Replicable and Reproducible Research with Workflow

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Agenda

❑ **Background**

❑ **Data Access with Workflow**

❑ **Case Study with Workflow**

❑ **Discussion**

Motivation

REPRODUCIBILITY, REPLICABILITY, AND GENERALIZATION IN THE SOCIAL, BEHAVIORAL, AND ECONOMIC SCIENCES

REPRODUCIBILITY: the ability of a researcher to duplicate the results of a prior study using the same materials and procedures as were used by the original investigator.

REPLICABILITY: the ability of a researcher to duplicate the results of a prior study if the same procedures are followed but new data are collected.

GENERALIZABILITY: whether the results of a study apply in other contexts or populations that differ from the original one

Challenges

A survey conducted by *Nature* found that more than **70%** of researchers have failed to reproduce another scientist's studies, and more than **50%** have failed to reproduce their own experiments (Baker, 2016).

- ❑ **Unavailable dataset**
- ❑ **Different environment**
  - Operation system
  - Computing environment
  - Software
  - Library versions
- ❑ **Lacks documentation**

Reproducibility, Replicability, and Expansion with Workflow

Data Science Workflow Tool KINME

Open for Innovation
KNIME

https://www.knime.com/

- ❑ Workflow is displayed as connected nodes which makes it easy to troubleshoot and visualize
- ❑ Easy to use without much knowledge of coding
- ❑ Great extensions for data preprocessing, analysis, and visualization
- ❑ Connection to other languages, such as JS, R, Python, etc.
- ❑ Open-source
- ❑ Cross platform interoperability
- ❑ Has a decent size community that supports Q&A.

Read
- Excel Reader (XLS)
- File Reader
- ARFF Reader
- CSV Reader
- Line Reader
- Table Reader
- PMML Reader
- Model Reader
- Fixed Width File Reader
- List Files
- Read Excel Sheet Names (XLS)
- Read Images
- Explorer Browser

Mining
- Bayes
- Clustering
- Rule Induction
- Neural Network
- Decision Tree
- Decision Tree Ensemble
- Misc Classifiers
- Ensemble Learning
- Item Sets / Association Rule
- Linear/Polynomial Regressic
- Logistic Regression
- MDS
- PCA
- PMML
- SVM
- Feature Selection
- Scoring

Statistics
- Hypothesis Testing
- Cronbach Alpha
- Standardized Cronba
- Rank Correlation
- Statistics
- Crosstab (local)
- Value Counter
- Linear Correlation
- Numeric Outliers
- Numeric Outliers (Ap

Geospatial Operations
- Geometry IO and visualization
  - Shapefile reader
  - Shapefile writer
  - GeoJSON reader
  - GeoJSON writer
  - WFS connector
  - Map viewer
- Geometry conversion
  - Transform
  - Snap to grid
  - Polygon to line
  - Line to polygon
  - Geometries to multi-geometries
  - Multi-geometry to geometries
  - Filter geometry by type
  - Vertices to points
  - Line endpoints
  - Line merge
- Geometry procesing
  - Buffer
  - Concave Hull

Spatial Data Lab

- ☐ Integrated hundreds of datasets with thousands of variables
- ☐ Developed more than 60 workflow-based case studies for spatiotemporal research
- ☐ Comprehensive documents for easy reproducibility, and replicability

Data Access with Workflows

- ❑ **China Data Online platform**
- ❑ **Database (Postgres)**
- ❑ **External Platforms with Rest API**
- ❑ **Harvard Dataverse**
- ❑ **Data on GitHub**

Database

Web API

Open Data Repository

Data Access with Workflows

2. Access Large-scale Patent Data from Platform Database

1) Import Workflow from Public Folder **\\CDI\Case Study\00_Example\00_database\patent_db**
2) The imported workflow is shown as below. There are five components: PostgreSQL database settings; DB Table selector; DB Query; read data from DB to get results.

字段名	Field	字段名	Field	字段名	Field
标题（O)	Tio	公开（公告）日	Publication Date	引证类别(backward)	Citation Origin Code
摘要（O)	Abo	转让执行日	Assignment ExecutionDate	X引证文献	ct-X
专利价值度	Vlstar	专利有效性	status	家族引证次数(backward)	Family Citation Number of Times
申请人(原始)	AP-OR	当前法律状态	CN status lite	家族被引证次数（forward)	Family Citation-Forward Number of Times
发明(设计)人(原始)	in-or	法律状态文字信息	Legal Free Text	非专利引证	Citation-Nonpatent
代理人姓名	Attorney	引证信息（backward)	Citation	优先权日	Priority Date
代理机构	Agency	被引证信息（forward)	Citation-Forward	申请人省市	Applicant province
IPC分类	IPC	引证次数（backward)	Citation Number of Times	中国省市代码	PC-CN
IPC主分类	IPC Main	被引证次数（forward)	Citation-Forward Number of Times	中国申请人省市代码	AP-PC
洛迦诺分类	Locarno Classification	家族引证（backward)	Family Citation	中国申请人地市	City
CPC分类	CPC	家族被引证（forward)	Family Citation-Forward	中国申请人区县	County
申请人地址	Applicant Address Information	引证申请人（backward)	Citation Applicant	受让人	Assignee
申请号	Application Number	被引证申请人（forward)	Citation-Forward Applicant	转让人	Assignor
优先权号	Priority Number	家族引证申请人(backward)	Family Citation Applicant	行业门类	Bclas1
公开类型	Publication Type	家族被引证申请人（forward)	Family Citation-Forward Applicant	行业大类	Bclas2
简单同族	MainFamily	引证号码(backward)	Citation Number	行业中类	Bclas3
扩展同族	CompleteFamily	被引证号码（forward)	Citation-Forward Number	公开(公告)号	Publication Number
同族国家	Fa-Country	引证国别(backward)	Citation Authority	授权公告日	Grant Date
申请日	Application Date	被引证国别（forward)	Citation-Forward Authority	首项权利要求	First Claim

Data Access with Workflows

3. Access **Public** COVID-19 Data from **Harvard Dataverse**

Import workflow from public case study folder \\CDI\Case Study\00_Example\01_dataverse\dataverse_api.knwf

Data Access with Workflows

4. Access External Human Mobility Index Data via Rest API

Data Access with Workflows

5. Access External Data via GitHub API   https://github.com/stccenter/COVID-19-Data

Case Study 1: Air Pollution Data Visualization

Objectives

o Develop a prototype for spatiotemporal data visualization with dynamic maps

o Build a workflow for efficient China Data Online data visualization

o Make the data analysis and visualization replicable, reproducible and expandable

o Lower the barrier for spatiotemporal data visualization

Data Sources

o Harvard Dataverse (https://doi.org/10.7910/DVN/XETLSS)

Data

o Daily PM2.5 emissions by China cities (Jan-Feb, 2020)

o Province boundary basemap of Mainland China

Method and Flowchart

Methodology

Plotly Python Open-Source Graphing Library https://plotly.com/python/

Mapbox Choropleth   Lines on Mapbox   Filled Area on Maps   Bubble Maps

Flowchart

Data Inputs

- Daily PM2.5 emissions by city
- China City Base map

Data Processing

- Merge PM2.5 data with map
- Data Transformation
- Parameters Settings

Outputs

- HTML Map
- GIF Map
- MP4 Map

Workflow Implementation by KNIME

Steps for Running the Workflow

Step 1: **Download data** from \01_dynamic_maps\01_data\
Step 2: **Download workflow** from \01_dynamic_maps\02_workflow\environment_dynamic_map.knwf
Step 3: **Open KNIME** from local PC or China Data Lab Cloud Platform (in building)
Step 4: **Import KNIME workflow** file (environment_dynamic_map.knwf)
Step 5: **Launch the workflow** by double clicking the imported workflow
Step 6: **Configure "Input Data"**
Step 7: **Configure "Set Variables"**
- Select Geojson file 'China_admin_1.json' path;
- Set Output html, GIF, and MP4 file path;
- Set Option: 1->html; 2->GIF; 3->mp4
- Set Title: name of the html file
- Set Days interval: default 3;

Step 8: **Configure path in "Image Write" node**
Step 9: Click **Run** 🔘 function from the top menu
Step 10: **Display the outputs**:
- HTML Map
- GIF Map
- MP4 Map
- Chart

*** Please install Anaconda as the Python environment and set Python path in the KNIME preference
*** install python libraries following commands below
  ➢ conda install –c plotly plotly
  ➢ conda install –c plotly plotly-orca
  ➢ conda install –c plotly python-kaleido
  ➢ conda install -c conda-forge imageio
  ➢ conda install -c anaconda opencv

*** Please set Chrome as default browser
*** Please install suggested extensions when opening workflow

Summary

https://covid-19.stcenter.net/index.php/global-countries/

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Short communication

COVID-19 spatiotemporal research with workflow-based data analysis

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ABSTRACT

Given the pertinence and acceleration of the spread of COVID-19, there is an increased need for the replicability of data models to verify the veracity of models and visualize important data. Most of these visualizations lack reproducibility, credibility, or accuracy, and are static, which makes it difficult to analyze the spread over time. Furthermore, most current visualizations depicting the spread of COVID-19 are at a global or country level, meaning there is a dearth of regional analysis within a country. Keeping these issues in mind, a replicable, efficient, and simple method to generate regional COVID-19 visualizations mapped with time was created by using the KNIME software, an open-source data analytics platform that can create user-friendly applications or workflows. For this analysis, Albania, Sweden, Ukraine, Denmark, Russia, India, and Australia were closely observed. Among the maps generated for the aforementioned countries, it was noticed that regions with a high population or high population density were often the epicenters within their respective country. The regions caused the virus to spread to their neighboring regions: kickstarting the "domino effect", leading to the infection of another region until the country is overwhelmed with cases—what we call a proximity trend. These dynamic maps are crucial to fighting the pandemic because they can provide insight as to how COVID-19 spreads by providing researchers or officials with an accurate and insightful tool to aid their analysis. By being able to visualize the spread, health and government officials can dive deeper to identify the sources of transmission and attempt to stop or reverse them accordingly.

COVID-19 Rapid Response Research with Workflow-based Data Analysis

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[1] Chintala, S., Dutta, R., & Tadmor, D. (2021). COVID-19 spatiotemporal research with workflow-based data analysis. Infection, Genetics and Evolution, 88, 104701.
[2] Tadmor, D. (2020). COVID-19 Rapid Response Research with Workflow-based Data Analysis. Available at SSRN 3643621.

Wu, X., Nethery, R. C., …, & Dominici, F. (2020). Air pollution and COVID-19 mortality in the United States: Strengths and limitations of an ecological regression analysis. Science Advances, 6(45)

Objective: Assessing whether long-term exposure to air pollution increases the severity of COVID-19 health outcomes, including death, is an important public health objective.

Data Sources: Harvard Dataverse, NASA, Census Bureau

Data: COVID-19 Cases, PM 2.5, Population density, income, percent of owner-occupied housing, adult population, age distribution, black residents, et al.

Table S2: Characteristics of the study cohort up to and including June 18, 2020, mean (standard deviation).

	Total (3,087 counties)	$PM_{2.5} < 8$ $\mu g/m^3$ (1,217 counties)	$PM_{2.5} \geq 8$ $\mu g/m^3$ (1,870 counties)
COVID-19 death rate (per 100,000)	15.5 (31.2)	7.0 (19.7)	21.0 (35.7)
Average $PM_{2.5}$ ($\mu g/m^3$)	8.4 (2.5)	5.7 (1.4)	10.1 (1.2)
Rate of hospital beds (per 100,000)	300.8 (428.4)	338.8 (548.2)	276.1 (325.3)
Days since first case	76.9 (21.1)	68.2 (27.8)	82.6 (12.2)
Days since stay-at-home order	59.4 (38.1)	52.4 (41.6)	63.9 (34.9)
% Smokers	17.4 (3.5)	15.8 (3.1)	18.5 (3.4)
% Obese	32.9 (5.4)	31.2 (5.1)	34.0 (5.3)
% In poverty	10.5 (5.9)	9.6 (5.8)	11.0 (5.9)
% Less than high school education	21.3 (10.7)	16.6 (8.8)	24.4 (10.6)
% Owner-occupied housing	75.0 (8.3)	76.4 (7.6)	74.1 (8.6)
% Hispanic	7.5 (12.3)	9.6 (13.6)	6.1 (11.1)
% Black	8.0 (14.1)	1.0 (1.9)	12.6 (16.5)
% ≥65 years of age	16.0 (4.1)	17.4 (4.6)	15.0 (3.4)
% 45-64 years of age	26.4 (3.0)	26.9 (3.8)	26.1 (2.4)
% 15-44 years of age	37.6 (6.5)	35.2 (8.2)	39.2 (4.5)
Population density (person/km²)	149.5 (699.2)	46.1 (146.9)	216.9 (884.4)
Median household income ($1,000)	49.3 (13.4)	50.6 (11.1)	48.4 (14.6)
Median house value ($1,000)	135.7 (89.9)	140.4 (87.8)	132.7 (91.1)
Average summer temperature (°F)	86.0 (5.7)	83.7 (6.7)	87.4 (4.4)
Average winter temperature (°F)	45.1 (11.9)	39.4 (11.4)	48.7 (10.7)
Average summer relative humidity (%)	89 (9.6)	83.2 (11.5)	92.8 (5.5)
Average winter relative humidity (%)	87.5 (4.8)	88.0 (5.6)	87.2 (4.1)

Methodology

Methodology:

o Employ *Ecological Regression Analysis* to investigate relation between air pollution and COVID-19 health outcomes

o Fit a **negative binomial mixed model** using COVID-19 mortality rates as the outcome

o *Generalized linear mixed-effects model (GLMM)*

Flowchart

Workflow Implementation

Summary

Findings

o The higher historical PM2.5 exposures are positively associated with higher county-level COVID-19 mortality rates after accounting for many area-level confounders.

o It also found that population density, days since the first COVID-19 case was reported, median household income, percent of owner-occupied housing, percent of the adult population with less than high school education, age distribution, and percent of Black residents are important predictors of the COVID-19 mortality rate in the model.

Discussion

o Integrate more datasets from multiple data sources

o Develop more case studies with workflow tools, including KNIME, R AnalyticalFlow, Jupyter Notebook (Python/R)

o Collaborate with global scholars to replicate publications

o Build a case study repository for easy access and query

o Organize training webinars for students, researchers, and educators to promote cross-disciplinary reproducible, replicable, and generalizable research

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Thank you !

Questions/Comments?

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