Programming Principles in Python (CSCI 503/490)

Machine Learning

Dr. David Koop

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

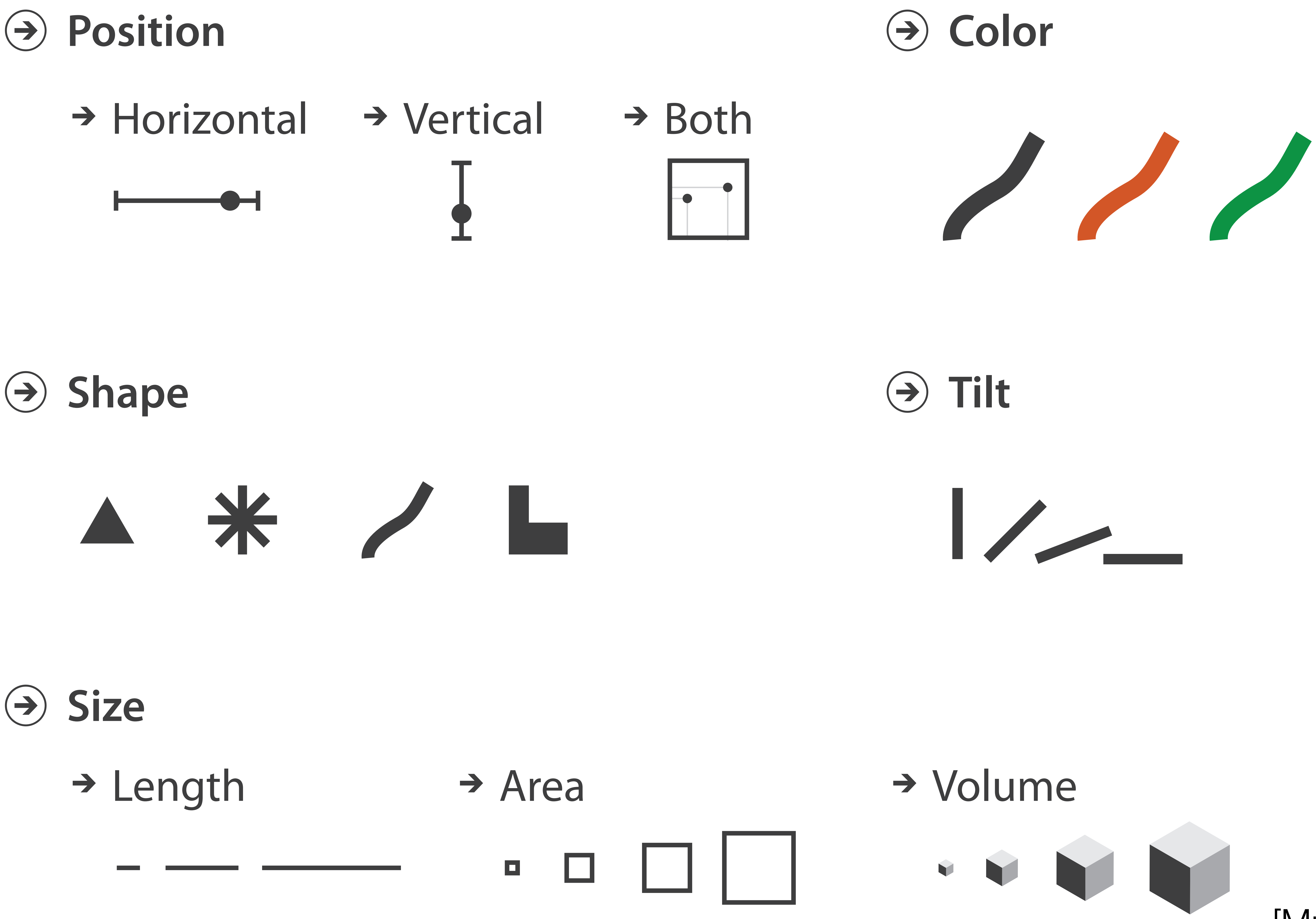
- ```
  import altair as alt
  import pandas as pd
  data = pd.DataFrame({'x': [1,3,4,6,10],'y': [1,5,2,7,3]})
  alt.Chart(data).mark_line().encode(x='x', y='y')
  ```
- Easiest to use data from a pandas data frame
  - Another option is a csv or json file
  - Can support geo_interface, too
- `Chart` 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:

- 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

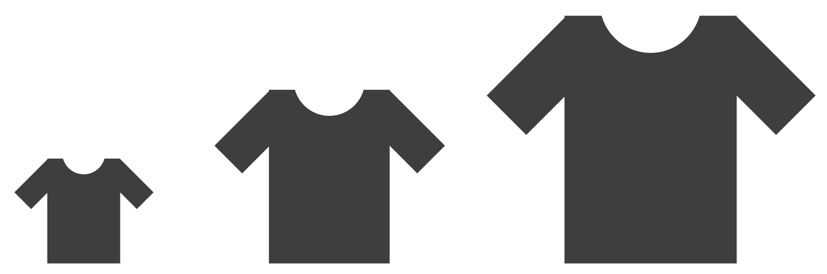


[Munzner (ill. Maguire), 2014]

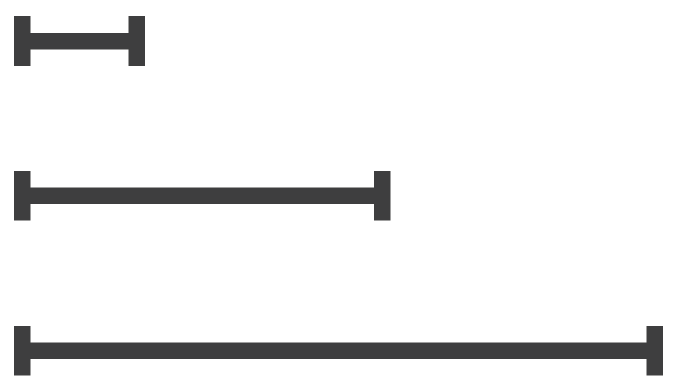
Data Attributes and Altair Types

- Categorical

- Ordered
  - *Ordinal*

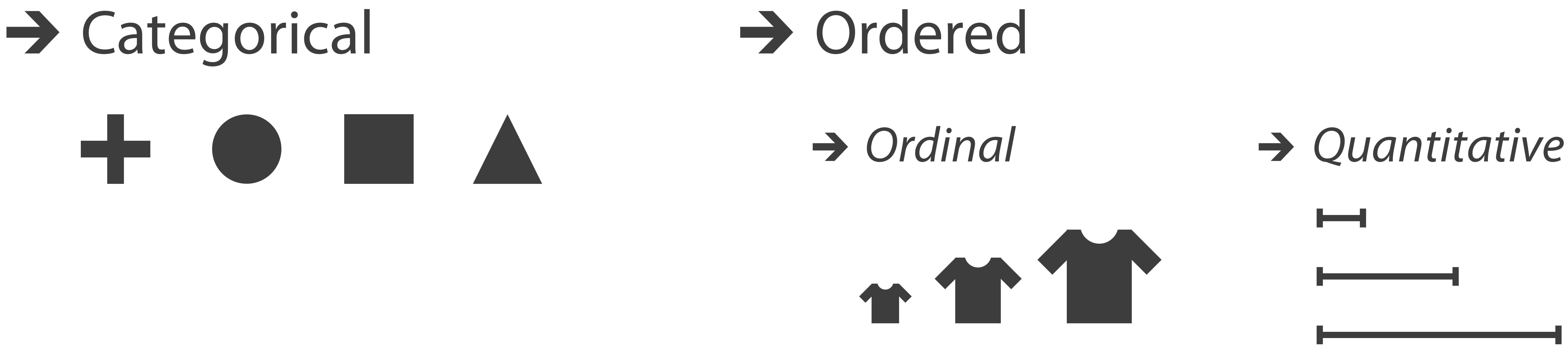


  - *Quantitative*



[Munzner (ill. Maguire), 2014]

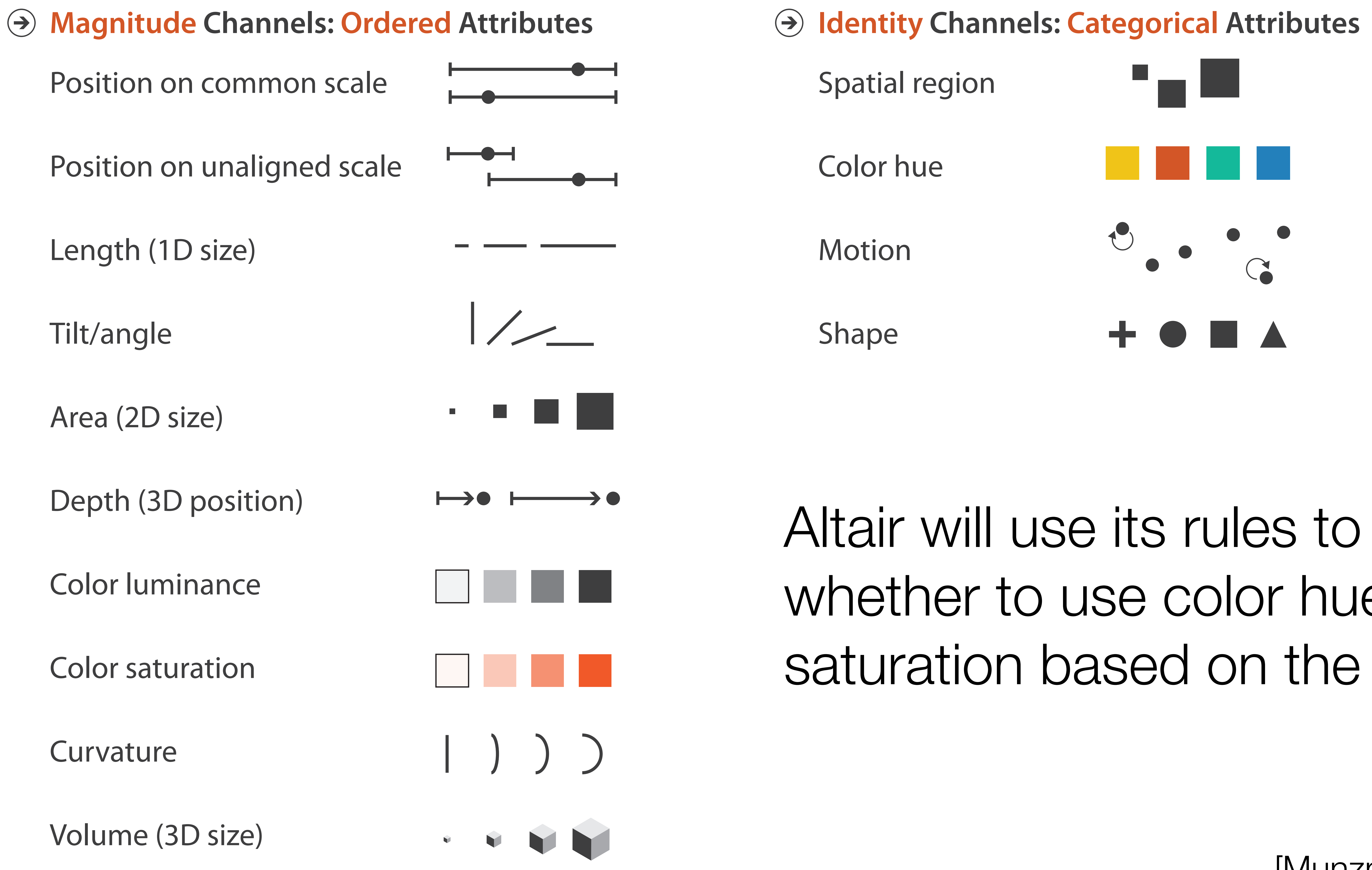
Data Attributes and Altair Types



- 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



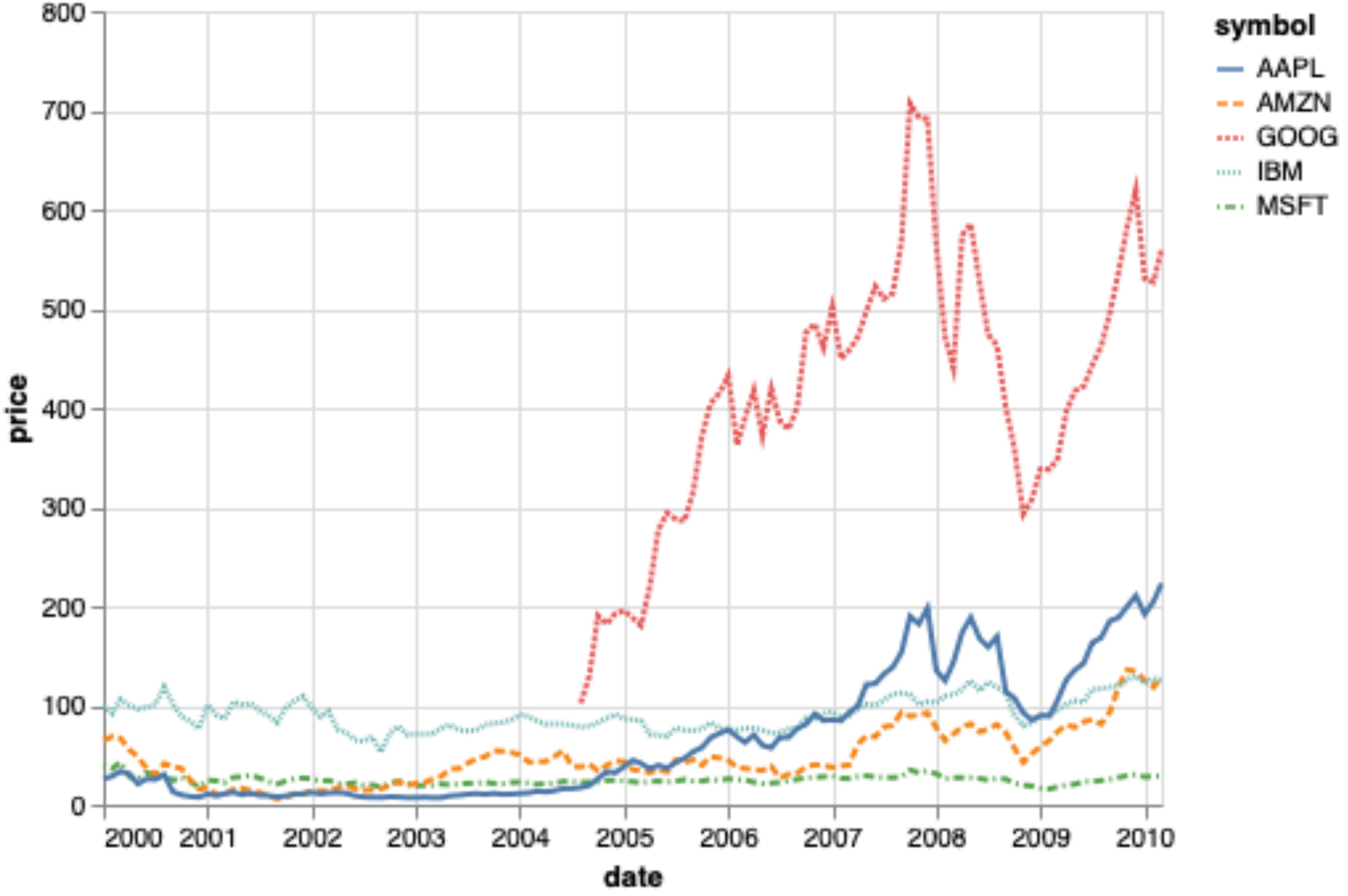
Altair will use its rules to pick whether to use color hue or saturation based on the type

[Munzner (ill. Maguire), 2014]

Altair Supports Concatenation, Layering, & Repetition

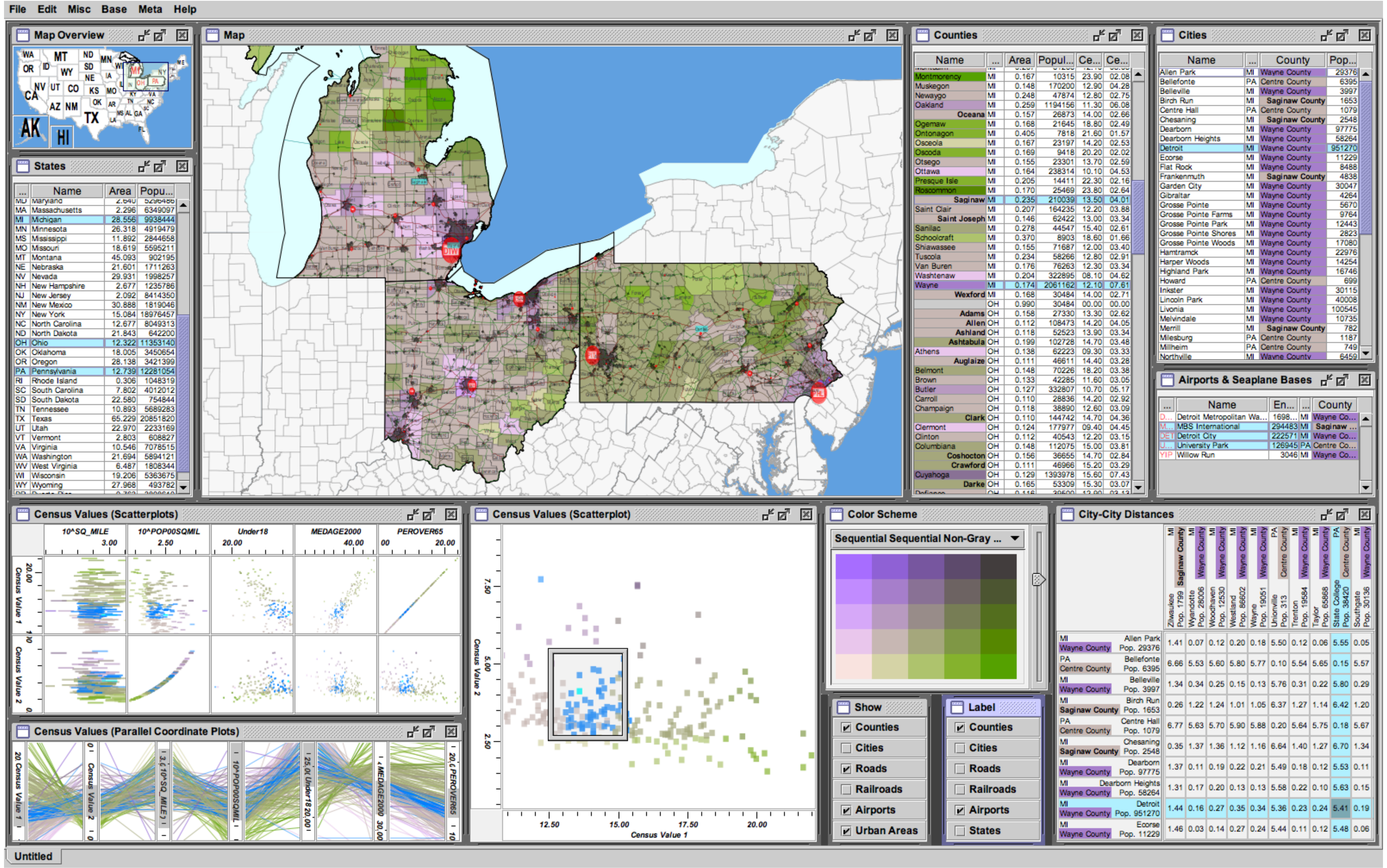
- Layering:
  - + Operator
- Concatenation:
  - Horizontal: | operator
  - Vertical: & operator
- Repetition
  - Use of .repeat for layout
  - Reference repeated variables in the encoding

Layering



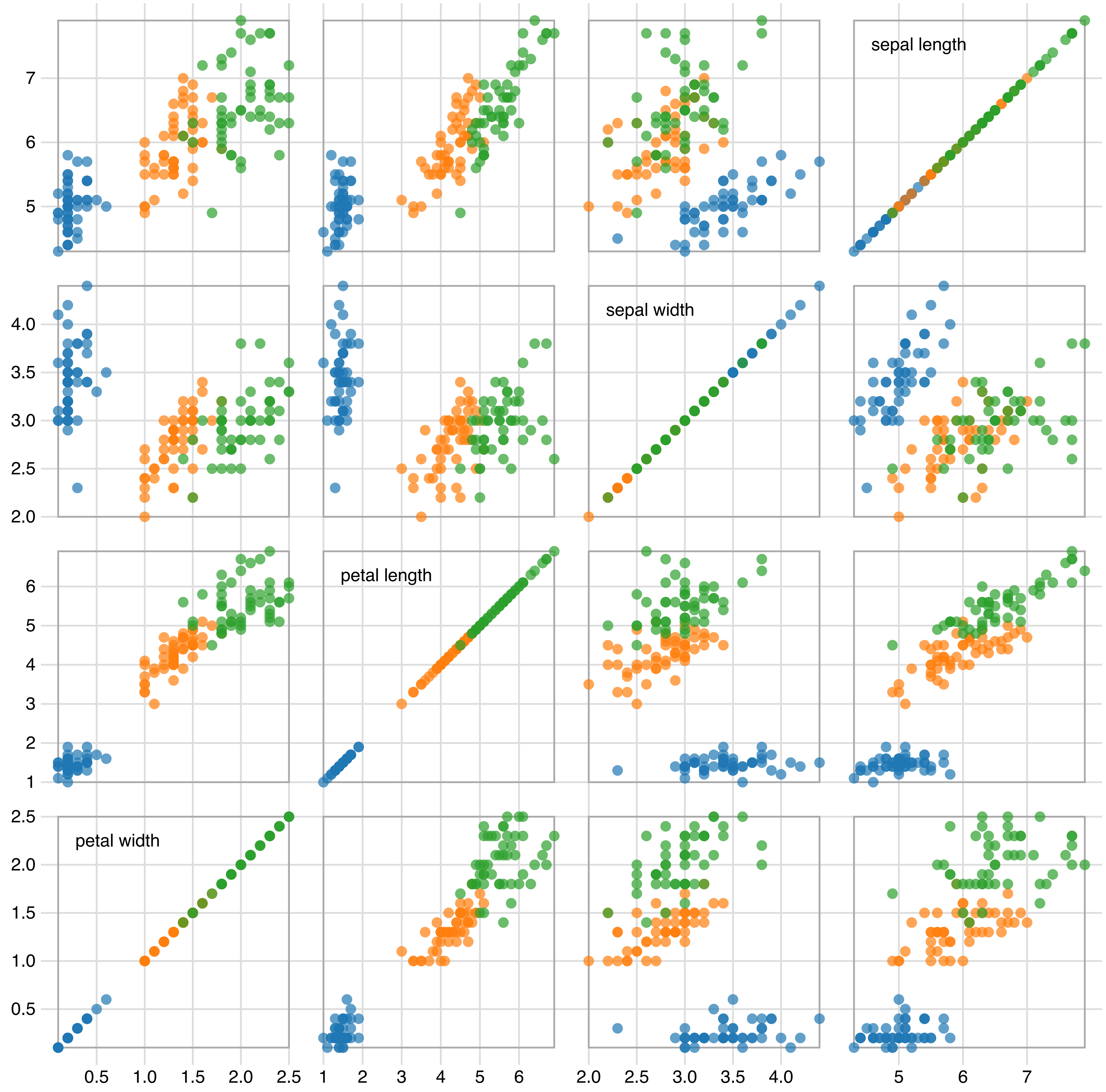
[Altair]

Concatenation



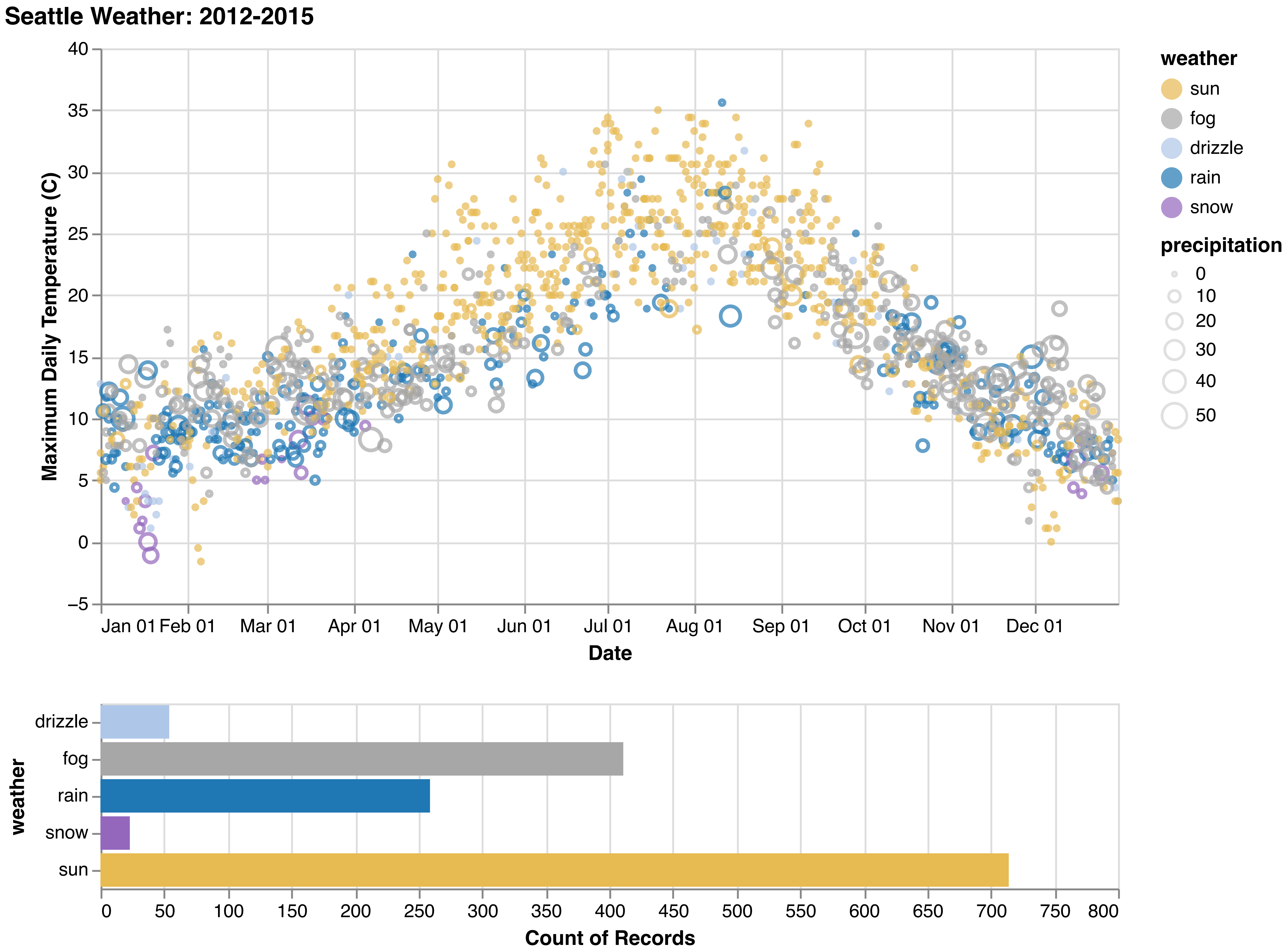
[Improvise, Weaver, 2004]

Repetition



[M. Bostock]

Interaction



Assignment 8

- Due Today
- Data and Visualization
- Pokemon Data

Final Exam

- Wednesday, May 10, **10:00**-11:50am 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

Machine Learning in Python

Tasks Machine Learning can Help With

- Identifying the zip code from handwritten digits on an envelope

- 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…

[E. Alpaydin via E. Eaton]

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?

[A. Müller & S. Guido]

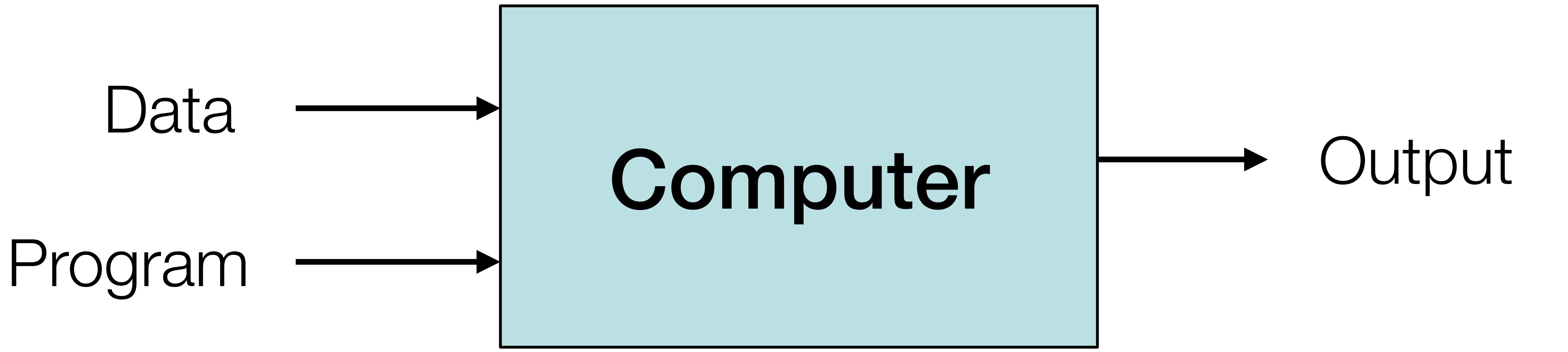
Machine Learning Workflow Overview

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).

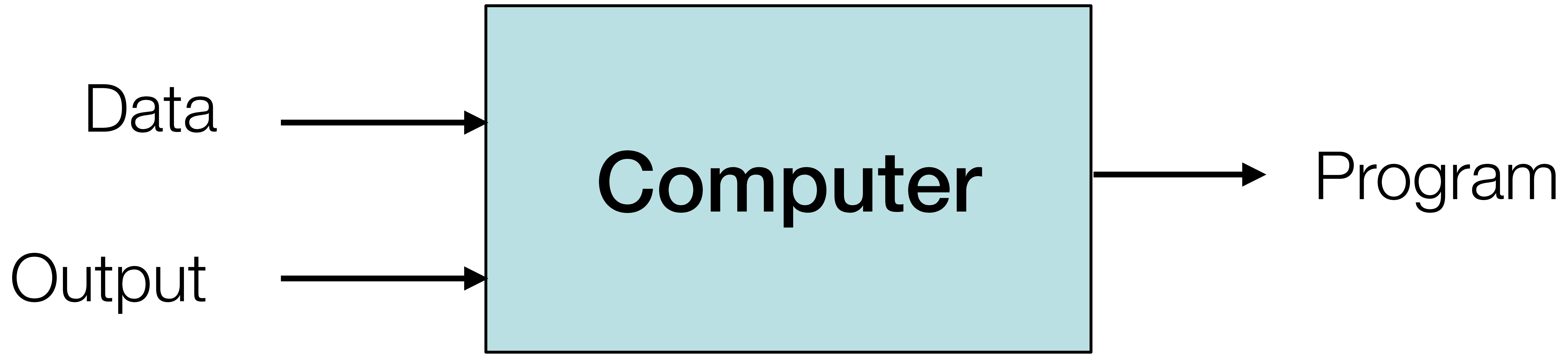
[R. Grosse et al.]

Machine Learning

- Traditional Programming



- Machine Learning



[P. Domingos]

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.

[P. Domingos]

Evaluation

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

[P. Domingos]

Optimization

- Combinatorial optimization
  - E.g.: Greedy search
- Convex optimization
  - E.g.: Gradient descent
- Constrained optimization
  - E.g.: Linear programming

[P. Domingos]

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

[P. Domingos]

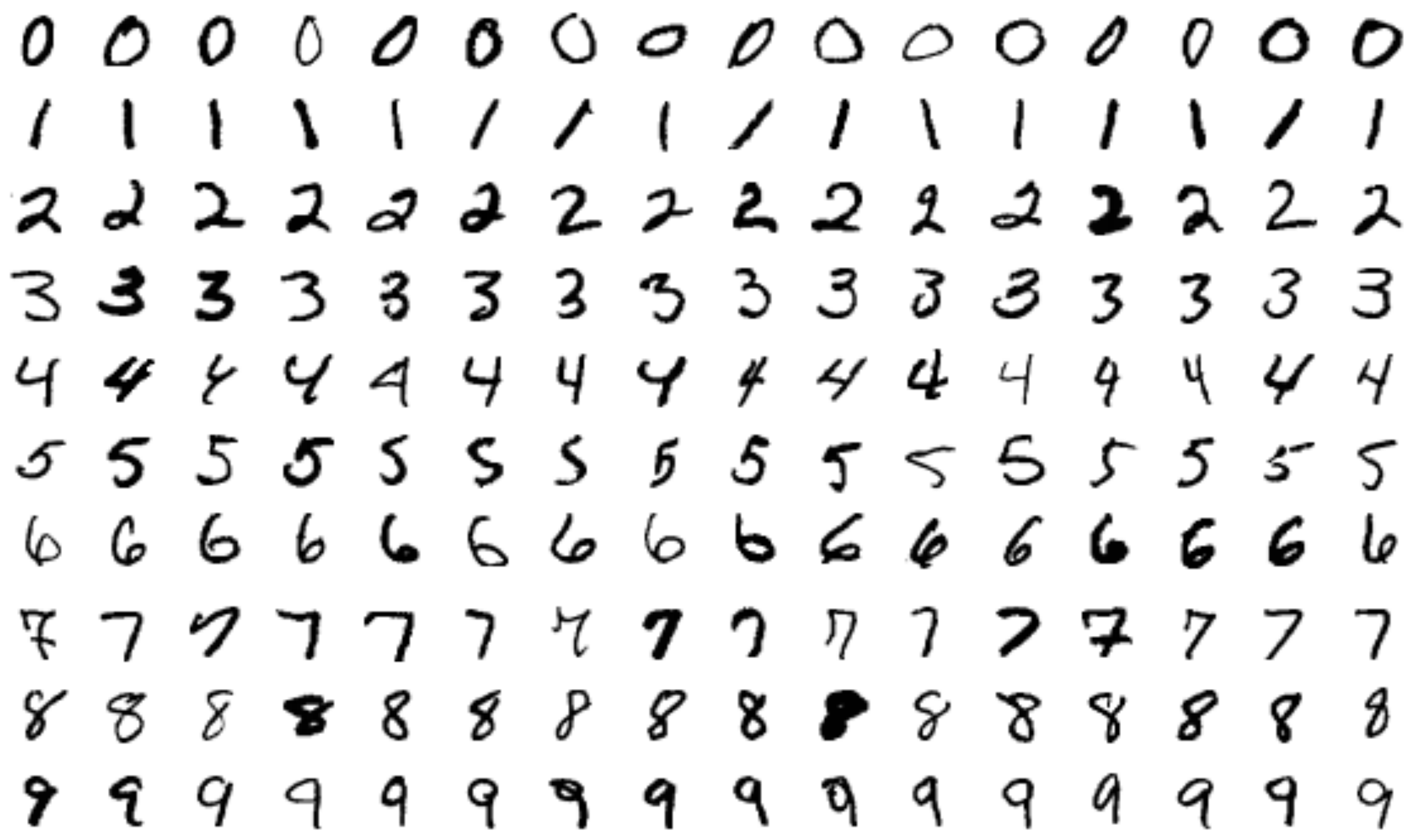
Areas of Machine Learning

- 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

[P. Domingos]

Supervised & Unsupervised Tasks

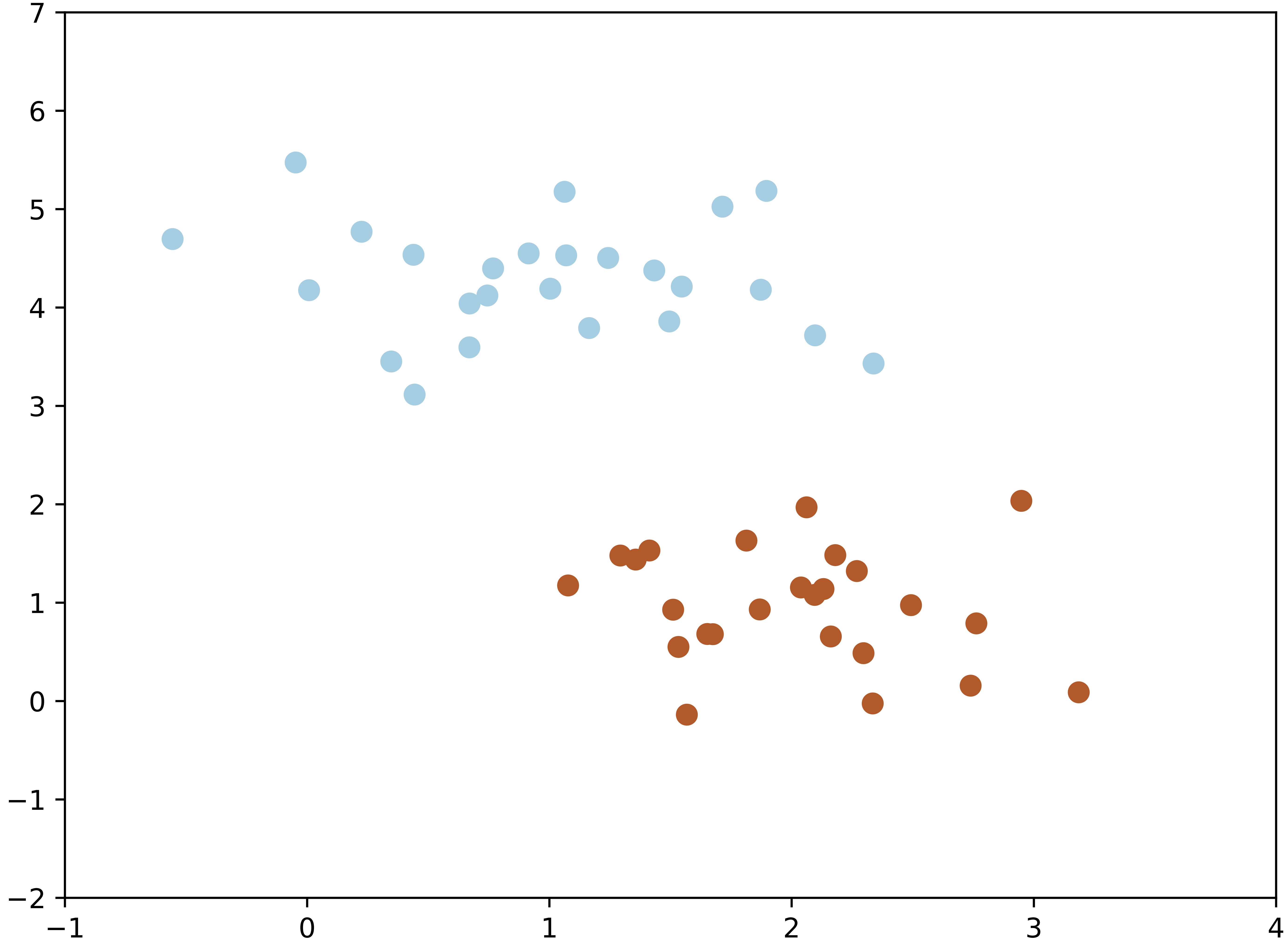
- Identifying the zip code from handwritten digits on an envelope (**supervised**)



- Detecting fraudulent activity in credit card transactions (**supervised**)
- Identifying topics in a set of blog posts (**unsupervised**)
- Grouping customers with similar preferences (**unsupervised**)

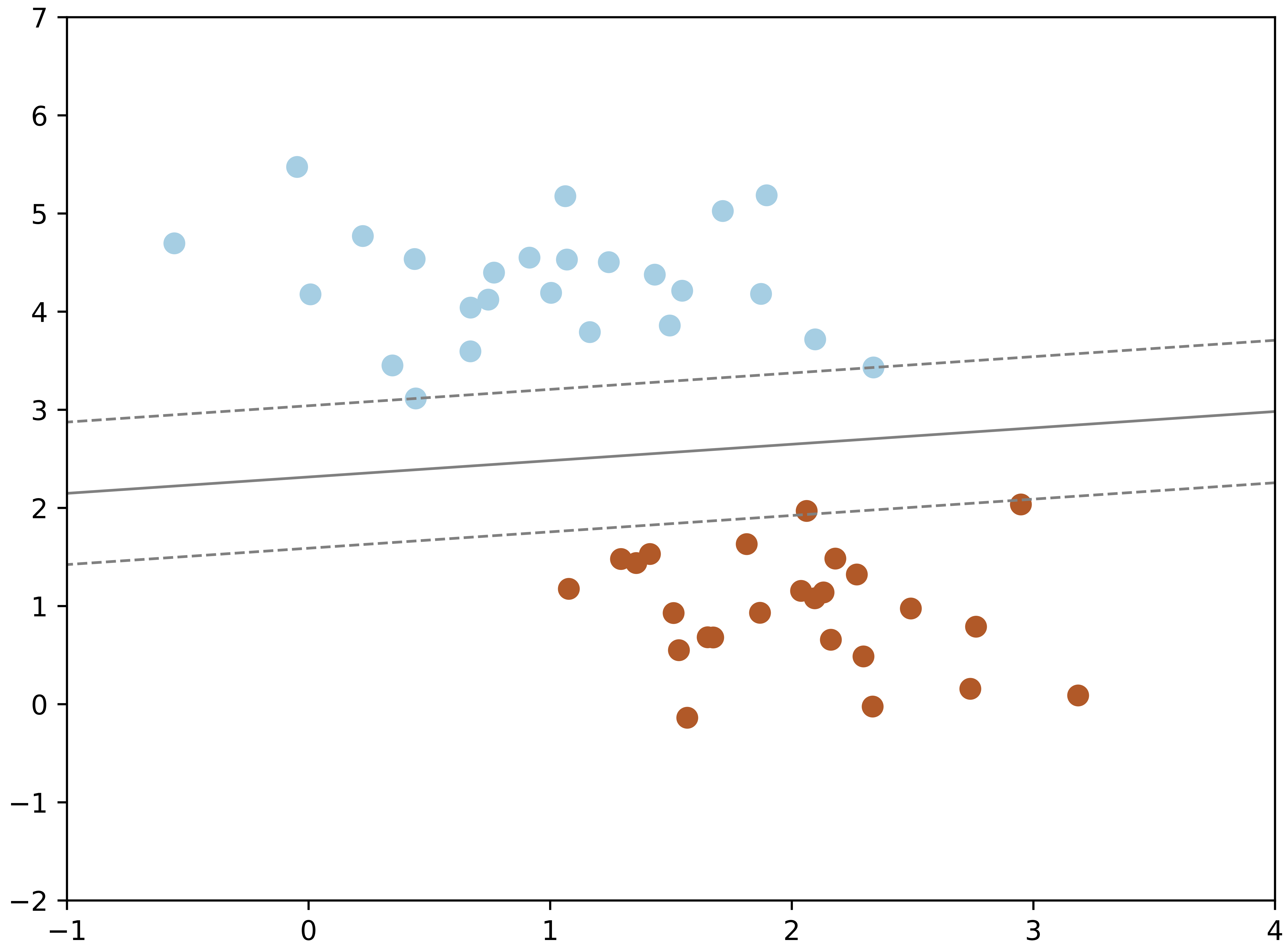
[A. Müller & S. Guido, Introduction to Machine Learning with Python, J. Steppan (MNIST image)]

Supervised Learning



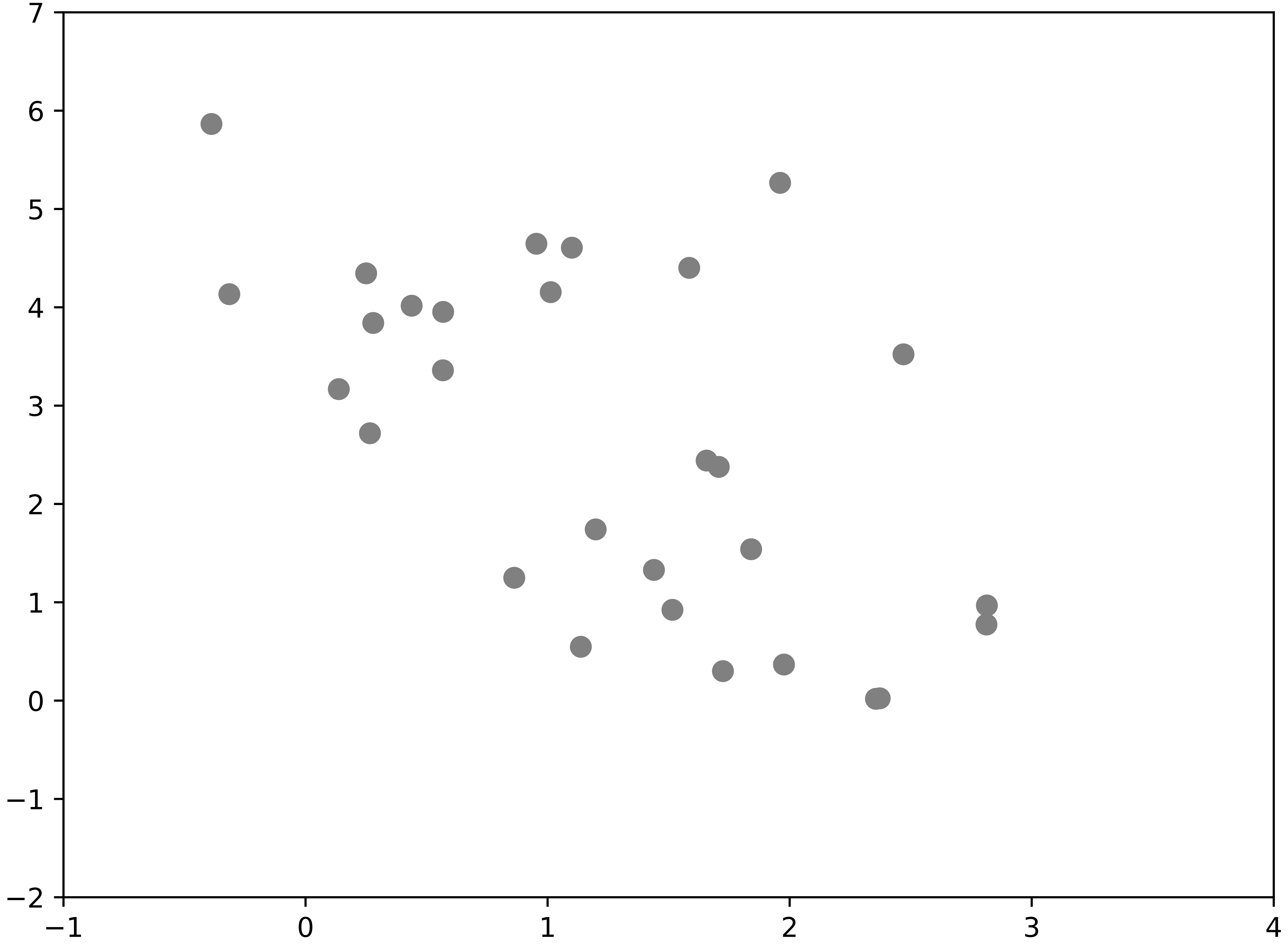
[J. VanderPlas]

Supervised Learning: Learned Algorithm (Fit)



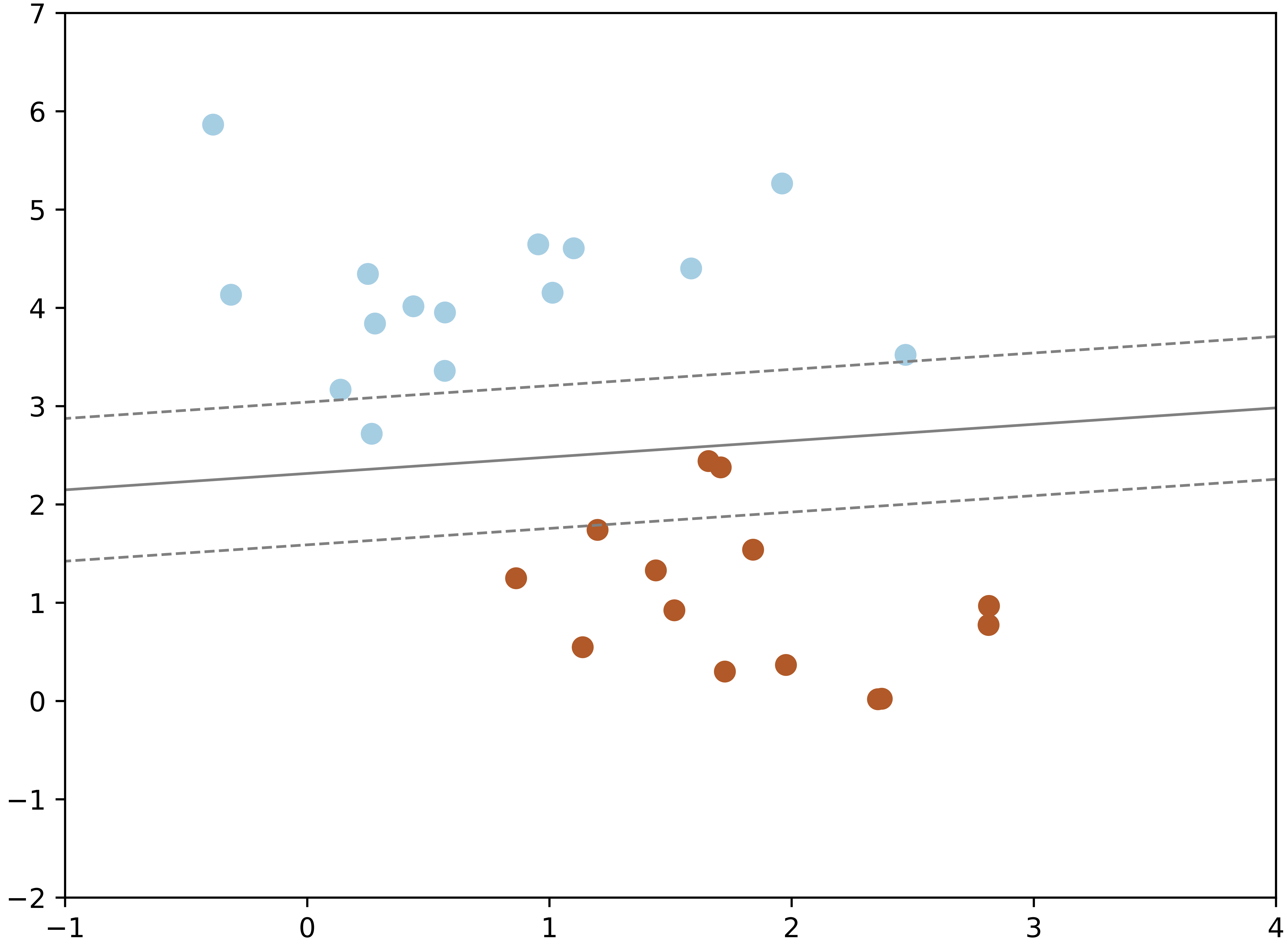
[J. VanderPlas]

Supervised Learning: Prediction



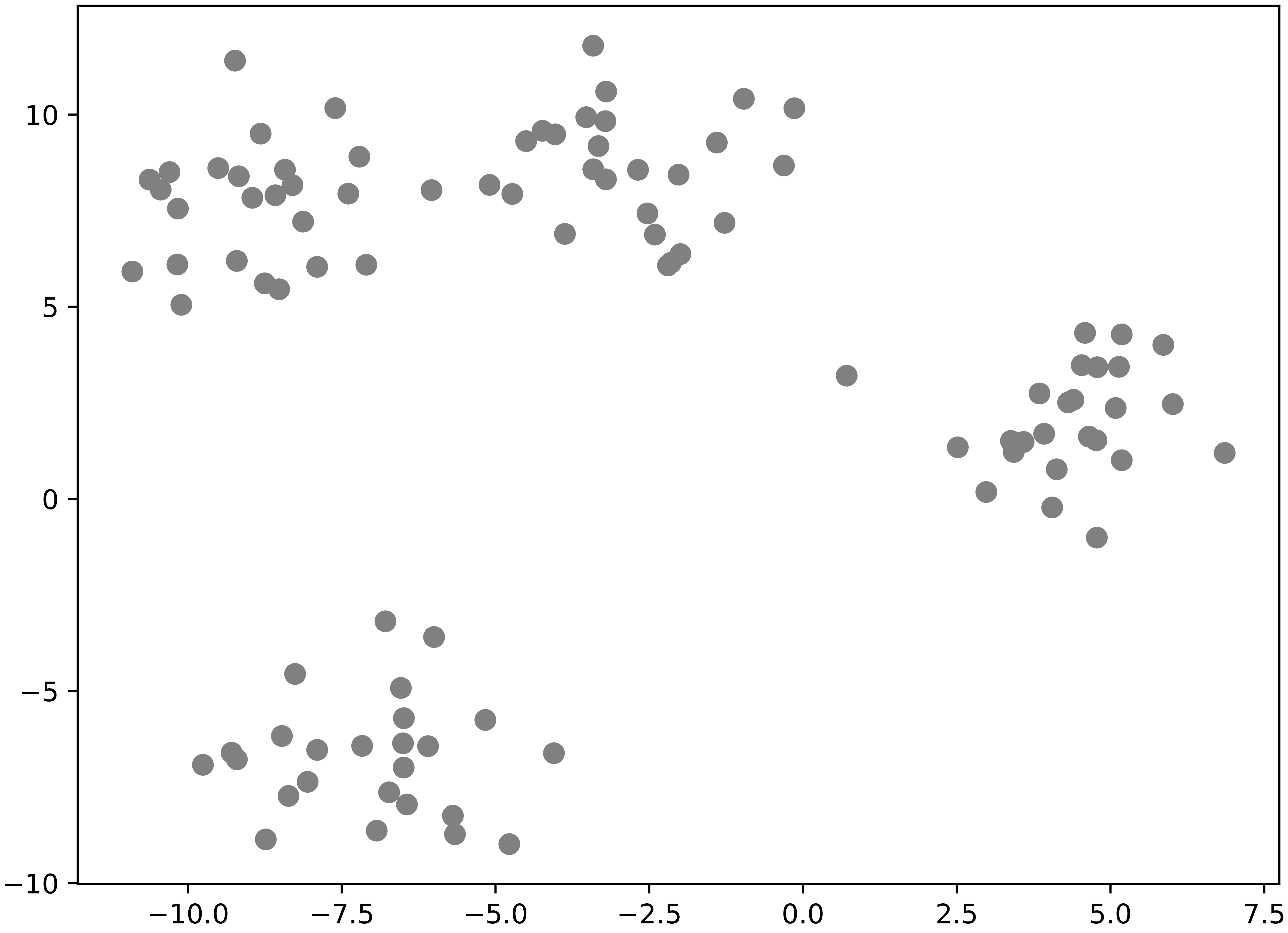
[J. VanderPlas]

Supervised Learning: Prediction



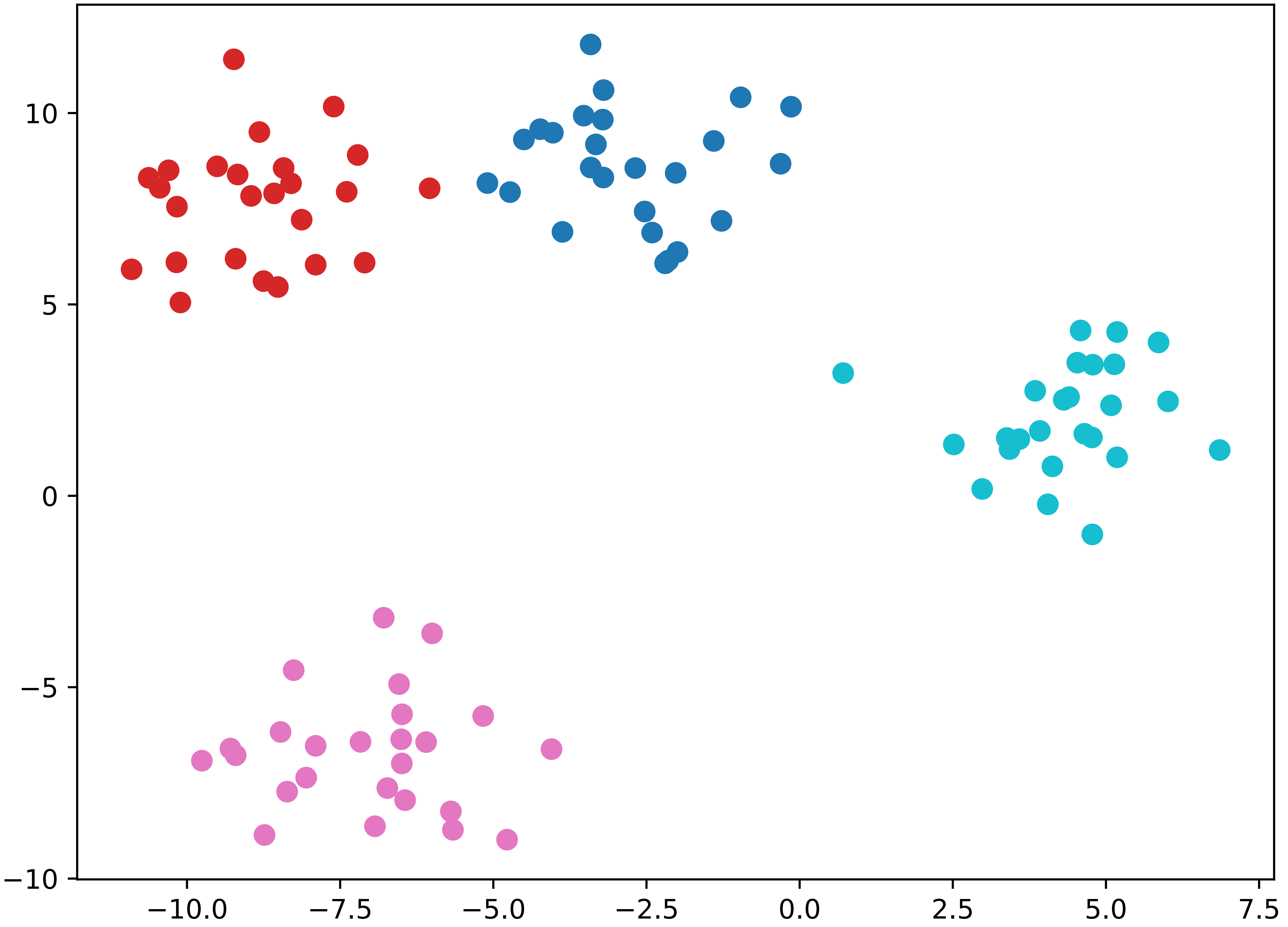
[J. VanderPlas]

Unsupervised Learning: Input



[J. VanderPlas]

Unsupervised Learning: Output



[J. VanderPlas]

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]

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

[L. Buitinck et al.]

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 vis `transform` method
  - Can combine `fit` and `transform` via `fit_transform`

[L. Buitinck et al.]

Penguin Example

scikit-learn Template

1. Choose model class
2. Instantiate model
3. Fit model to data
4. Predict on new data

```
from sklearn.naive_bayes import GaussianNB
model = GaussianNB()
model.fit(Xtrain, ytrain)
y_model = model.predict(Xtest)
```

5. (Check accuracy)

```
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