Programming Principles in Python (CSCI 503/490)

Machine Learning

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Grammar of Graphics & Altair

- "Grammar of Graphics", L. Wilkinson
- "A Layered Grammar of Graphics" + ggplot, H. Wickham
- Vega: "Declarative language for creating, saving, and sharing interactive visualization designs"
- Vega-Lite: higher-level language than Vega, carefully crafted rules for defaults
- Altair: Python interface to Vega-Lite
  - "spend more time understanding your data and its meaning"
  - Specify the what, minimize the amount of code directing the how
  - Python can write JSON specification just as well as any other language
  - Bindings make it more Python-friendly, integrate with pandas, add support for Jupyter, etc.
Basic Example

• import altair as alt
  import pandas as pd
  data = pd.DataFrame({'x': [1, 3, 4, 6, 10], 'y': [1, 5, 2, 7, 3]})
  alt.Chart(data).mark_line().encode(x='x', y='y')

• Easiest to use data from a pandas data frame
  - Another option is a csv or json file
  - Can support geo_interface, too

• Chart is the basic unit

• Mark: .mark_*() indicates the geometry created for each data item

• Encode: .encode() allows visual properties to be set to data attributes
Visual Marks

• **Marks** are the basic graphical elements in a visualization
• Marks classified by dimensionality:
  
  - **Points**
  - **Lines**
  - **Areas**

• Also can have surfaces, volumes
• Think of marks as a mathematical definition, or if familiar with tools like Adobe Illustrator or Inkscape, the path & point definitions
• Altair: area, bar, circle, geoshape, image, line, point, rect, rule, square, text, tick
  - Also compound marks: boxplot, errorband, errorbar
Encode via Visual Channels

- **Position**
  - Horizontal
  - Vertical
  - Both

- **Color**
  - Black
  - Red
  - Green

- **Shape**
  - Triangle
  - Asterisk
  - Slash
  - L Shape

- **Tilt**
  - Angle 1
  - Angle 2

- **Size**
  - Length
  - Area
  - Volume

[Munzner (ill. Maguire), 2014]
Data Attributes and Altair Types

- Categorical
- Ordered
- Ordinal
- Quantitative

[Munzner (ill. Maguire), 2014]
Data Attributes and Altair Types

- Categorical data = Nominal (N)
- Ordinal data = Ordinal (O)
- Quantitative data = Quantitative (Q)
- Temporal data = Temporal (T)

[Munzner (ill. Maguire), 2014]
Different Channels for Different Attribute Types

**Magnitude Channels: Ordered Attributes**
- Position on common scale
- Position on unaligned scale
- Length (1D size)
- Tilt/angle
- Area (2D size)
- Depth (3D position)
- Color luminance
- Color saturation
- Curvature
- Volume (3D size)

**Identity Channels: Categorical Attributes**
- Spatial region
- Color hue
- Motion
- Shape

Altair will use its rules to pick whether to use color hue or saturation based on the type.

[Munzner (ill. Maguire), 2014]
Altair Supports Concatenation, Layering, & Repetition

• Layering:
  - + Operator

• Concatenation:
  - Horizontal: | operator
  - Vertical: & operator

• Repetition
  - Use of .repeat for layout
  - Reference repeated variables in the encoding
Layering
Concatenation

[Improvise, Weaver, 2004]
Repetition
Seattle Weather: 2012-2015

Date

Maximum Daily Temperature (°C)

Count of Records

weather
- sun
- fog
- drizzle
- rain
- snow

precipitation
- 0
- 10
- 20
- 30
- 40
- 50

Interaction

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Assignment 8

• Due Thursday, May 2
• Data and Visualization
• Same Utility Data
  - Group by, data transformation
  - matplotlib visualization
  - altair visualization
Final Exam

- Monday, May 6, **12:00-1:50pm** in PM 110
- **More comprehensive** than Test 2
- Expect questions from topics covered on Test 1 and 2
- Expect questions from the last four weeks of class (data, visualization, machine learning)
- Similar format

- Bring questions on Wednesday!
Machine Learning in Python
Tasks Machine Learning can Help With

• Identifying the zip code from handwritten digits on an envelope

![MNIST Image](https://www.csie.ntu.edu.tw/~cjlin/liblinear/mnist.png)

• Detecting fraudulent activity in credit card transactions
• Identifying topics in a set of blog posts
• Grouping customers with similar preferences

[A. Müller & S. Guido, Introduction to Machine Learning with Python, J. Steppan (MNIST image)]
When to Use Machine Learning?

• ML is used when:
  - Human expertise does not exist (navigating on Mars)
  - Humans can’t explain their expertise (speech recognition)
  - Models must be customized (personalized medicine)
  - Models are based on huge amounts of data (genomics)

• ML isn’t always useful:
  - Calculating payroll…
Questions when building a machine learning solution

• What question(s) am I trying to answer? Do I think the data collected can answer that question?
• What is the best way to phrase my question(s) as a machine learning problem?
• Have I collected enough data to represent the problem I want to solve?
• What features of the data did I extract, and will these enable the right predictions?
• How will I measure success in my application?
Machine Learning Workflow Overview

1. Should I use ML on this problem?
   - Is there a pattern to detect? Can I solve it analytically? Do I have data?
2. Gather and organize data.
   - Preprocessing, cleaning, visualizing.
3. Establishing a baseline.
4. Choosing a model, loss, regularization, …
5. Optimization (could be simple, could be a Phd…).
6. Hyperparameter search.
7. Analyze performance & mistakes, and iterate back to step 4 (or 2).
Machine Learning

- Traditional Programming

  Data → Computer → Output
  Program →

- Machine Learning

  Data → Computer → Program
  Output →
Machine Learning

- Every machine learning algorithm has three components:
  - Representation
  - Evaluation
  - Optimization
Representation

- Decision trees
- Sets of rules / Logic programs
- Instances
- Graphical models (Bayes/Markov nets)
- Neural networks
- Support vector machines
- Model ensembles
- Etc.
Evaluation

- Accuracy
- Precision and recall
- Squared error
- Likelihood
- Posterior probability
- Cost / Utility
- Margin
- Entropy
- K-L divergence
- Etc.
Optimization

• Combinatorial optimization
  - E.g.: Greedy search

• Convex optimization
  - E.g.: Gradient descent

• Constrained optimization
  - E.g.: Linear programming
Types of Learning

- Supervised (inductive) learning
  - Training data includes desired outputs
- Unsupervised learning
  - Training data does not include desired outputs
- Semi-supervised learning
  - Training data includes a few desired outputs
- Reinforcement learning
  - Rewards from sequence of actions
Areas of Machine Learning

- Supervised learning
  - Decision tree induction
  - Rule induction
  - Instance-based learning
  - Bayesian learning
  - Neural networks
  - Support vector machines
  - Model ensembles
  - Learning theory

- Unsupervised learning
  - Clustering
  - Dimensionality reduction
Supervised & Unsupervised Tasks

• Identifying the zip code from handwritten digits on an envelope (supervised)

• Detecting fraudulent activity in credit card transactions (supervised)

• Identifying topics in a set of blog posts (unsupervised)

• Grouping customers with similar preferences (unsupervised)

[A. Müller & S. Guido, Introduction to Machine Learning with Python, J. Steppan (MNIST image)]
Supervised Learning
Supervised Learning: Learned Algorithm (Fit)
Supervised Learning: Prediction
Supervised Learning: Prediction
Unsupervised Learning: Input
Unsupervised Learning: Output

- J. VanderPlas

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Scikit-Learn

• Started as a Google Summer of Code project! (D. Cournapeau, 2007)
• Rewritten by scientists at INRIA (France) in 2010
• Written in Python using numpy, some optimizations using C (cython)
• The "gold standard" for machine learning in python
scikit-learn Principles

• Consistency: all objects share consistent, documented interface
• Inspection: parameters and parameter values determined by learning algorithms are stored and exposed as public attributes
• Non-proliferation of classes: only learning algs are classes, not datasets or parameters; easier to combine with other libraries
• Composition: create and reuse building blocks
• Sensible defaults: user-defined parameters should have meaningful defaults
scikit-learn entities

- Data: numpy matrices (also pandas series, data frames), process batches
- Estimators: all supervised & unsupervised algs implement common interface
  - estimator initialization does not do learning, only attaches parameters
  - fit does the learning, learned parameters exposed with trailing underscore
- Predictor: extends estimator with predict method
  - also provides score method to return value indicating prediction quality
- Transformer: help modify or filter data before learning
  - Preprocessing, feature selection, feature extraction, and dimensionality reduction with transform method
  - Can combine fit and transform via fit_transform
Penguin Example
scikit-learn Template

1. Choose model class
2. Instantiate model
3. Fit model to data
4. Predict on new data
   ```python
   from sklearn.naive_bayes import GaussianNB
   model = GaussianNB()
   model.fit(Xtrain, ytrain)
   y_model = model.predict(Xtest)
   ```
5. (Check accuracy)
   ```python
   from sklearn.metrics import accuracy_score
   accuracy_score(ytest, y_model)
   ```
Deep Learning

• Deep learning is tied to neural networks, attempting to mimic how human neurons work together
• Hierarchical with multiple layers
• Usually takes advantage of GPUs
• Frameworks:
  - pytorch
  - TensorFlow
  - keras
  - theano
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