Building Student Confidence in STEM – Programs that Promote Student Success

Dr. Lisa Dierker
Dr. Ashley McDonald

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Building Student Confidence in STEM – Programs that Promote Student Success

Dr. Lisa Dierker
Dr. Ashley McDonald
Passion-Driven Statistics
Course-Based Undergraduate Research Experience (CURE)

Lisa Dierker
AAAS-IUSE, August 10, 2023
NS&B

Government

Biology

Economics

Psychology

Mathematics

E&ES

Sociology

College/Social Science
Design

Students
- feasible
- attractive
- inspirational

Instructors
- easy
- attractive
- inspirational

Institution
- feasible/sustainable
- affordable
- policy
- flat/shrinking resources
- “boxes”
- “priority fear”

Large numbers
- Diverse backgrounds
- Competing pressures

Small numbers
- Diverse backgrounds
- Competing pressures
1. Selecting a research question from existing data
2. Examining frequency distributions for the variables you have chosen
3. Data management
4. Graphing one variable at a time
5. Graphing relationships between two variables (and adding a third)
6. Inferential statistics and testing relationships between two variables
7. Examining these relationships by stratifying the sample by a third variable.
8. Multivariate modeling
Dissemination Sites
The Association between Smoking Quantity and Nicotine Dependence among Young Adults with and without Psychiatric Disorders

Lisa Dierker, Quantitative Analysis Center, Wesleyan University

Introduction
- Psychiatric disorders are a potent group of risk factors consistently implicated in the development of nicotine dependence (Rohde et al., 2003, 2004).
- While the association has been well established in the literature, less is known about the ways in which psychiatric disorders may play a role in the emergence of nicotine dependence.
- Most recent research has focused on heavy smoking factors e.g. the self medication hypothesis (Khanbali, 1997).
- Alternatively, however, psychiatric disorders may signal a greater sensitivity to nicotine dependence at low levels of smoking (i.e. individuals with psychiatric disorders may develop nicotine dependence symptoms at lower levels of smoking than those without psychiatric disorders).

Research Questions
- Which psychiatric disorders are associated with nicotine dependence? Are there differences in comorbidity?
- Does the association between smoking quantity and nicotine dependence differ for individuals with and without these psychiatric disorders?

Methods
Sample
- Young adults (age 18 to 25) who reported daily smoking in the past year (n=1520) were drawn from the first wave of the National Epidemiologic Study of Alcohol and Related Conditions (NESARC).
- NESARC is a nationally representative sample of non-institutionalized adults in the U.S.

Measures
- Lifetime psychiatric conditions were assessed using the NIAAA, Alcohol Use Disorder and Associated Disabilities Interview Schedule – DSM-IV (AUDADIS-IV).
- The tobacco module includes questions on symptom criteria for DSM-IV nicotine dependence.
- Current smoking was evaluated through quantity (“On the days that you smoked in the last year, about how many cigarettes did you usually smoke?”).

Results
- Univariate
  - Fully 61% of smokers met criteria for DSM-IV nicotine dependence.
  - A total of 55% met criteria for nicotine dependence for any psychiatric disorders.
- Bivariate
  - Chi-square analysis showed that daily, young adult smokers with a psychiatric disorder were significantly more likely to meet criteria for nicotine dependence (76.9%) than those without a psychiatric disorder (60.7%).
- As expected, the number of cigarettes smoked per day was significantly associated with DSM-IV nicotine dependence, OR=1.04 (1.03-1.06).
- Multivariate
- Major depression (MDD), specific phobia, alcohol dependence, and antisocial personality disorder (ASPD) were more associated with DSM-IV nicotine dependence after controlling for comorbidity.
- The interaction between number of cigarettes smoked per day and four specific psychiatric disorders and MDD was not found to be significant in the presence of nicotine dependence.
- At each level of use, the probability of nicotine dependence is significantly higher among those with the disorder than those without (Figure 1).
- In contrast, the interaction between alcohol dependence and number of cigarettes smoked per day was statistically significant when predicting nicotine dependence (Figure 2).

Discussion
- Individuals with major depression, specific phobia, and ASPD may be more sensitive to nicotine dependence across levels of smoking.
- Individuals with alcohol dependence are more sensitive to nicotine dependence at low levels of daily smoking, but not at the highest levels when compared to nicotine dependence.

Further research is needed to determine whether sensitivity to nicotine dependence is based on physical and/or psychological differences related to psychiatric disorders.

References

Figure 1: Smoking and Nicotine Dependence by Major Depressive Disorder

Figure 2: Smoking and Nicotine Dependence by Alcohol Use Disorders among Daily, Young Adult Smokers
The Association between Sexual Assault and Subsequent Marijuana Use
Charlotte Mittenthal
Wesleyan University

INTRODUCTION
- Sexual assault is an epidemic that one in five women and one in thirteen men will experience at some point during their college careers (RAINN.org, 2014).
- Previous studies have found a significant relationship between sexual assault trauma and sedative-drug use, such that many survivors use sedative drugs or “downers” after the event (Ullman et al., 2013).
- A person’s likelihood of using marijuana after having been sexually assaulted increases if they have been subjected to retraumatization (Wash et al., 2014).

RESEARCH QUESTIONS
1) Is a person’s likelihood of using and abusing marijuana higher if they have been a victim of sexual assault at some point in their adolescent life?
2) Does depression confound the relationship between sexual assault and drug use?
3) Is gender a moderating factor in the relationship between sexual assault and marijuana use?

METHODS
- Data were drawn from the 2008 Add Health survey, which is a nationally representative longitudinal study including 15,701 participants documenting adolescent to adult health.
- The sample was young adults aged 24-32 (n=15,701).
- Measures:
  - Sexual assault was measured by whether or not participants had been forced into sexual activities against their will.
  - Marijuana abuse symptoms were measured by asking participants if they have ever continued to use marijuana after realizing that it was causing emotional or health problems, problems with their family and friends, or problems at work or school.
  - Marijuana was also measured by whether or not participants have been under the influence when they could have put themselves or others at risk.

RESULTS
Univariate:
- Of those surveyed, 12.8% (n=1931) reported that they have, at some point in their adolescent life, been sexually assaulted.
- Of those surveyed, 20.15% (n=947) of participants who have smoked marijuana continued to use it after realizing it was causing them continuous health problems.

Bivariate:
- When examining the association between past year marijuana abuse and sexual assault, a chi-square test of independence revealed that among people that answered yes to smoking marijuana, people that have been sexually assaulted are 27% more likely to continue to use marijuana after realizing that is causing them emotional problems and/or health problems than people who have not been sexually assaulted. X2 = 8.9081, 1 df, p = 0.003

RESULTS CONT.
Moderation:
- Gender does moderate the association between sexual assault and marijuana. It was insignificant for men (p=0.85), however, it remained significant for women (p=0.007).

DISCUSSION
- Individuals who have experienced either physical or non-physical coercion into sexual activity are more susceptible to marijuana abuse and dependence.
- Individuals who are survivors of sexual assault may use marijuana such as marijuana to cope with the trauma of sexual assault, as a means of dissipating with reality, or as a sedative to be able to sleep.
- The Add Health survey fails to provide a holistic and accurate representation of sexual assault, as it asks participants to exclude experiences with parents or adult caregivers, which could be a major source of childhood sexual assault and abuse. Therefore, further research is needed to provide a more accurate estimation of individuals who have experienced sexual assault at some point in their adolescent lives.
- Further research is needed to provide alternative methods of coping such as prescription medications, therapy, and melded such that survivors of sexual assault may not need to abuse substances.

REFERENCES
- Rape and Sexual Victimization Among College-Aged Females, 1995-1996. From Department of Justice. Office of Justice Programs, Bureau of Justice Statistics
Propensity for Adult Children of Alcoholics to Seek Treatment for Alcohol Abuse
Frances Williams, Quantitative Analysis Center, Wesleyan University

Introduction
- Twin, adoption, and family studies demonstrate that genetic factors account for 50-60% of the variance in risk for developing alcoholism (Fournier et al., 2010).
- Children of alcoholics (COAs) progress more quickly from initial adolescent alcohol use to onset of disorder than matched controls (Hussong & Chassin, 2008).
- Exposure to maternal problem drinking in childhood is positively associated with psychiatric symptoms in adulthood (Greenfield et al., 1993).
- Significant differences reported between genders for all disorders (Morgan et al., 2010).
- While literature focuses on psychopathology of COAs, little has been documented on adult alcohol abuse tendencies in COAs.

Research Questions
- Is seeking treatment for alcohol abuse associated with having at least one alcoholic or problem drinking parent?
- Is this association influenced by number of alcoholic parents?
- Does this association differ for individuals with adoptive parents?

Methods
- Sample: Adults who reported suffering from alcohol abuse at one or multiple points in their life (n=33944) were drawn from the National Epidemiologic Study of Alcohol-Related Conditions (NESARC).
- NESARC is a nationally representative sample of non-institutionalized adults in the United States.
- Diagnostic classifications were based on the Alcohol Use Disorder and Associated Disabilities Interview Schedule-DSM-IV Version (AUDADIS-IV).
- Logistic regression was used to test moderating effects of gender, personal income, and level of schooling.
- Chi-square test used to evaluate significance of associations.

Results

Part 1: Bivariate and Multivariate
- Chi-square test revealed a significant relationship between having at least one alcoholic parent and seeking treatment for alcohol abuse, consistent for both biological parents (X²=4725.5, df= 1, p<.0001) and adoptive parents (X²=10.25, df=1, p=.0014).
- Personal income was positively associated with seeking alcoholic treatment for alcoholic biological parents (OR=0.98, CI 0.97-0.99, p=.0097) but not alcoholic adoptive parents.
- Men with at least 1 alcoholic parent were more likely to seek treatment than women, with both biological parents (OR=0.29, CI 0.26-0.33, p<.0001) and adoptive parents (OR=0.32, CI 0.29-0.35, p<.0001).
- Adjusting for moderators (personal income, gender, schooling) individuals with alcoholic biological/adoptive parents are 3.22/2.85 times more likely to seek treatment for alcohol abuse (CI 2.92-3.59/2.45-3.58, p<.0001).

Part 2: Comparison
- Chi-square test revealed a significant relationship between number of alcoholic parents and seeking treatment for alcohol abuse for both biological parents (X²=796.9, df=3, p<.0001) and adoptive parents (X²=15.8, df=3, p<.0005).
- Men were more likely to seek treatment than women, with both biological parents (OR=0.29, CI 0.259-0.324, p<.0001) and adoptive parents (OR=0.319, CI 0.287-0.353, p<.0001).
- Personal income was positively associated with seeking treatment for alcoholic biological parents (OR=0.98, CI 0.97-0.99, p=.0097) but not adoptive parents.

- Individuals with 2 alcoholic parents were found to be 1.97 more times more likely to seek treatment than those with only 1 alcoholic parent (CI 1.66-2.34, p<.0001) and 3.58 times more likely than those with 0 alcoholic parents (CI 4.92-6.85, p<.0001).
- Individuals with 2 alcoholic adoptive parents were 5.02 times more likely to seek treatment than those with 0 alcoholic adoptive parents (CI 1.04-24.29, p<.002).

Discussion
- Adult children of alcoholics (COAs), both biological and adoptive, are more likely to seek treatment for alcohol abuse than those of non-alcoholics.
- Number of alcoholic parents is positively associated with COAs seeking treatment, with the exception of female children of adoptive parents.
- Significant differences in gender are seen throughout this association.
- Now that a significant association has been identified, further research is needed to examine relationships between alcohol abuse and psychiatric disorders in COAs, as well as to examine specific forms of treatment utilized.

References
GOD AND GUNS: THE RELATIONSHIP BETWEEN SPIRITUALITY AND VIEWS ON GUN CONTROL

Jackie Marginelli, Quantitative Analysis Center, Wesleyan University

Introduction

- Studies have shown that people who are more spiritual tend to oppose more restrictions on gun rights.
- This is especially true for individuals who identify themselves as either Protestant or Catholic.
- In a survey of 650 adults in a North Carolina county, 68% of Protestants, 6% of Catholics, and 26% of “other religious groups” owned handguns.
- However, in a study of the relationship between gun ownership and firearm rates between 1981-2010, researchers found a substantial correlation.

Research Questions

- Is an increase in an individual’s spirituality associated with an individual’s views on gun restrictions?
- Does this relationship change based on an individual’s gender and/or an individual’s race?

Methods

Sample:
- The General Social Surveys (GSS) were conducted in February, March, and April from 1972-2004.
- There are a total of 56,087 interviews from the survey from 1977-2010 and 2,812 interviews were conducted in 2004—the year of this study.

Measures:
- Spirituality was measured with a binary analysis of individuals who considered themselves moderately religious and individuals who considered themselves very religious.
- If individuals were deeply religious they said they felt close to a god almost all the time.
- Those who were moderately religious said they felt close to a god sometimes.
- Individual views on gun restrictions was measured with a binary analysis with 1 representing supporting more restrictions on guns and 2 representing supporting less.

Results

Univariate
- After performing a univariate analysis on the variable of how individuals viewed restrictions on guns, more individuals in the study prefer more restrictions on guns (52%), however those who did not prefer more restrictions on guns was not insignificant (30%).
- After performing a univariate analysis on the variable of spirituality, more individuals in the study self-identified as spiritual (87%), however, those who self-identified as less spiritual (41%) could still be used to visualize this relationship.

Bivariate
- Chi-squared test showed a slight association between an individual’s spirituality and their views on gun restrictions (X^2 = 5.095, p-value < 0.005 or p < .05).
- Chi-squared test for moderation showed that gender does not moderate the relationship between spirituality and views on gun control (Men, X^2 = 1.003, p < .05 / Women, X^2 = 0.03717, p = .50)
- Chi-squared test for moderation showed that race does not moderate the relationship between spirituality and views on gun control

Discussion

- Although there is a slight relationship between spirituality and views on gun control, upon further evaluation, this relationship is confounded by both race and gender.
- It is interesting to note that those who are more religious support more restrictions on guns. It is important to subset this population to better understand this relationship as spirituality deepens.
- Although as an individual gets more spiritual, they are more likely to oppose more restrictions, there is a small population who identifies as incredibly spiritual who support more restrictions.
- Perhaps instead of studying the relationship between individual spirituality and views on gun regulations one should instead study the relationship between gender and views on gun restrictions or race and views on gun restrictions.

References

[References provided in the image]
The Association between Religiosity and Likelihood of Contracting Sexually Transmitted Infections among Young Adults

Margaret Sullivan Wesleyan University, Psychology Statistics

INTRODUCTION

Young adults count for almost 1 in 2 of every diagnosis of sexually transmitted infections in the United States (Spain 2017).

In the United States, a survey study found that the more religious, the less likely a college student was to accept the attitude that having casual or caretaker sex was acceptable. However, these individuals were found to be less likely to endorse a strong agreement with the use of birth control, increasing their vulnerability to STIs (Muiray et al. 2007).

Certain studies suggest that the relationship between religiosity and sexually transmitted infections is complex and moderated by factors such as drug use (Wabino et al. 2015).

Recent studies do not look at specific diagnoses of sexually transmitted infections among young people with variant levels of religiosity across for both gender demographics. Because an individual’s opinion on sexual activity is often affected by religious affiliation and identity, additional research is warranted.

RESEARCH QUESTIONS

Is there a significant relationship between an individual’s level of religiosity and diagnosis of a sexually transmitted infection?

How does the association differ by gender? By religion?

METHODS

Data were drawn from nationally representative of United States adolescents in adulthood, National Longitudinal Survey of Adolescent Health (Add Health).

The wave IV interviews were primarily conducted at respondents’ homes using Blaise Survey Software, a computer-assisted interview software, to reduce bias.

The sample used in this analysis contains relevant data on 6,504 respondents aged 24-32 and 46% of this sample is male. A history of STIs was measured. Example: “Have you ever been told by a doctor, nurse, or other health professional that you had any of the following sexually transmitted infections?” (HIV/STD)

Religiosity was measured with the question: “How important is your religious faith to you?” (RelSci) Possible responses ranged from 1 (not important) to 4 (more important than anything else).

RESULTS

UNIVARIATE

24.30% of young adults have been reported to have had one or more sexually transmitted disease.

14.2% of young adults reported that religious faith was ‘not important’ while 12.4% reported that religious faith was ‘more important’ than anything else. 23.9% reported it being ‘somewhat important’. 43.3% reported faith was ‘very important’ to them.

BIVARIATE

Chi-square analysis reveals that religiosity and STI diagnosis are related. Post hoc testing revealed that individuals who reported faith as ‘somewhat’ or ‘very important’ to them and their diagnosis of one or more STIs was related. p-value = 0.003, 1 df, X^2 = 8.5669 (Figure 1)

In contrast, attendance of religious services in the past year was not associated with likelihood of contraction of STIs in the past year. p-value = 0.959.

MULTIVARIATE

Logistic regression analysis reveals that being Christian (christ_gender) confounds the relationship between religiosity and a personal history of STIs.

Sexually Transmitted infections and Religiosity were still associated after controlling for: number of partners; use of condoms as birth control or infection prevention; gender; and frequency of use birth control when engaging in sexual activity.

After testing for moderation across religious affiliations, religiosity and diagnosis of an STD was only moderated by one religion: Christian protestanism (hetero=1). An individual’s tendency to turn to their faith for help did not moderate the relationship.

USE OF CONDOMS

Gender moderated the association between condom use and importance of religion for men (bic = sex*1), but not for women (bic = sex*2). 1 df, p<0.012 (Figure 2)

DISCUSSION

There is an association between religiosity and the likelihood of contracting STIs. Surprisingly, the only confounders discovered in this study were related to religious attitudes and identities. No contraceptive behaviors confounded the relationship.

It is important to consider how religious teaching dually effects vulnerability to STIs when discussing the data. Although a very religious individual may be engaging in less ‘social’ sexual activity because it is condemned by their religion, they are also probably less likely to have the resources to be educated on proper measures to engage in safe sex.

More observational research should be conducted to better understand how religion affects an individual’s attitude towards sex and level of knowledge on contraceptive use and STI prevention.

REFERENCES


Project-Based Approach

Public Access Data

Faculty Data

Community Data
# Code-Based Software

<table>
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<th>SPSS</th>
<th>UNIANOVA QuantResponseVar BY CategExplanatoryVar.</th>
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<td>STATA</td>
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<td>class CategExplanatoryVar;</td>
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<td>model QuantResponseVar = CategExplanatoryVar;</td>
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<td>myAnovaResults &lt;- aov(QuantResponseVar ~ CategExplanatoryVar, data = myData)</td>
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<td>summary(myAnovaResults)</td>
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<td>model1 = smf.ols(formula='QuantResponseVar ~ C(CategExplanatoryVar)', data=myData)</td>
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<td>results1 = model1.fit()</td>
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</table>
Taking Students out of their comfort zone...

....and then loving them through the fall out!
Key findings...

Attracts higher rates of under-represented minority (URM) students compared to a non-CURE statistics course.

Attracts higher rates of both URM and female students compared to an introductory programming course.

Passion-Driven Statistics students are more likely to report increased confidence in working with data and increased interest in pursuing advanced statistics coursework compared to a non-CURE statistics course.

Using causal inference techniques to achieve matched comparisons, students originally enrolled in Passion-Driven Statistics were significantly more likely to take additional undergraduate courses focused on statistical concepts, applied data analysis, and/or use of statistical software compared to students taking either a psychology statistics course or math statistics course. 

more useful, more rewarding, accomplished more than expected
METHOD

N=1882 students taking CURE or MATH STAT between fall semester 2009 and spring semester 2018 at NE Liberal Arts College

N=907 responded to the survey

<table>
<thead>
<tr>
<th>CURE Statistics</th>
<th>Math Statistics</th>
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<tr>
<td>n=551</td>
<td>n=356</td>
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Propensity score matching = OneToManyMTCH SAS Macro and specifying a 1:1 nearest neighbor match.

<table>
<thead>
<tr>
<th>CURE Statistics</th>
<th>Math Statistics</th>
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<td>n=272</td>
<td>n=272</td>
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Table 1. Demographic and Background Characteristics of Respondents.

<table>
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<th>CURE Statistics n=551</th>
<th>Math Statistics n=356</th>
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</thead>
<tbody>
<tr>
<td>Age of university enrollment</td>
<td>M=18.8 (s.d. 1.65)</td>
<td>M=18.6 (s.d. 0.69)</td>
</tr>
<tr>
<td>Gender (% female)</td>
<td>312 (56.6%)</td>
<td>215 (60.4%)</td>
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<tr>
<td><em>Ethnicity</em></td>
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<tr>
<td>Hispanic</td>
<td>62 (11.3%)</td>
<td>42 (11.8%)</td>
</tr>
<tr>
<td>Black</td>
<td>67 (12.2%)</td>
<td>32 (9.0%)</td>
</tr>
<tr>
<td>Native Hawaiian/Pacific Islander</td>
<td>1 (0.18%)</td>
<td>3 (0.84%)</td>
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<tr>
<td>American Indian/Native American</td>
<td>9 (1.63%)</td>
<td>1 (0.28%)</td>
</tr>
<tr>
<td>Asian</td>
<td>104 (18.9%)</td>
<td>72 (20.2%)</td>
</tr>
<tr>
<td>White</td>
<td>338 (61.3%)</td>
<td>218 (61.2%)</td>
</tr>
<tr>
<td>Other</td>
<td>3 (0.54%)</td>
<td>1 (0.28%)</td>
</tr>
<tr>
<td>International student</td>
<td>50 (9.1%)</td>
<td>21 (5.9%)</td>
</tr>
<tr>
<td>First generation college student</td>
<td>91 (16.5%)</td>
<td>61 (17.1%)</td>
</tr>
<tr>
<td>Pell grant eligible</td>
<td>106 (19.2%)</td>
<td>66 (18.5%)</td>
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<tr>
<td><em>Year of enrollment in statistics course</em></td>
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<tr>
<td>First year</td>
<td>60 (10.9%)</td>
<td>142 (39.9%)</td>
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<tr>
<td>Second year</td>
<td>219 (39.8%)</td>
<td>122 (34.3%)</td>
</tr>
<tr>
<td>Third year</td>
<td>155 (28.1%)</td>
<td>52 (14.6%)</td>
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<tr>
<td>Fourth year</td>
<td>117 (21.2%)</td>
<td>40 (11.2%)</td>
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<tr>
<td>Number of years since graduation</td>
<td>M=5.3 (s.d. 2.57)</td>
<td>M=4.5 (s.d. 2.83)</td>
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<td>UG data courses</td>
<td>CURE Statistics n=272</td>
<td>Math Statistics n=272</td>
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<td>----------------------------------------------------------</td>
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<tr>
<td>Took additional data-oriented courses as UG</td>
<td>148 (54%)</td>
<td>85 (31.3%)</td>
</tr>
<tr>
<td>Number of data-oriented courses taken as UG</td>
<td>M=2.2 (s.d. 1.69)</td>
<td>M=1.5 (s.d. 0.96)</td>
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<tr>
<td>Data as primary job responsibility in current/most recent job</td>
<td>55 (20.2%)</td>
<td>33 (12.1%)</td>
</tr>
<tr>
<td>Confidence in working with data (1=never to 5=very frequently)</td>
<td>M=3.5 (s.d. 0.97)</td>
<td>M=3.3 (s.d. 0.96)</td>
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<tr>
<td>Salary (% &gt; $100K/year)</td>
<td>94 (34.7%)</td>
<td>69 (25.5%)</td>
</tr>
<tr>
<td>More useful than other college courses preparing for a job or graduate school</td>
<td>114 (42.1%)</td>
<td>37 (13.8%)</td>
</tr>
</tbody>
</table>
No differences were found…

1. Having completed a degree or certificate program beyond UG

2. Self-reported frequency of working with data in the context of collecting data, analyzing data, communicating the results of data, making decisions based on data, and how often they would like to work with data in the future.

3. Average number of hours worked each week or respondents’ satisfaction with number of hours worked.
Mediating and Direct Effects for CURE statistics course on post UG outcomes

CURE vs. MATH STAT

Additional UG data-oriented courses

- Data Job
- Data Confidence
- >100K salary
- Judge course as more useful
E-book

https://ldierker1.github.io/passiondrivenstatistics/
What makes it a transformative experience

• The students set the topic and make the decisions
• Didactic portions heavier out of class and support for one-on-one engagement in class
• As much one-on-one support as needed
• Just in time (need to know) content knowledge
• Flexible content for all types of learners
• Everyone involved in designing and running the course bringing their best stuff.
What makes it a transformative experience

- Students on laptops in flexible use classroom
- Peer mentors (1:10)
- Instructor
- Skype/zoom in-class support
- Staffed discussion forums
- Instructor/instructor support
PASSIONDRIVENSTATISTICS.COM

ldierker@wesleyan.edu
Integrating Programming into the Molecular Sciences Curriculum

Ashley Ringer McDonald

The Molecular Sciences Software

California Polytechnic State University
San Luis Obispo, CA, USA
Integrated Programming Education Promotes Student Success and Equity

• Students who have programming and computational data analysis skills are at an advantage over students who do not.

• Integrating these computational skills into STEM curriculum broadly promotes student success and equity.

• Faculty development and training is key.
The Molecular Sciences Software Institute (the MolSSI)

• National Science Foundation Center (launched 2016, renewed 2021)

• Collaborative effort by nine institutions in the United States

• Goals: Improve software, education, and training computational molecular science – a broad domain that includes quantum chemistry, computational materials science, and biomolecular simulation.
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Teresa Head-Gordon, U.C. Berkeley, Co-Director for Laboratory, Industrial, and Academic Outreach and Education

Shantenu Jha, Rutgers U., Co-Director for Software Engineering Process, Middleware, and Infrastructure

Anna Krylov, U. Southern California, Co-Director for Quantum Chemistry

Theresa Windus, Iowa State U., Deputy Director and Co-Director for Code and Data Interoperability

Dominika Zgid, U. Michigan, Co-Director for Materials Science

Ashley McDonald, Cal Poly SLO., Co-Director for Education, Training, and Faculty Development
MolSSI Education’s Mission

To Provide Education and Training...

- MolSSI serves as an education and outreach nexus for the worldwide CMS community.
- MolSSI organizes summer schools, targeted workshops, high-school and undergraduate training programs, and on-line resources and classes to provide current and future CMS students with a modern and complete set of programming skills.
- MolSSI provides faculty development to help faculty upskill their own computational skills and develop discipline-specific curriculum.
Since 2017, **over 2000 students** have participated MolSSI Education workshops.

MolSSI Education engages audiences who are... **geographically and demographically diverse**

- International: 15%
- Hispanic: 62%
- Mixed Race: 4%
- Caucasian: 8%
- American: 11%

Partnerships and Collaboration

Student demographics for the 2021 MolSSI Workshop in collaboration with the Tapia Center at Rice University. Students in this program were **58% female**.

Programming languages and tools...

- Python
- Pandas
- C++
- Git

...in the context of computational molecular science.

Online Lessons

[http://education.molssi.org/resources](http://education.molssi.org/resources)
MolSSI Python Data and Scripting

Audience: Beginner to beginner+ programmers

How do I get started with Python?

• Jupyter notebooks
• Python syntax and control structures
• Reading and writing files
• File manipulation and parsing
•Analyzing and graphing data
• Writing functions
• Creating command line programs from Python scripts

Also a version of biochemists.
Data Analysis and Data Visualization

Audience: Beginner+

How do I use python to analyze data?

• Numpy arrays
• Pandas for data analysis
• SciPy and Data Fitting
• File manipulation and parsing

• Advanced data visualization
• Plots and subplots
• Multi-dimensional and interactive plotting

Schedule

<table>
<thead>
<tr>
<th>Time</th>
<th>Topic</th>
<th>Questions</th>
</tr>
</thead>
<tbody>
<tr>
<td>00:00</td>
<td>1. Working with Numpy Arrays</td>
<td>What are the differences between numpy arrays and lists?</td>
</tr>
<tr>
<td></td>
<td></td>
<td>How can I use NumPy to do calculations?</td>
</tr>
<tr>
<td>01:05</td>
<td>2. Using pandas for data analysis</td>
<td>What is pandas?</td>
</tr>
<tr>
<td></td>
<td></td>
<td>How do I access data in a pandas dataframe?</td>
</tr>
<tr>
<td>01:05</td>
<td>3. Using scipy for data fitting</td>
<td>How do I fit data to a specified function?</td>
</tr>
<tr>
<td></td>
<td></td>
<td>How do I assess the quality of my fit?</td>
</tr>
<tr>
<td></td>
<td></td>
<td>How do I determine the standard error for my fit parameters?</td>
</tr>
</tbody>
</table>

Scientific Visualization Using Python
MolSSI Best Practices in Python Development

Audience: Intermediate programmers

How do I share my code?

- Conda and Python environments
- How to structure your project?
- Version control using git
- Python Coding Style
- Code collaboration and repositories.
- Writing tests.
- Automatically running test.
- Documentation.
Finding MolSSI Tutorials Online

MolSSI Education Resources

MolSSI offers 1-2 day workshops as well as online tutorial materials. Most tutorials are hosted on GitHub in the MolSSI Education GitHub organization. Workshops and materials here may still be under development. Outside contribution is welcomed and encouraged!

- Programming
- Software Development
- Machine Learning
- High Performance Computing
- Molecular Modeling
- External Resources

Python Data and Scripting Workshop

Description: The Python Data and Scripting workshop is designed for students who are currently involved in, or planning to start computational chemistry research. This workshop is designed to help students develop practical programming skills that will benefit their undergraduate research, and will take students through introductory programming and scripting with Python to version control and sharing their code with others. NO prior programming experience is required.

- Workshop Topics
  - View Workshop Materials
  - View GitHub Repository
  - View Workshop Recording

Python Data and Scripting for Biochemists and Molecular Biologists

Description: The Python Scripting for Biochemistry and Molecular Biology Workshop is designed for students and faculty who are interested in getting started with coding as part of their teaching and research. The workshop provides hands-on python coding experience using examples relevant to biochemists. It includes parsing PDB files, data analysis, linear regression, nonlinear regression, and plotting data. No prior programming experience is necessary.

- Workshop Topics
  - View Workshop Materials
  - View GitHub Repository

We teach live workshops and webinars. But, if you can’t attend an event, our materials are available online.

Visit http://education.molssi.org/resources
Using MolSSI resources as a springboard for curriculum in your course
General Chemistry

- Grace Stokes and Hoda Mirafzel
  Santa Clara University, Santa Clara, CA, USA

- Activity: The energy levels of the Bohr Model

- MoISSI springboard: Python Data and Scripting Workshop
  Introduction & Plotting Lessons
The energy levels of the Bohr Model

The purpose of this exercise is to use Python to better understand the energy diagram for the Hydrogen Atom as described by the Bohr model.

Written for Santa Clara University by Elliott Anderson (Chemistry ’22), Dr. Hoda Mirafzal, and Dr. Grace Stokes

Part 1: Graphing the Bohr Atom Energy Levels

In Section 2.5 of the Tro textbook on pg. 94, we find Equation 2.6, which describes how energy changes with principal quantum number (n). The Rydberg constant \( R_H \) in Equation 2.6 comes from multiplying together a number of physical constants, as shown in the table below.

\[
E_n = -\frac{R_H}{n^2} = -\frac{m_e^2 e^4}{8\epsilon_0^2 h^2} \times \frac{1}{n^2} \tag{2.6}
\]

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Quantity</th>
<th>Value in SI units</th>
</tr>
</thead>
<tbody>
<tr>
<td>( m_e )</td>
<td>electron mass</td>
<td>( 9.109 \times 10^{-31} ) kg</td>
</tr>
<tr>
<td>( e )</td>
<td>electron charge</td>
<td>( 1.602 \times 10^{-19} ) C</td>
</tr>
<tr>
<td>( \varepsilon_0 )</td>
<td>vacuum permittivity</td>
<td>( 8.854 \times 10^{-12} ) C/(N m)</td>
</tr>
<tr>
<td>( h )</td>
<td>Planck’s constant</td>
<td>( 6.626 \times 10^{-34} ) J s</td>
</tr>
</tbody>
</table>

1. We will plug in physical constants from the table into Equation 2.6 to calculate energy in Joules for different integer values of \( n \) ranging from \( n = 1 \) to \( n = 10 \).
Physical Chemistry

- Ashley Ringer McDonald and John P. Hagen
  Cal Poly San Luis Obispo

- Activity: Using Numerical Integration to Solve Kinetics Problems

- MolSSI springboard: Python Data and Scripting Workshop
  Introduction & Plotting Lesson

  Functions Lesson
Kinetics Activity

Solving Differential Equations

A differential equation is an equation that contains a derivative. For example,

\[
\frac{dy}{dt} = y
\]

The solution to this differential equation is the function that shows the relationship between \( y \) and \( t \). In this example, the solution is \( y = e^t \). Using this solution, we could find the value of \( y \) at any given value of \( t \).

However, many differential equations are not solvable. (Or they are quite difficult to solve.) In science, we often don’t really need to know the actual equation showing the relationship between \( y \) and \( t \), we just need to know the value of \( y \) at a given value of \( t \). This is known as the numerical solution to the differential equation. In a numerical solution, you don’t know the actual equation that solves the differential equation, you just have the predictive power of that equation, without knowing the equation itself.

We will use a function called `solve_ivp` from the python library `scipy` to numerically integrate our differential equation. This will give us use the values of \( y \) at all the values of \( t \) we specify.

The basic steps to solving a DE are as follows:

1. Set up a function that calculates the value of the derivative. This function should have two inputs, the independent variable (in our example \( t \)) and the dependent variable (in our example \( y \)). You should list the independent variable first.
2. Choose the initial and final values of the independent variable.
3. Give the initial value of the dependent variable. You can specify more than one initial value, so this needs to be a list, even if you only have one value.
4. Use the `solve_ivp` function to solve the differential equation.
Kinetics Activity

import numpy as np
from scipy.integrate import solve_ivp
import matplotlib.pyplot as plt

def dydt(t, y):
    return y

# Set the initial and final time
t0 = 0
Tfinal = 1

# Set the initial value for y; this needs to be a list even if you only have one value
y0 = [1]

# Now solve the differential equation
solution = solve_ivp(dydt, [t0, Tfinal], y0)

# Get the list of times from the solution
solt = solution.t

# Get the list of values of y from the solution
soly = solution.y[0]

# Plot the results
plt.plot(solt, soly)

Practice 1:

As we discussed above, this is actually a differential equation that CAN be solved analytically, and we know the solution is $y = e^t$. Use the equation to calculate the values of $y$ for all the times in the evaluation times. Plot these points as dots on the same graph with the numerical solution.

Practice 2:

Consider a reaction that is second-order in one reactant A. The DE for the rate of this reaction is $\frac{d[A]}{dt} = -k[A]^2$. If the rate constant is 0.05 L mol$^{-1}$ s$^{-1}$ and the initial concentration of A is 1.5 M, what is the concentration of A after 10 seconds?
Software Course

- Nick Mayhall
  Virgina Tech

- Activity: Computing Thermodynamics Properties of the Ising Model

- MoISSI springboard: Best Practices Workshop
Package Development

• Develop programs to implement quantum algorithms

• Learn collaborative workflows

• Start developing in a notebook —> Convert to a package
TEACHING PROGRAMMING
ACROSS THE CHEMISTRY CURRICULUM

RING McDONALD
& NASH

ACS Symposium Series

ACS Publications

https://education.molssi.org
Computing Environments

- For introducing programming to students, we recommend using a cloud computing environment.

- Advantages:
  - Students do not have to install software on their own computer.
  - You only need a browser + internet access.

- Options:
  - chemcompute.org
  - nanohub.org

https://education.molssi.org
Conclusions

• MolSSI provides foundational programming lessons that can be incorporated into STEM curriculum.

• Outside of computer science, exposure to computational skills is extremely varied.

• Incorporating these skills into STEM disciplines ensures wider exposure for all students.

• Faculty professional development is key to widespread adoption.
Building Student Confidence in STEM – Programs that Promote Student Success

Dr. Lisa Dierker
Dr. Ashley McDonald

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Thank you for attending!

Slides and recording will be available in the coming days.

We value your feedback, please take a few minutes to complete the survey.

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