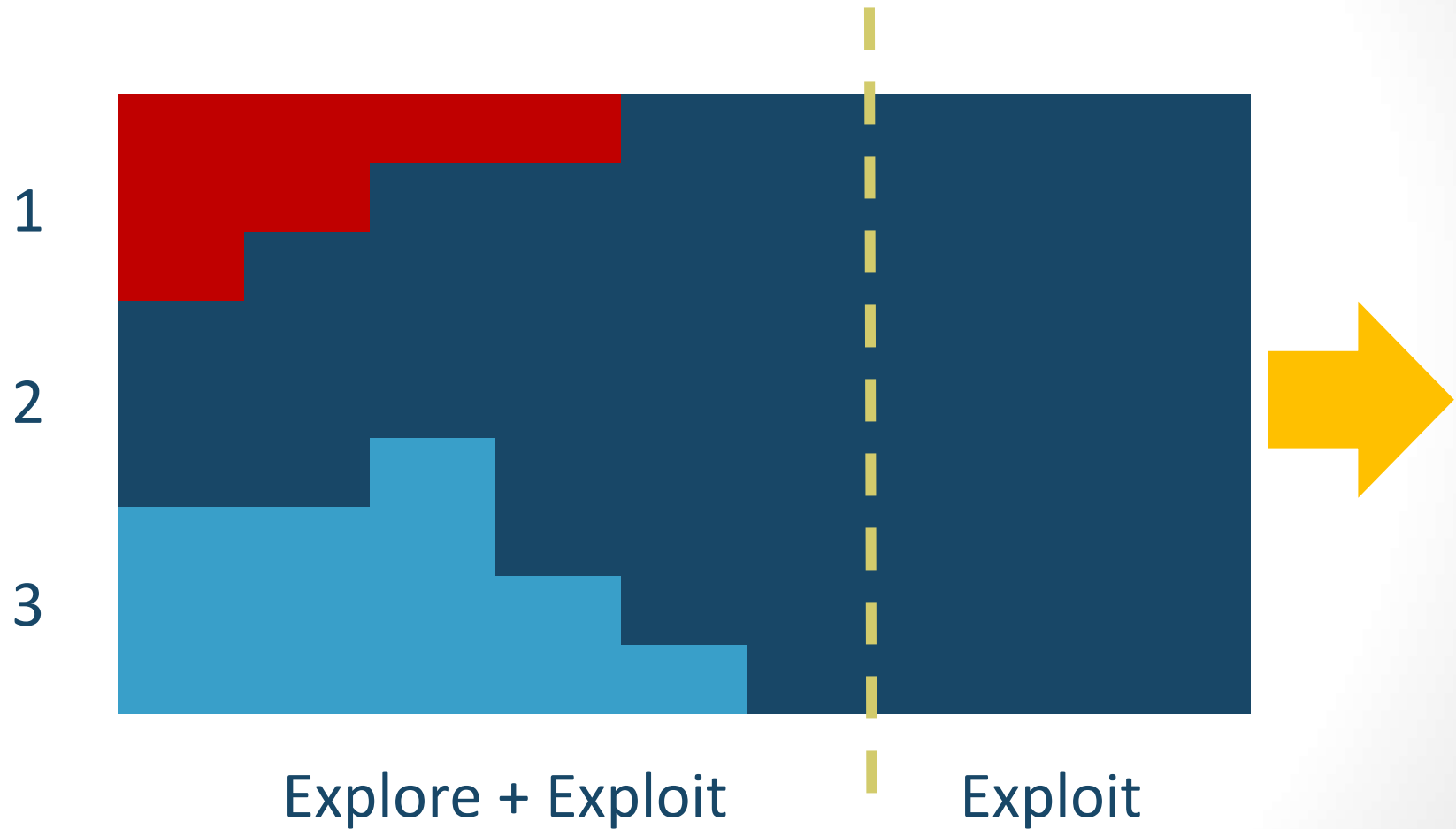
- **Idea:** we need to **explore** all of the conditions, and when the optimal one is found, we want to **exploit** it
- Classical experiments represent a 100% exploration phase after which a 100% exploitation phase begins
- **Multi-armed bandit experiments** are typified by a combination of both exploration and exploitation as the experiment is conducted



Multi-armed Bandit Experiments



Multi-armed Bandit Experiments



Multi-armed Bandit Experiments

- Thus the classical approach to the problem requires that we spend the entire experimental period “exploring” each condition at the same rate
- A multi-armed bandit experiment, on the other hand, does not provide equal allocation of units to conditions for the duration of the experiment
- At regular intervals the proportion of units allocated to each condition is updated to reflect the performance of each condition observed thus far



Multi-armed Bandit Experiments

- After an initial period of equal allocation, high performing conditions receive more units than lower performing conditions
- What does this updating rule look like specifically?
- In other words: How does this **adaptive allocation** of units to conditions work in practice?
 - Equal Allocation
 - Greedy Approach
 - Epsilon-Greedy Approach
 - Randomized Probability Matching



Multi-armed Bandit Experiments

Equal Allocation

- Each condition is allocated experimental units in equal proportions for the duration of the experiment
- This corresponds to the the classical experimental approach
- This represents 100% exploration during the experiment
- Detractors would say that this is inefficient and that the optimal condition can be found more quickly with an adaptive allocation strategy



Multi-armed Bandit Experiments

Greedy Approach

- Every experimental unit at a given point in time is assigned to the ‘best’ condition as determined by the data observed up to that point in time
- This approach is sometimes called “play-the-winner” and it represents 100% exploitation
- This approach may do a poor job at maximizing rewards as it does not adequately explore other conditions



Multi-armed Bandit Experiments

Epsilon-Greedy Approach

- This is a hybrid strategy that forces both exploration and exploitation
- Here allocation is performed via
 - the Greedy approach with probability $1 - \epsilon$
 - equal allocation with probability ϵ
- Thus a binary number is randomly generated using a Bernoulli distribution with probability of success/failure = $\epsilon/1 - \epsilon$)
 - If 1, perform greedy allocation
 - If 0, perform equal allocation



Multi-armed Bandit Experiments

Epsilon-Greedy Approach

- Notice that:
 - $\epsilon = 0$ corresponds to greedy allocation
 - $\epsilon = 1$ corresponds to equal allocation
- The choice of ϵ determines the desired balance of exploration and exploitation and is determined by the user
- Detractors would say that a drawback of the epsilon-greedy approach is that it will continue to explore even once an optimal condition has been found



Multi-armed Bandit Experiments

Randomized Probability Matching

Randomized probability matching (RPM) is a Bayesian alternative to the adaptive allocation strategies just discussed

- At successive time points, for each θ_j , the probability that θ_j is optimal is calculated
- This probability calculation is based on the joint posterior distribution of $(\theta_1, \theta_2, \dots, \theta_m)$
- These m probabilities are then used as allocation weights in the next round of allocation



Multi-armed Bandit Experiments

Randomized Probability Matching

- For example, consider a standard A/B (two-condition) test
- Suppose that based on the rewards observed thus far:
 - condition A has a 0.73 probability of being the superior condition, and
 - condition B has a 0.27 probability of being the superior condition
- Then, during the next allocation round, condition A would receive 73% of the experimental units and condition B would receive 27% of them



Multi-armed Bandit Experiments

Randomized Probability Matching

- The experiment continues until the probability of optimality dominates for one of the conditions, while the other probabilities of superiority tend to zero
- If the optimality probability does not dominate for one condition in particular, it suggests that multiple conditions are equally optimal
- In the case of two conditions, this result would be manifested as the two optimality probabilities stabilizing at roughly $1/2 = 0.5$



Multi-armed Bandit Experiments

Randomized Probability Matching

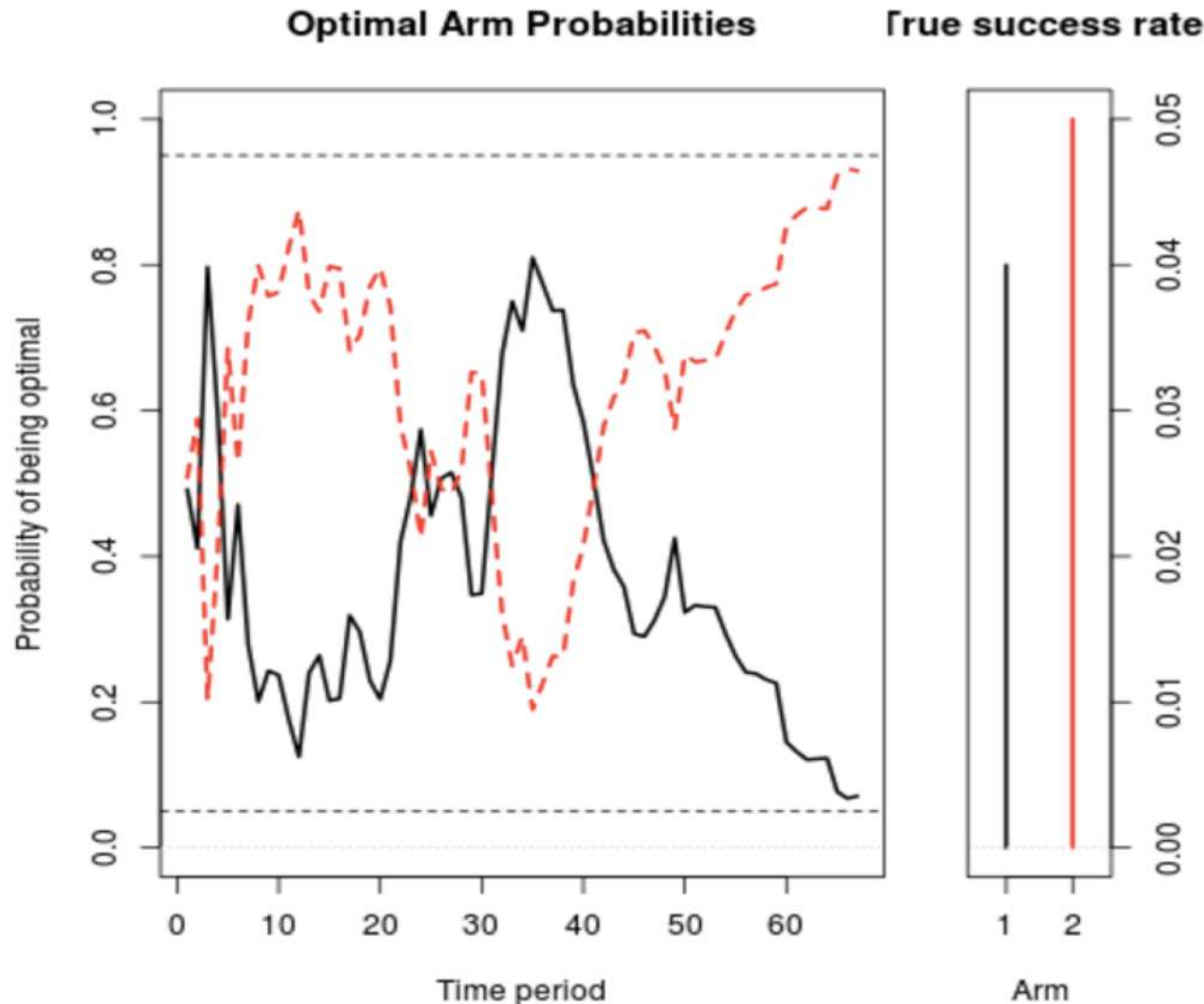


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Multi-armed Bandit Experiments

Randomized Probability Matching

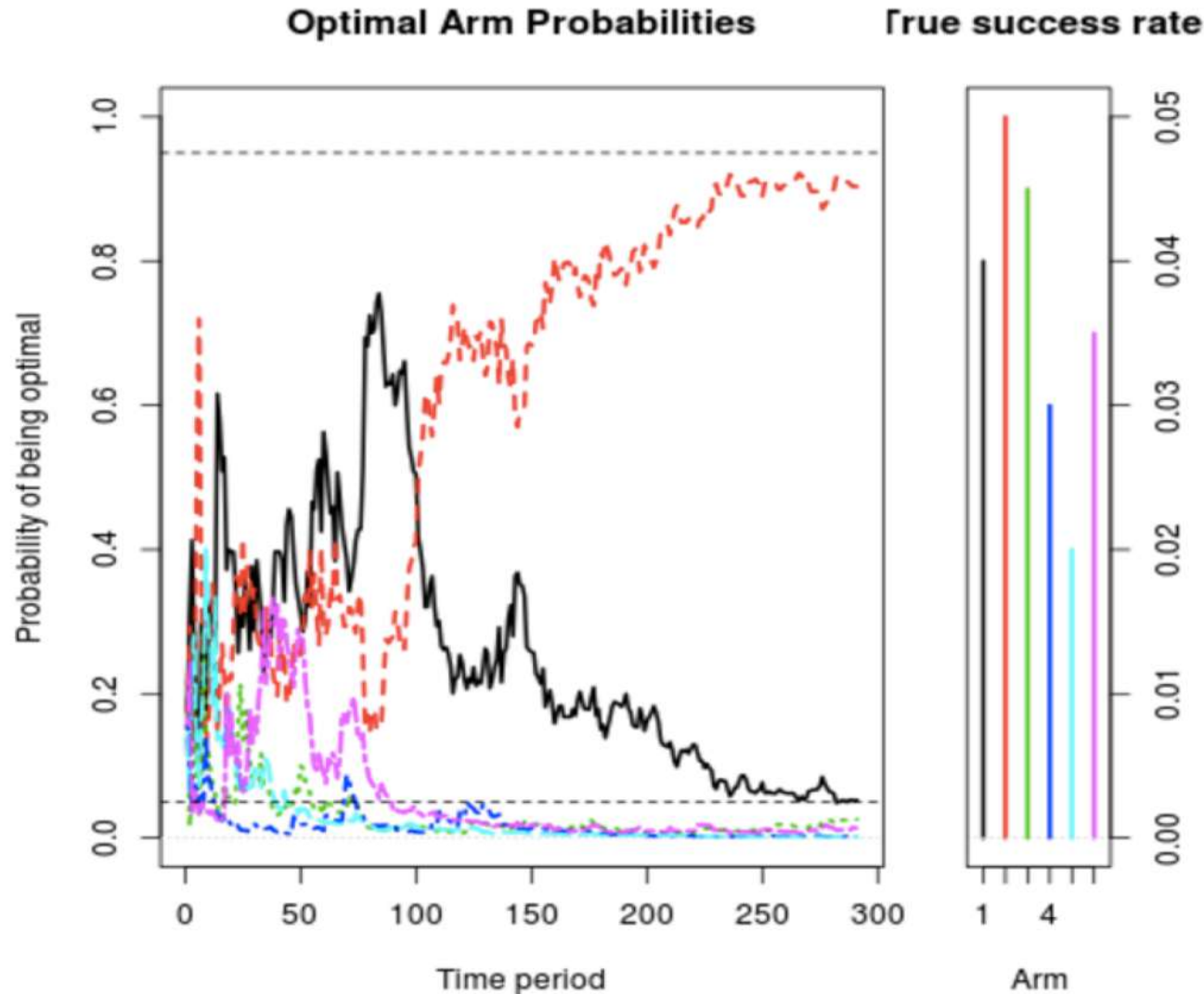


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Multi-armed Bandit Experiments

Randomized Probability Matching

- RPM has been shown to do a better job at balancing exploration and exploitation than other allocation strategies, and is able to more quickly find the optimal condition
- However, it relies on understanding Bayesian statistics and being able to sample from a posterior distribution obtained from **Markov chain Monte Carlo (MCMC)** simulation
- That said, it is available as the default design and analysis strategy in the **Google Analytics** experimentation platform



Multi-armed Bandit Experiments

Advantages

- Multi-armed bandit experiments purport to find the optimal condition more quickly than the classical experimental approach
- And due to the exploitation within the experiment itself, fewer units are assigned to suboptimal conditions
- As such, these approaches reduce the opportunity cost associated with experimenting with a risky or inferior condition



Multi-armed Bandit Experiments

Disadvantages

- **BUT** this approach ignores the impact of Type I errors
- By adopting the multi-armed bandit approach you, in a sense, must believe that the consequences associated with this type of error are of no practical importance
- It also requires quick feedback and so it doesn't work well when response observations are not obtained instantaneously
 - i.e., email advertising



See you next week!

