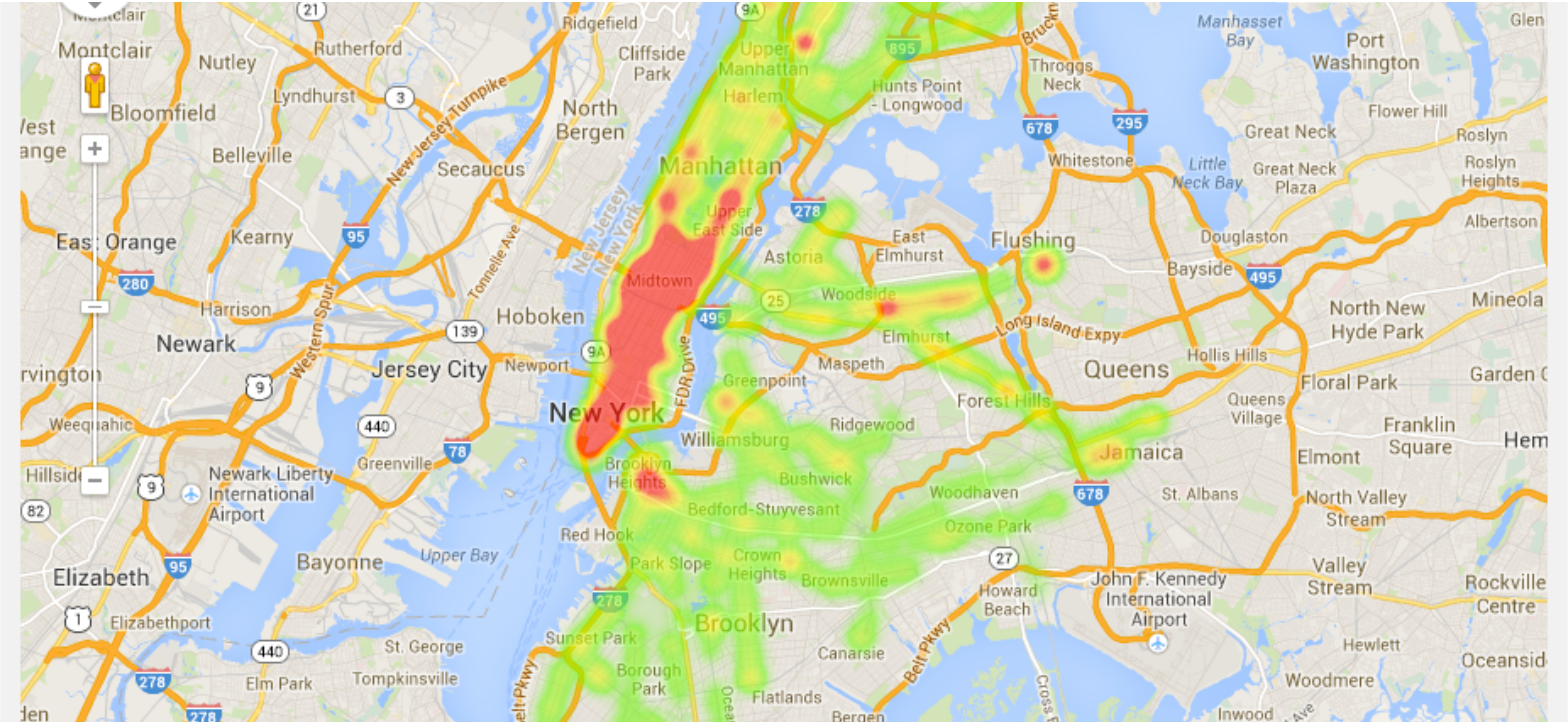
Programming Principles in Python (CSCI 503/490)

Visualization & Machine Learning

Dr. David Koop

Exploring Data through Visualization



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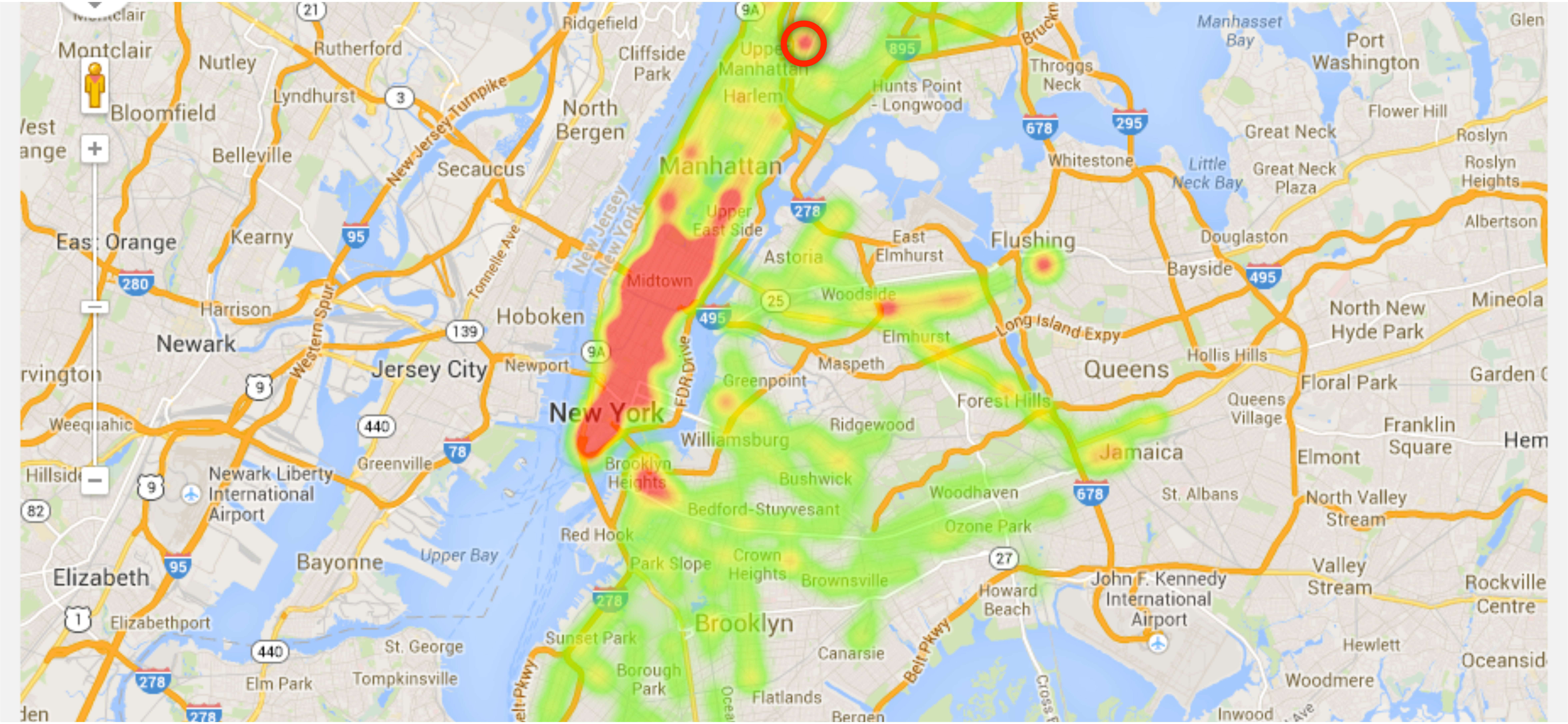
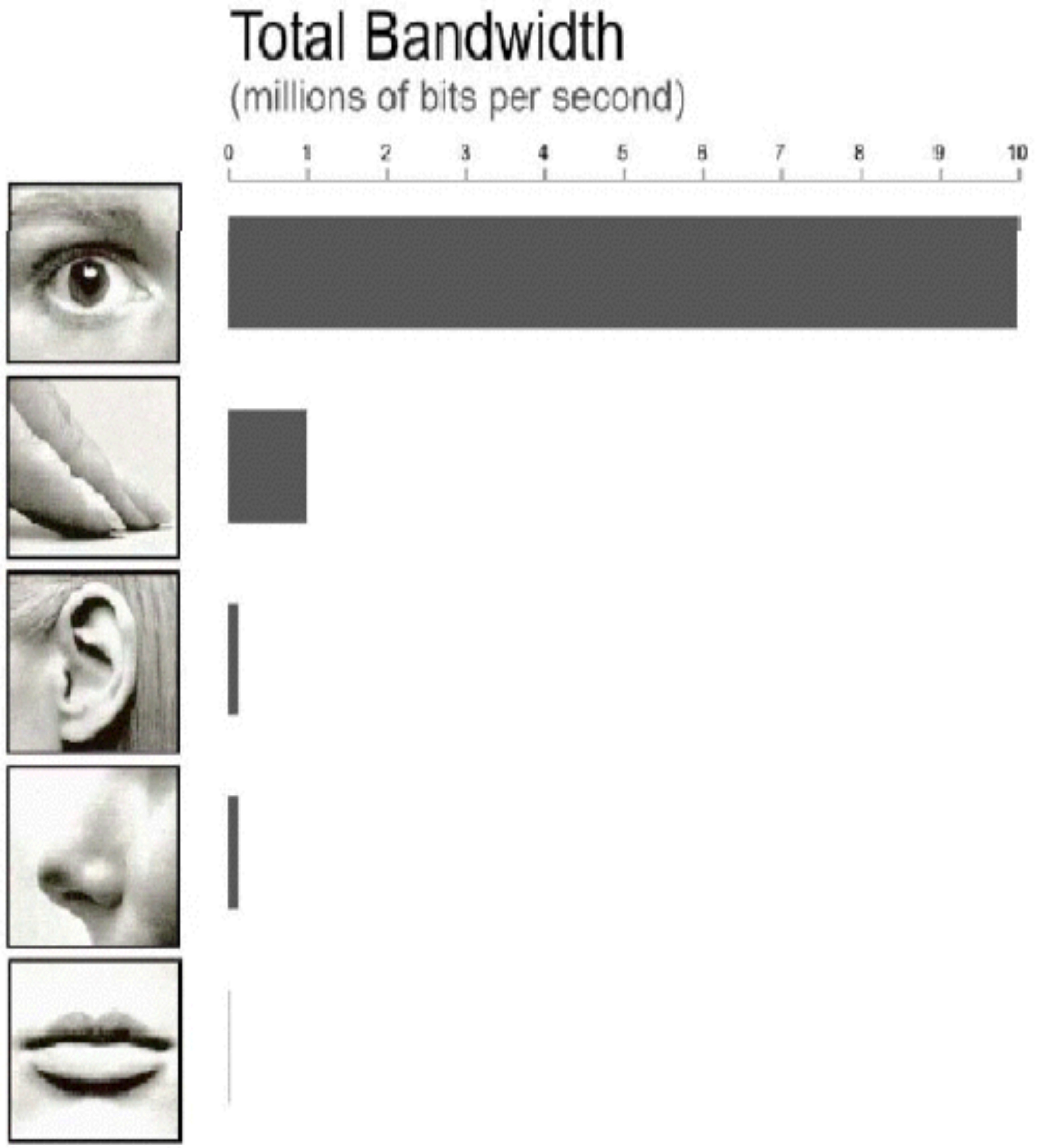
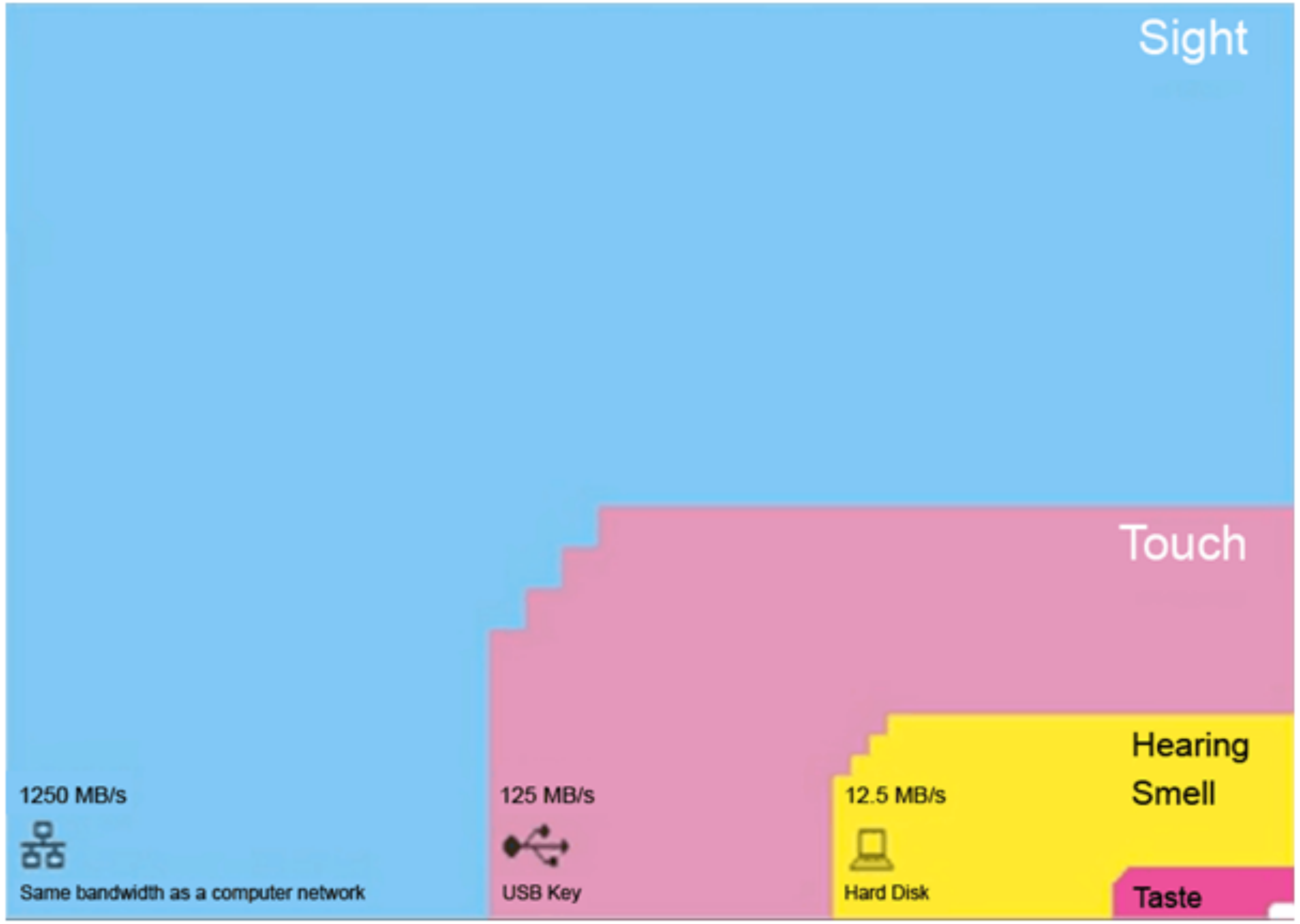


Why do we visualize data?





[via A. Lex]

[T. Nørretranders]

Why Visual?

I		II		III		IV	
x	y	x	y	x	y	x	y
10.0	8.04	10.0	9.14	10.0	7.46	8.0	6.58
8.0	6.95	8.0	8.14	8.0	6.77	8.0	5.76
13.0	7.58	13.0	8.74	13.0	12.74	8.0	7.71
9.0	8.81	9.0	8.77	9.0	7.11	8.0	8.84
11.0	8.33	11.0	9.26	11.0	7.81	8.0	8.47
14.0	9.96	14.0	8.10	14.0	8.84	8.0	7.04
6.0	7.24	6.0	6.13	6.0	6.08	8.0	5.25
4.0	4.26	4.0	3.10	4.0	5.39	19.0	12.50
12.0	10.84	12.0	9.13	12.0	8.15	8.0	5.56
7.0	4.82	7.0	7.26	7.0	6.42	8.0	7.91
5.0	5.68	5.0	4.74	5.0	5.73	8.0	6.89

[F. J. Anscombe]

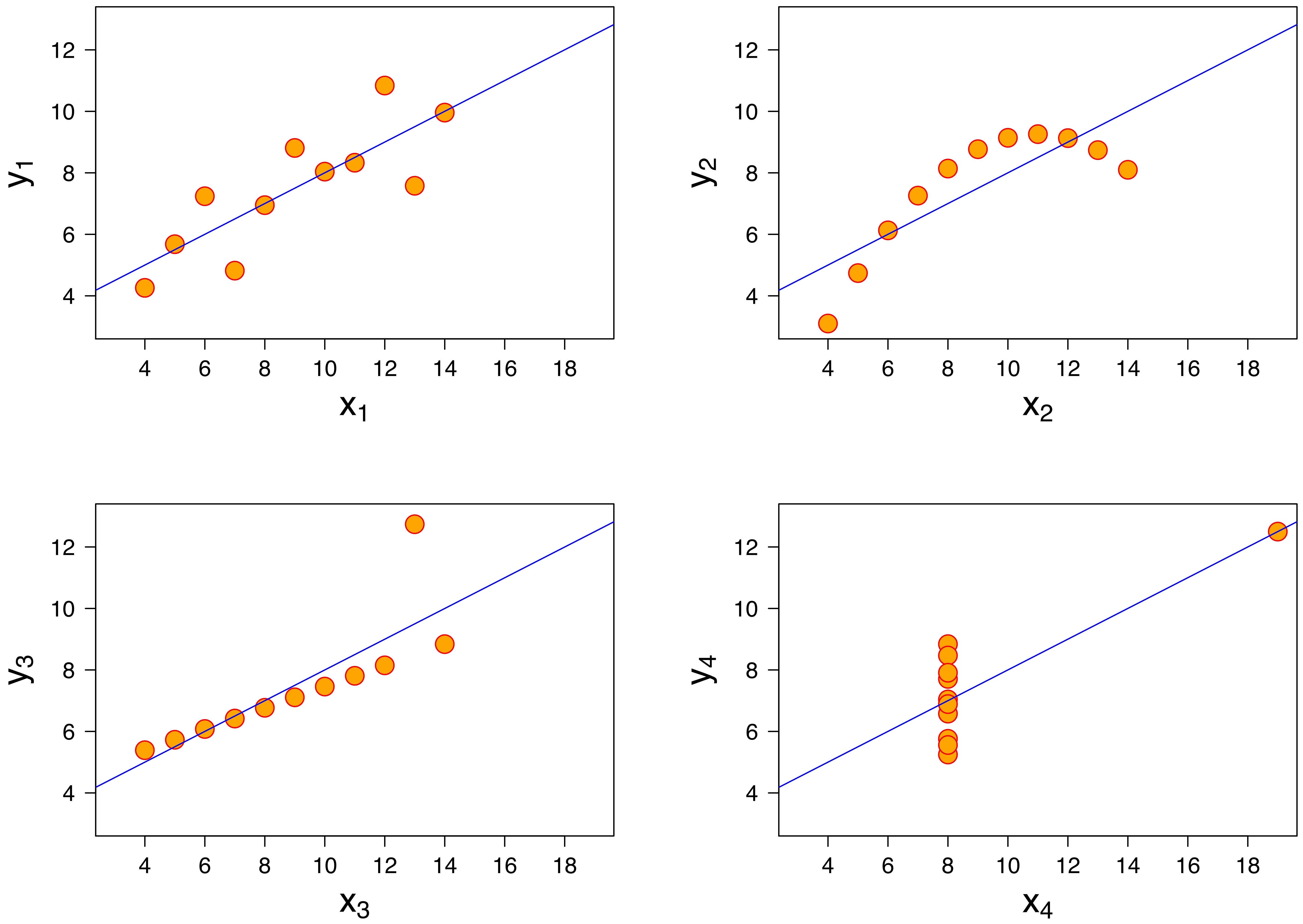
Why Visual?

I		II		III		IV	
x	y	x	y	x	y	x	y
10.0	8.04	10.0	9.14	10.0	7.46	8.0	6.58
8.0	6.95	8.0	8.14	8.0	6.77	8.0	5.76
13.0	7.58	13.0	8.74	13.0	12.74	8.0	7.71
9.0	8.81	9.0	8.77	9.0	7.11	8.0	8.84
11.0	8.33	11.0	9.26	11.0	7.81	8.0	8.47
14.0	9.96	14.0	8.10	14.0	8.84	8.0	7.04
6.0	7.24	6.0	6.13	6.0	6.08	8.0	5.25
4.0	4.26	4.0	3.10	4.0	5.39	19.0	12.50
12.0	10.84	12.0	9.13	12.0	8.15	8.0	5.56
7.0	4.82	7.0	7.26	7.0	6.42	8.0	7.91
5.0	5.68	5.0	4.74	5.0	5.73	8.0	6.89

Mean of x	9
Variance of x	11
Mean of y	7.50
Variance of y	4.122
Correlation	0.816

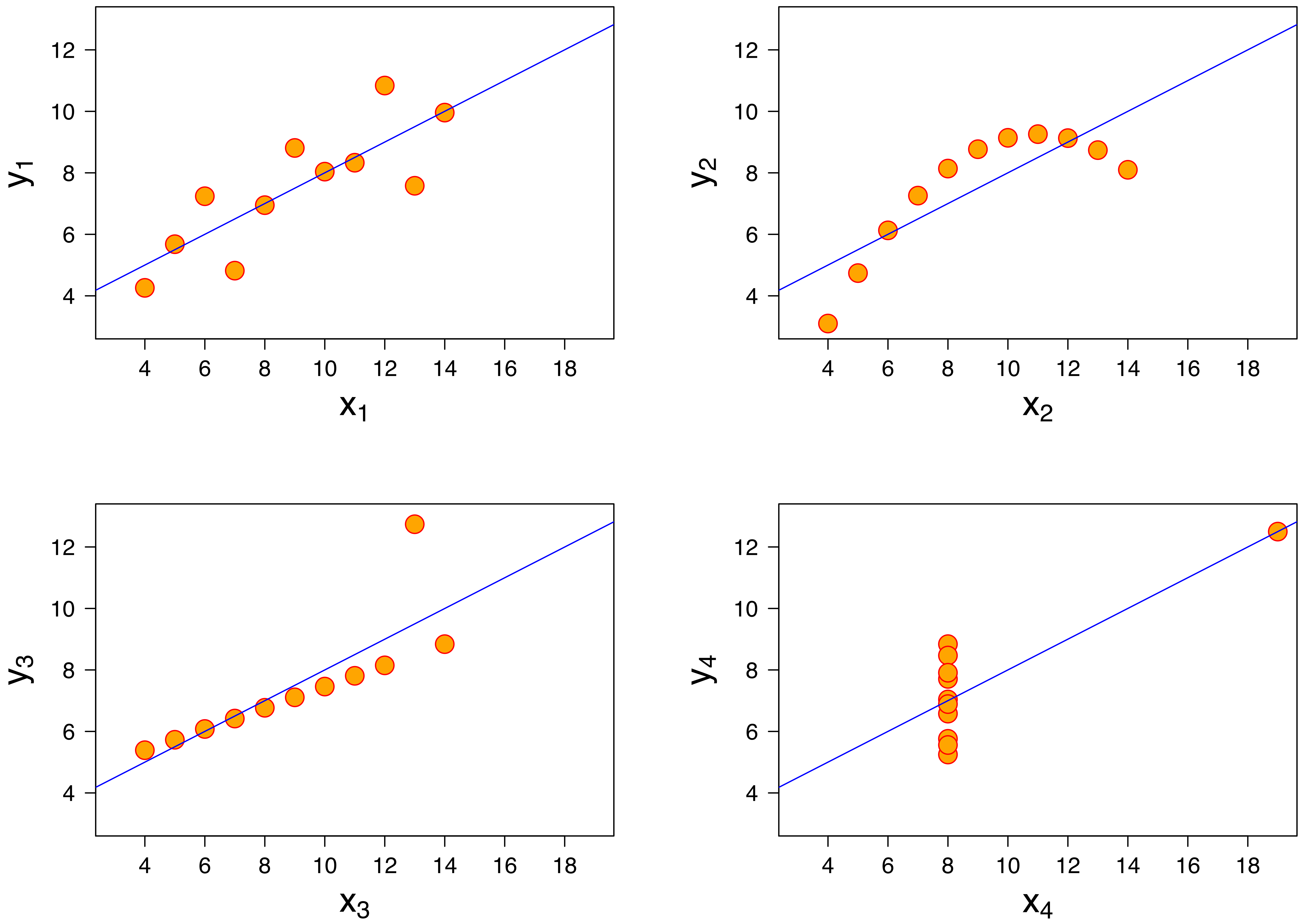
[F. J. Anscombe]

Why Visual?



[F. J. Anscombe]

Why Visual?



Mean of x	9
Variance of x	11
Mean of y	7.50
Variance of y	4.122
Correlation	0.816

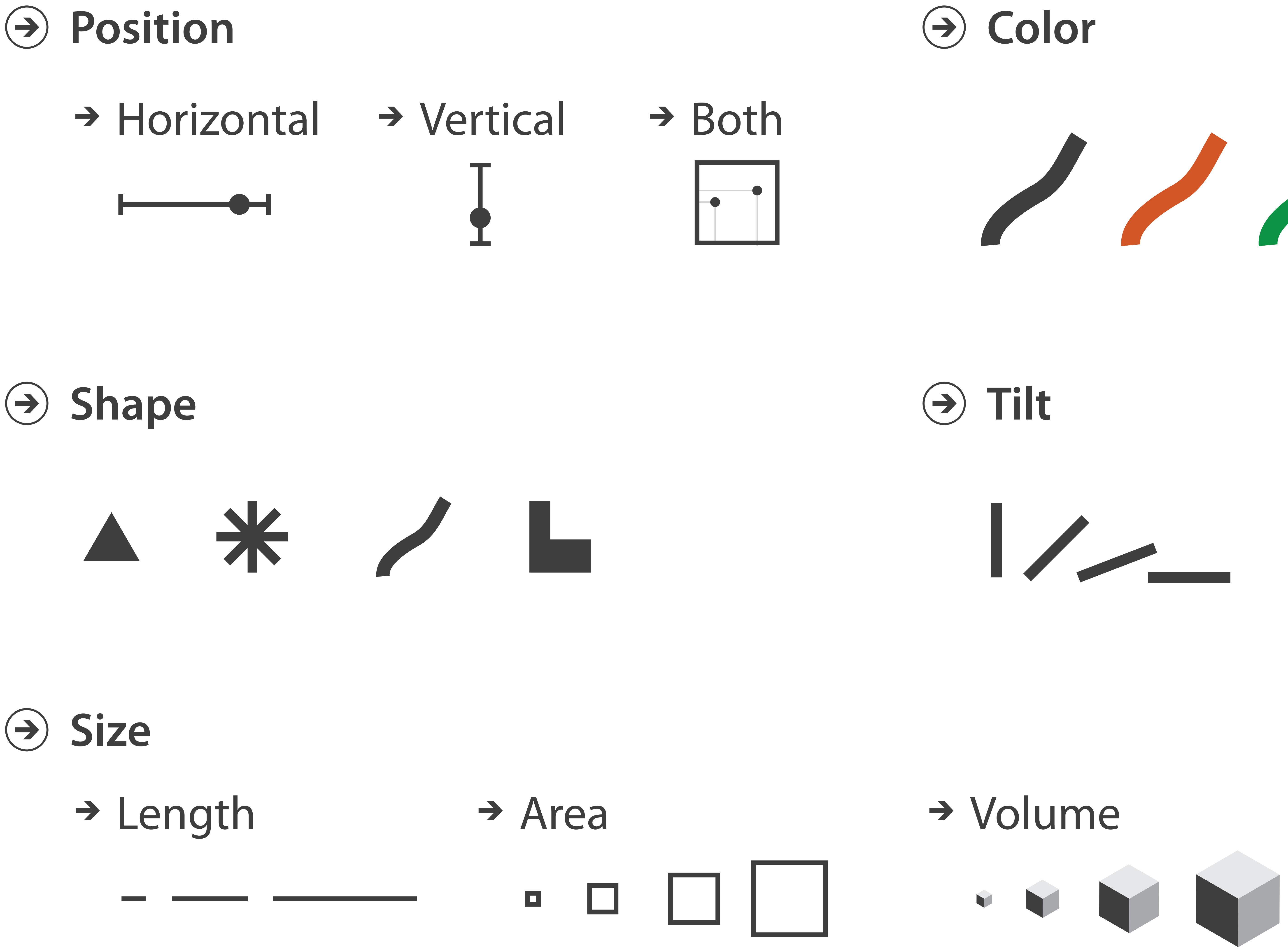
[F. J. Anscombe]

Visualization Goals

- "The purpose of visualization is **insight**, not pictures" – B. Schneiderman

- Identify patterns, trends
- Spot outliers
- Find similarities, correlation

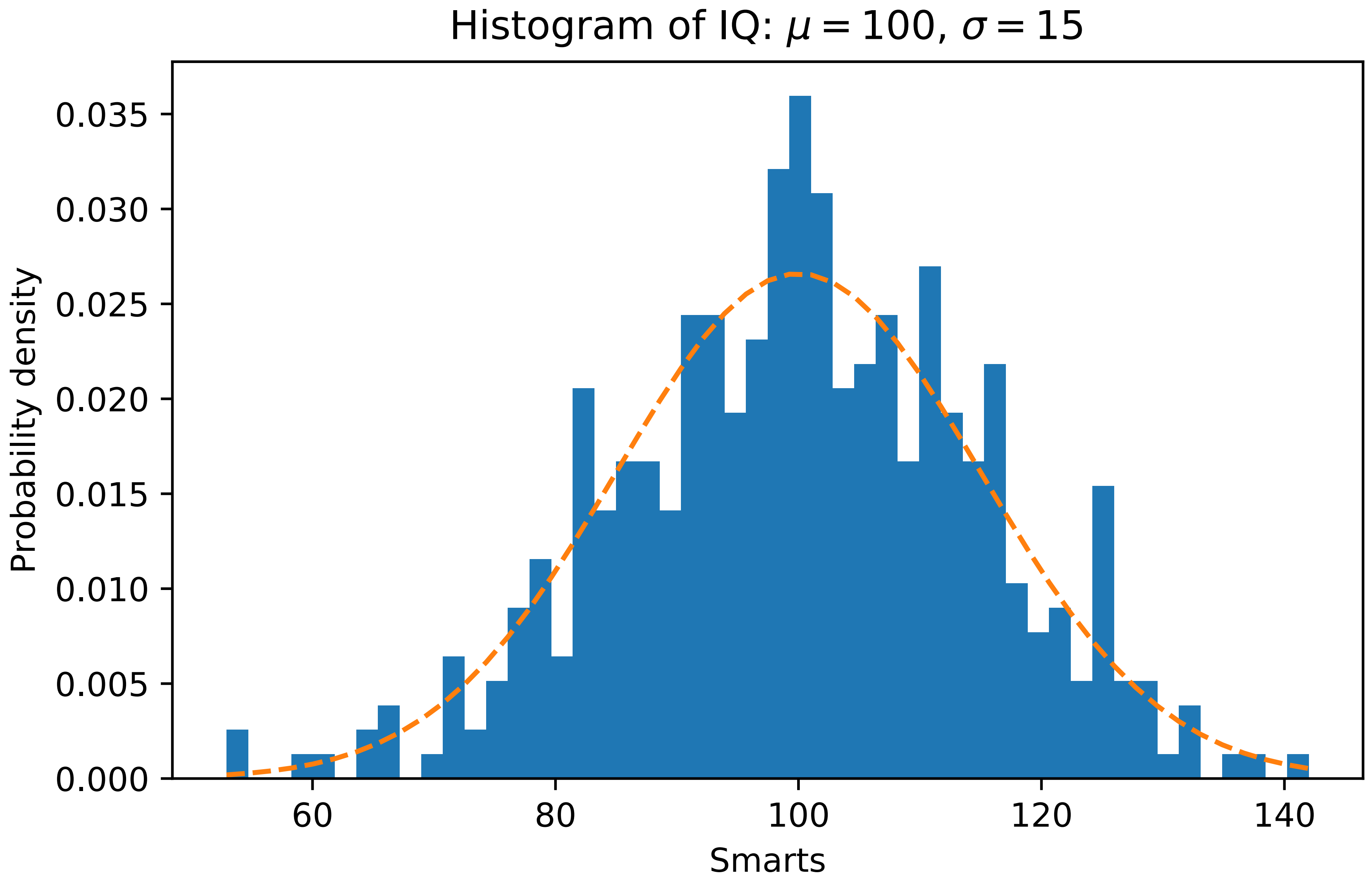
Data is Encoded via Visual Channels



[Munzner (ill. Maguire), 2014]

matplotlib

- Strengths:
  - Designed like Matlab
  - Many rendering backends
  - Can reproduce almost any plot
  - Proven, well-tested
- Weaknesses:
  - API is imperative
  - Not originally designed for the web
  - Dated styles



pandas Integration

- Can call many of these methods directly from pandas
- Handled through `kind` kwarg or `.plot` accessor
- It will try to guess a reasonable visualization, but may fail:
  - `fruit.plot()`
- Instead, specify x and y and other parameters:
  - `fruit.plot(kind='bar',x='name',y='price')`
  - `plt.bar(x='name',height='price',data=fruit) # SIMILAR`
  - `fruit.plot.scatter(x='price',y='count',c='name') # ERROR`
  -
    ```
    colors = {'Apple': 'red','Orange': 'orange',
              'Banana': 'yellow','Pear': 'green'}
    fruit.plot.scatter(x='price',y='count',
                       c=fruit['name'].map(colors))
    ```

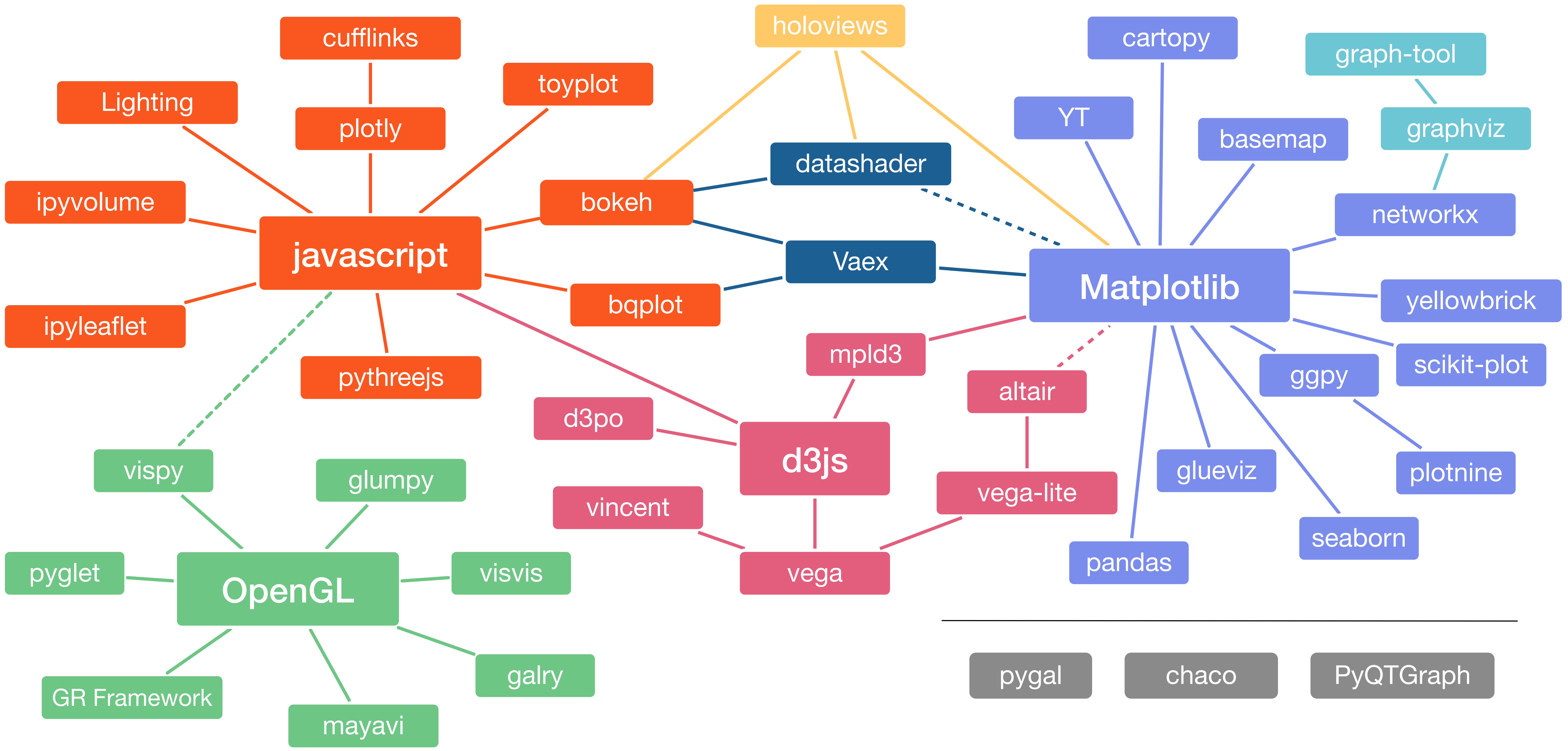
Assignment 8

- Due Friday
- Data and Visualization
- Port of Entry Data
- Part 1a: Month includes Year—the whole Data column (e.g. Jan 2022)

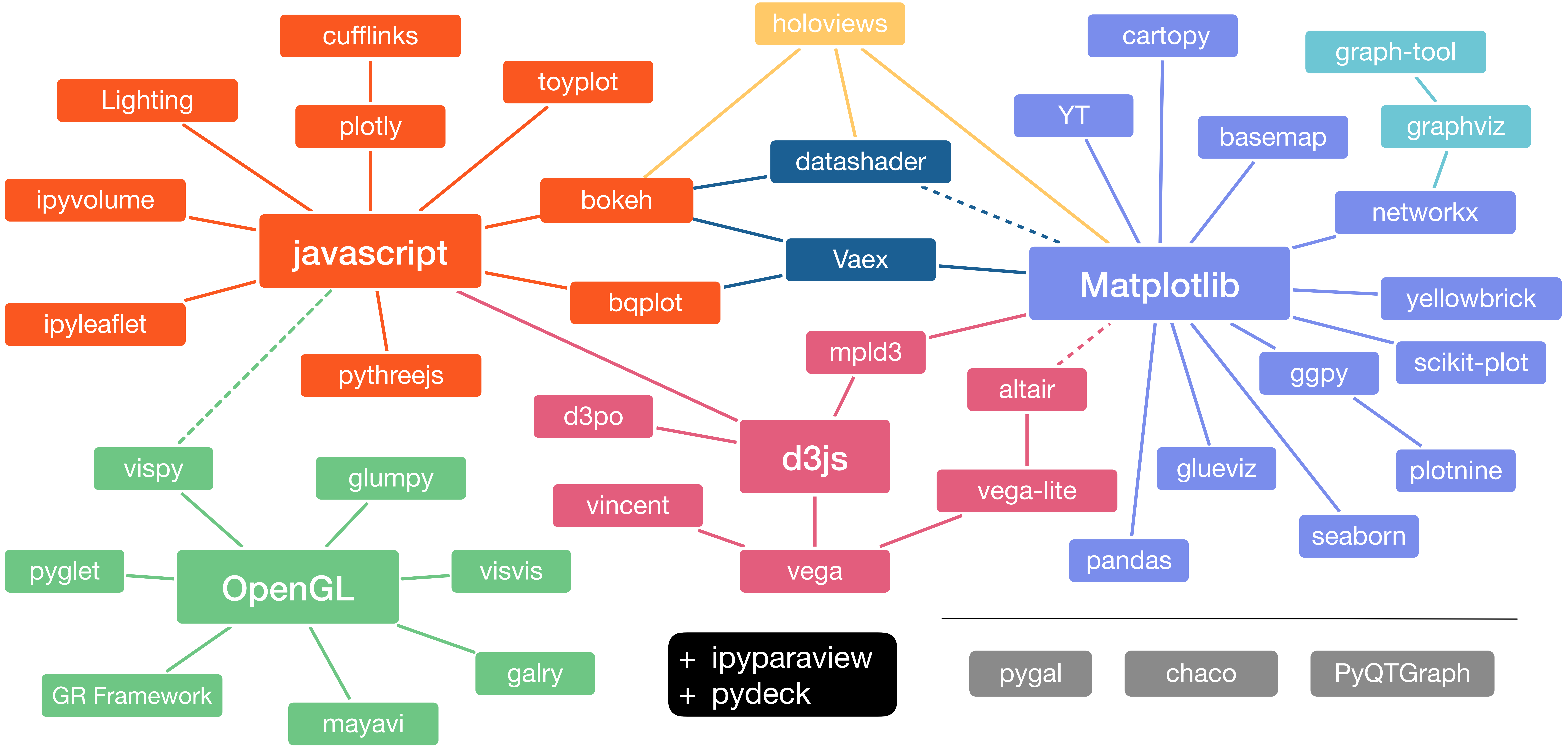
Final Exam

- Tuesday, December 6, **12:00**-1:50pm in PM 253
- **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

The Python Visualization Landscape



The Python Visualization Landscape



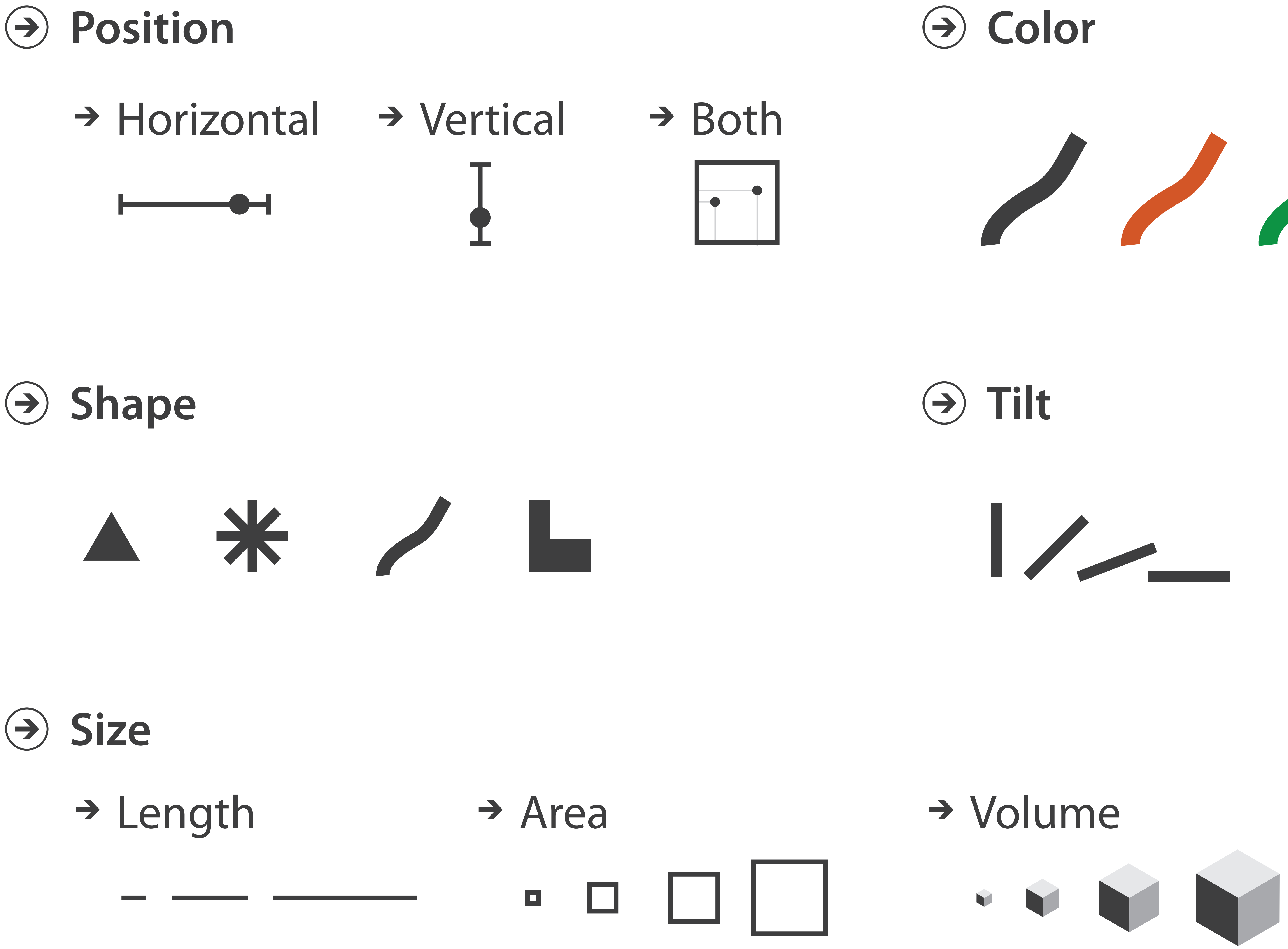
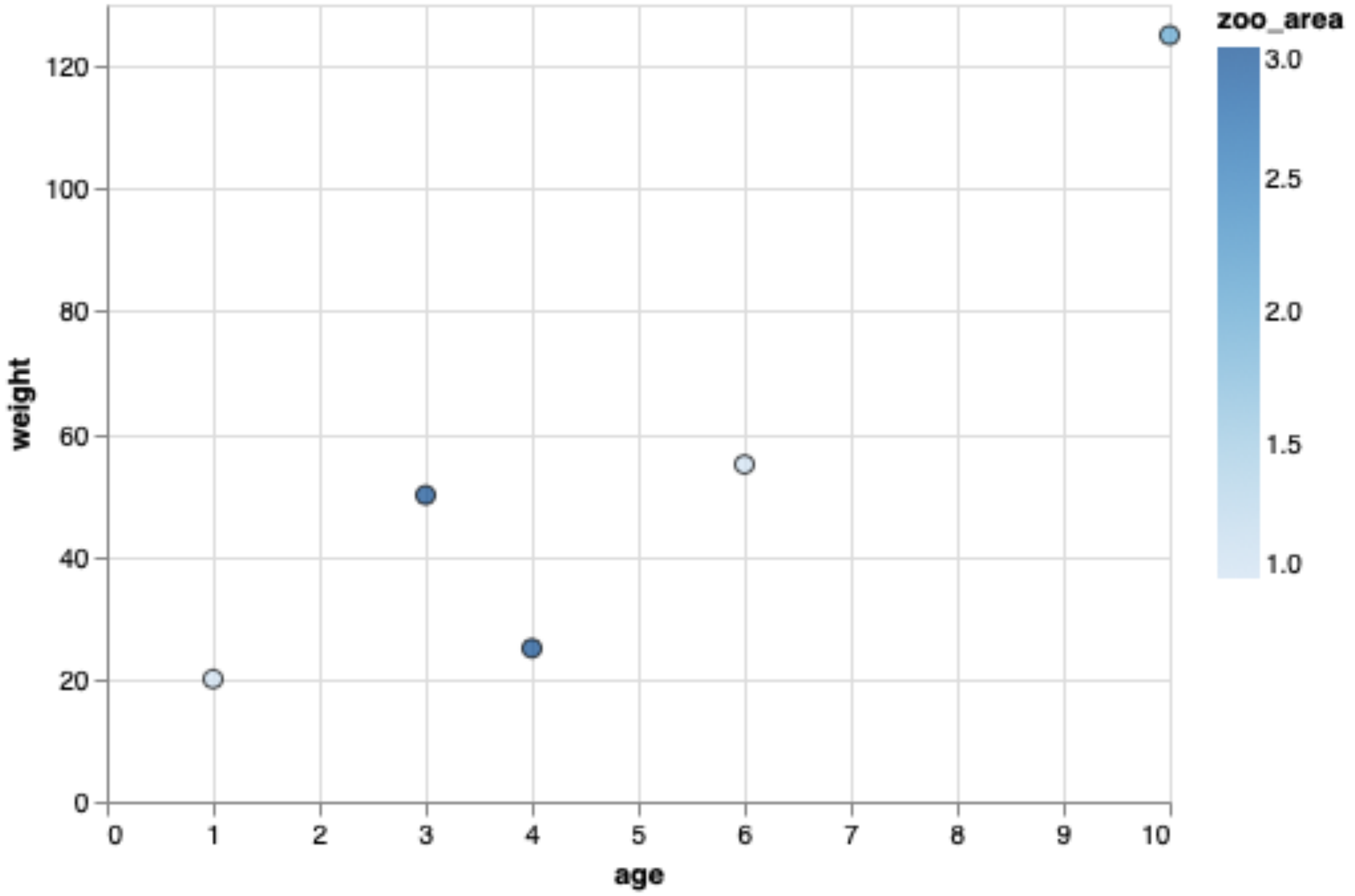
History of Vega-Lite & Altair

- "Grammar of Graphics", L. Wilkinson
- "A Layered Grammar of Graphics", H. Wickham
- ggplot: plotting library for R
- Vega: similar idea for Javascript/JSON (U. Washington, A. Satyanarayan)
  - "Declarative language for creating, saving, and sharing interactive visualization designs"
  - More focus on interaction and reactive signals
  - Separation between specification and runtime
- Vega-Lite: higher-level language than Vega (U. Washington, D. Moritz)
  - uses carefully designed rules to default settings

History of Vega-Lite & Altair

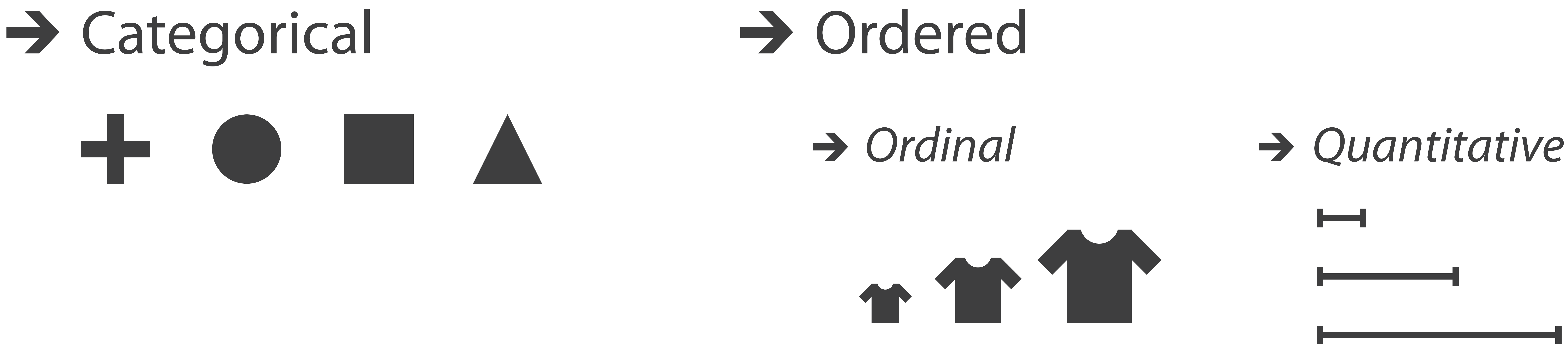
- Altair: Python interface to Vega-Lite (J. VanderPlas)
  - "spend more time understanding your data and its meaning"
  - Specify the what, minimize the amount of code directing the how
  - Python can write JSON specification just as well as any other language
  - Bindings make it more Python-friendly, 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]

Easily Explore Different Encodings

- ```
  data = pd.DataFrame({
        'age': [1,3,4,6,10],
        'weight': [20,50,25,55,125],
        'zoo_area': [1,3,3,1,2],
        'num_scoops': [3,2,4,2,3]
  })
  alt.Chart(data).mark_point(
        filled=True, size=50,
        stroke='black',strokeWidth=1
  ).encode(
        x='age',
        y='weight',
        color='zoo_area'
  )
  ```


  ```

Problem: zoo_area is not a continuous value, nor is it ordered in any way!

Data Attributes and Altair Types



[Munzner (ill. Maguire), 2014]

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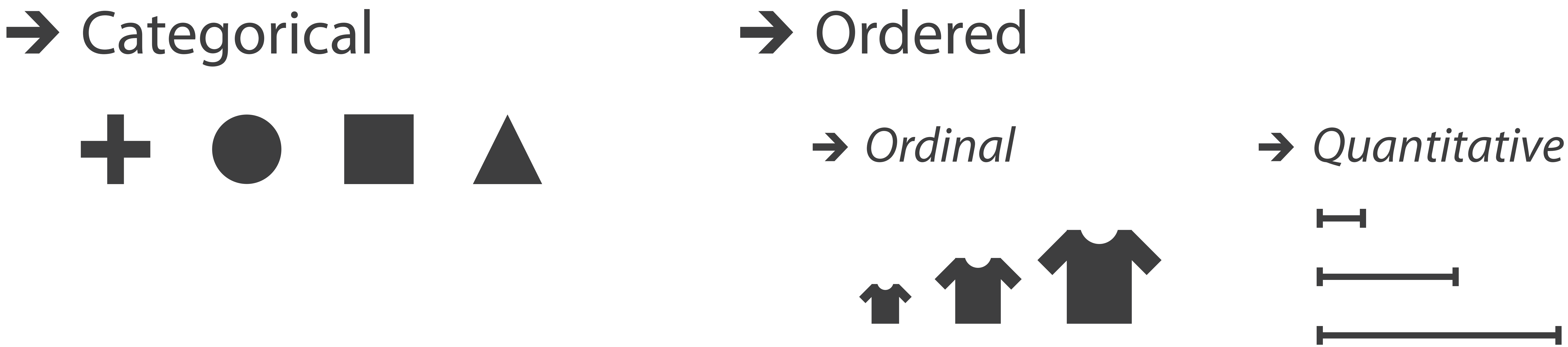
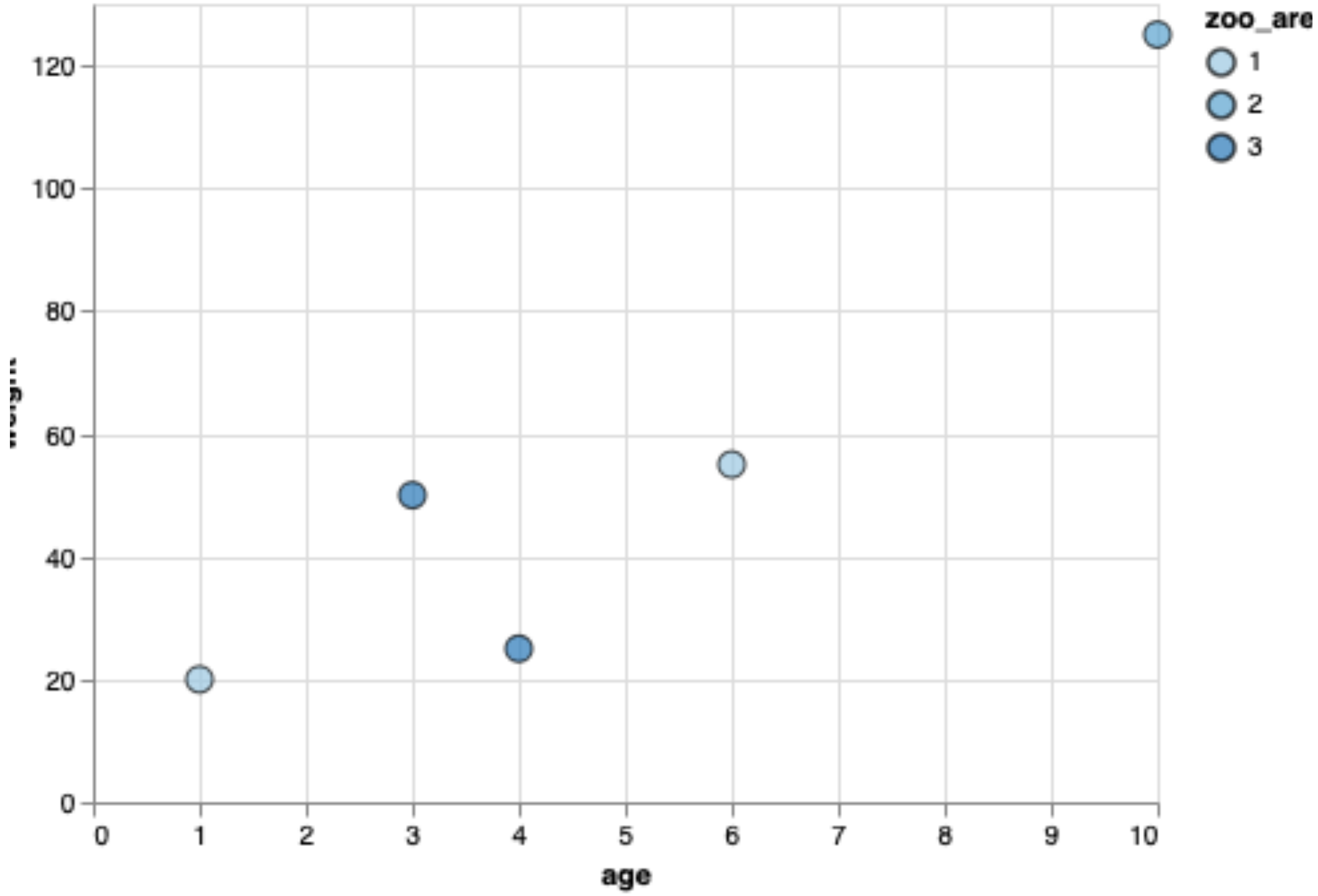


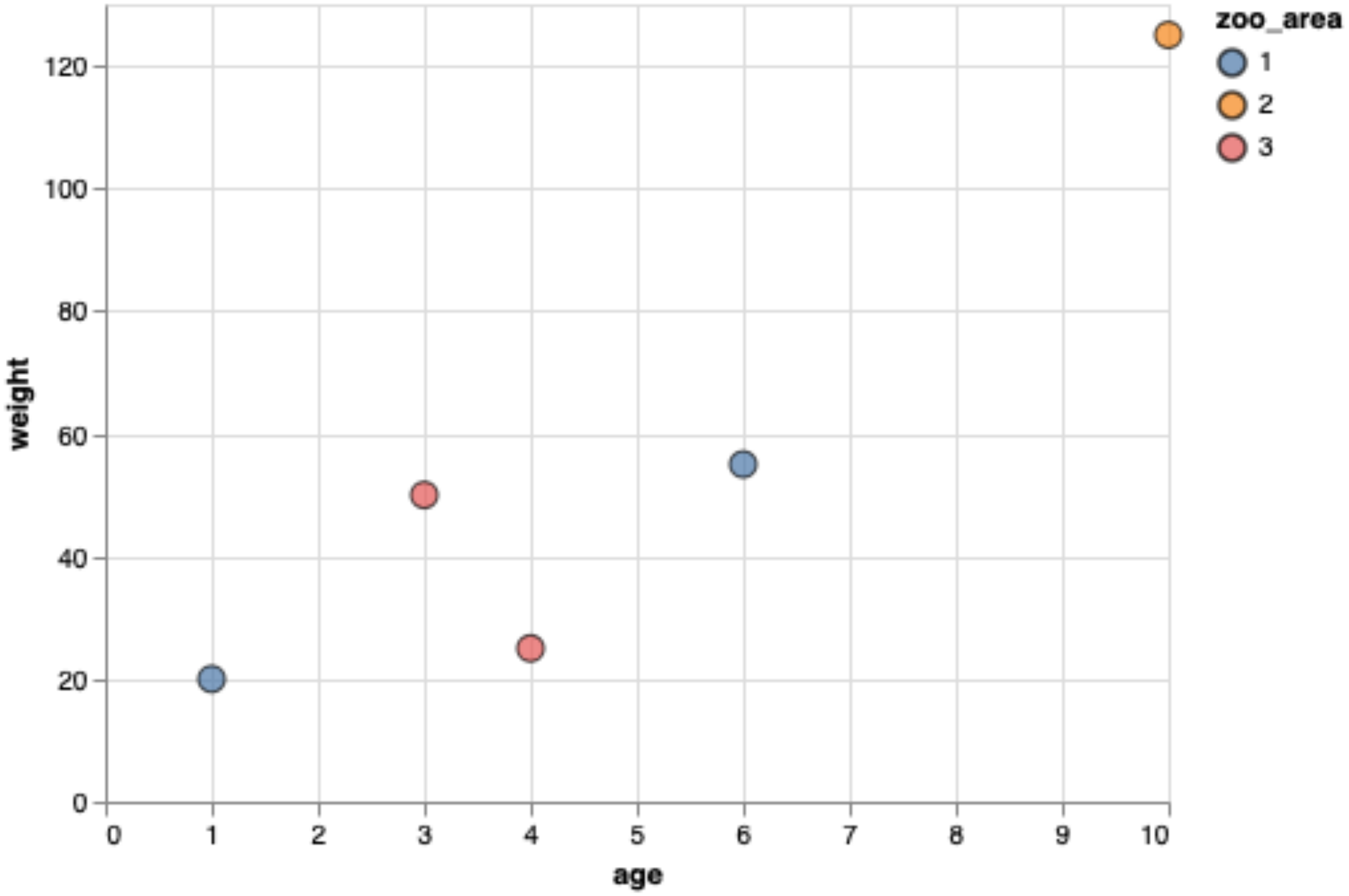
- Categorical data = Nominal (N)
- Ordinal data = Ordinal (O)
- Quantitative data = Quantitative (Q)
- Temporal data = Temporal (T)

[Munzner (ill. Maguire), 2014]

Specifying the Type

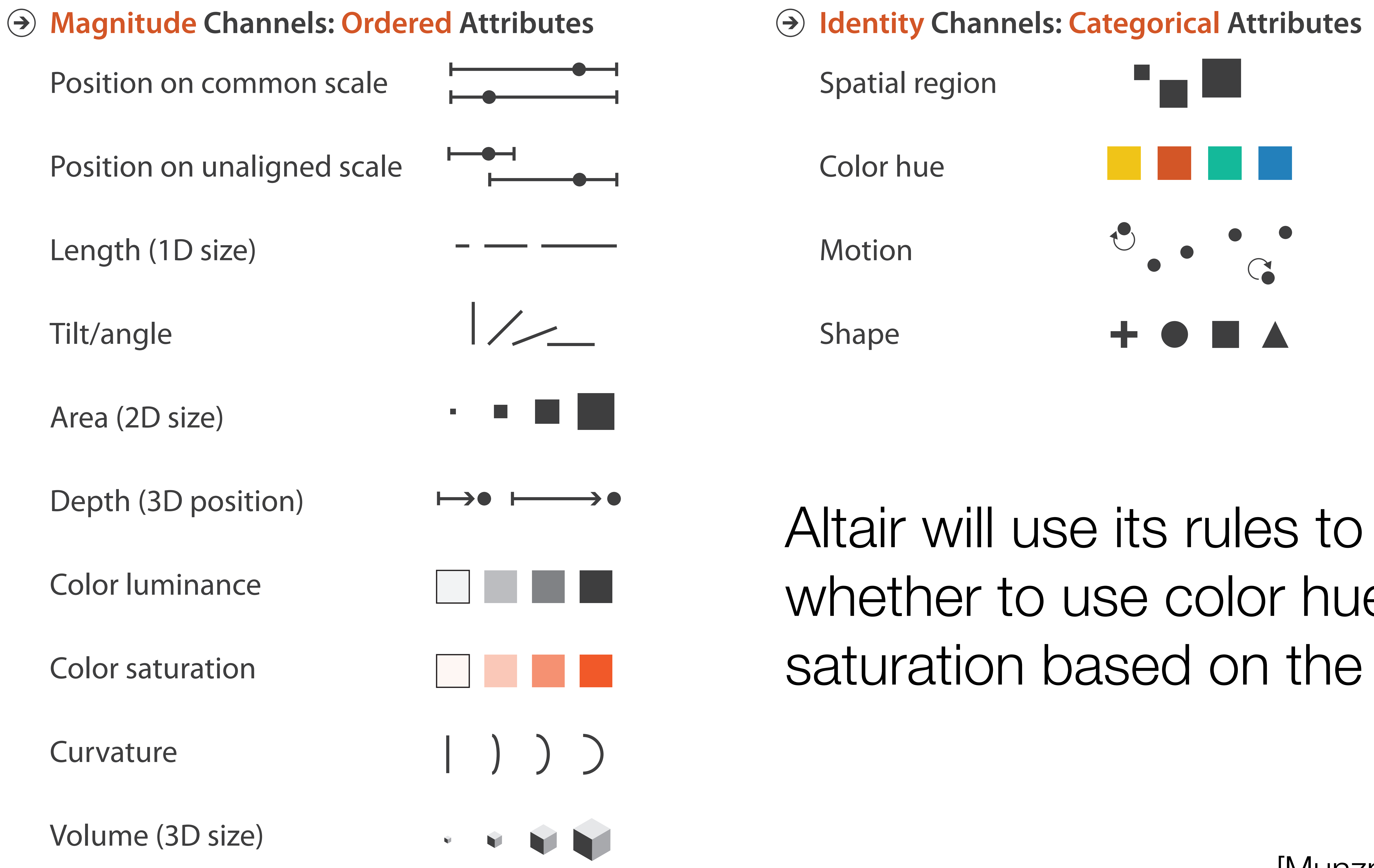


`zoo_area:O`



`zoo_area:N`

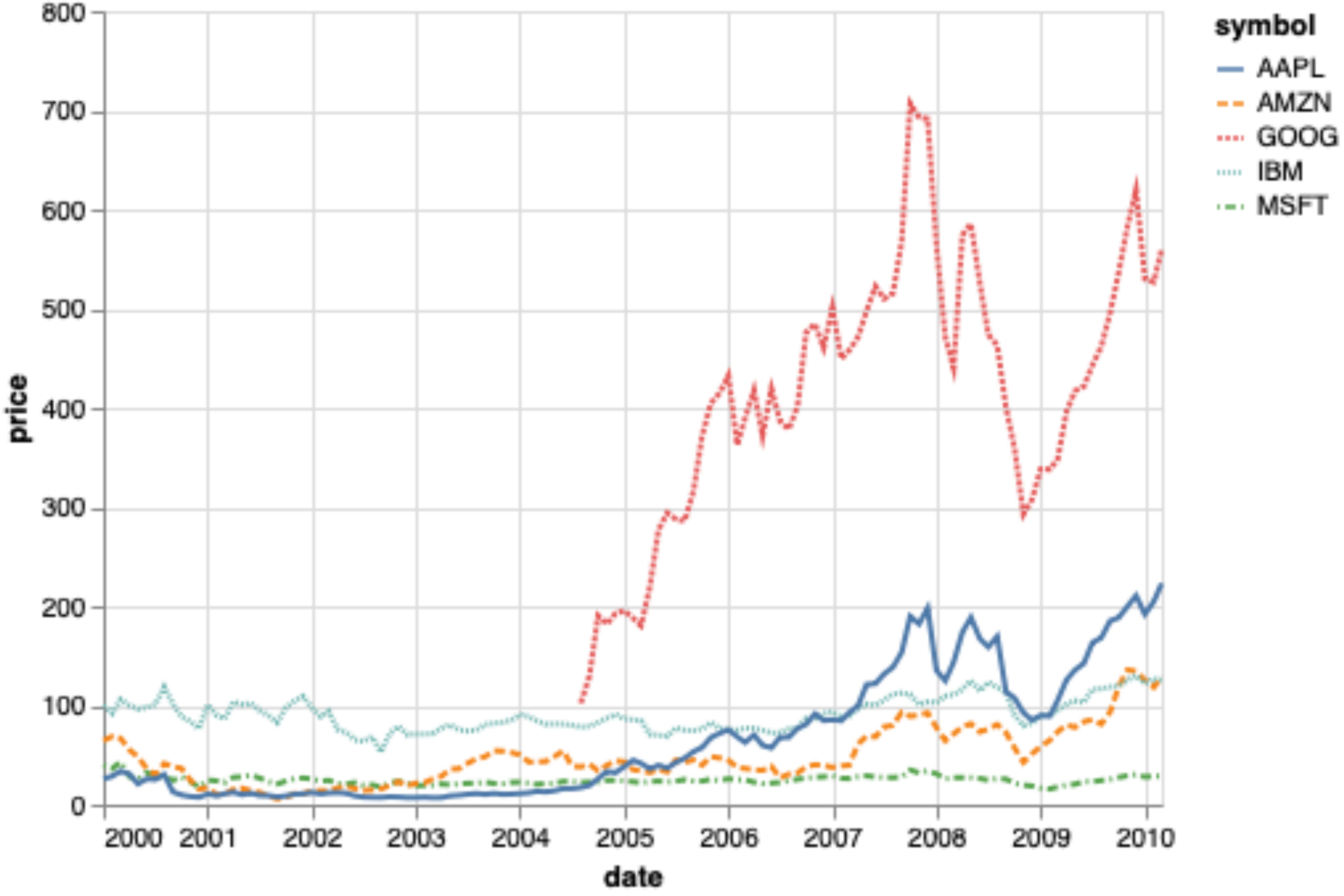
Different Channels for Different Attribute Types



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

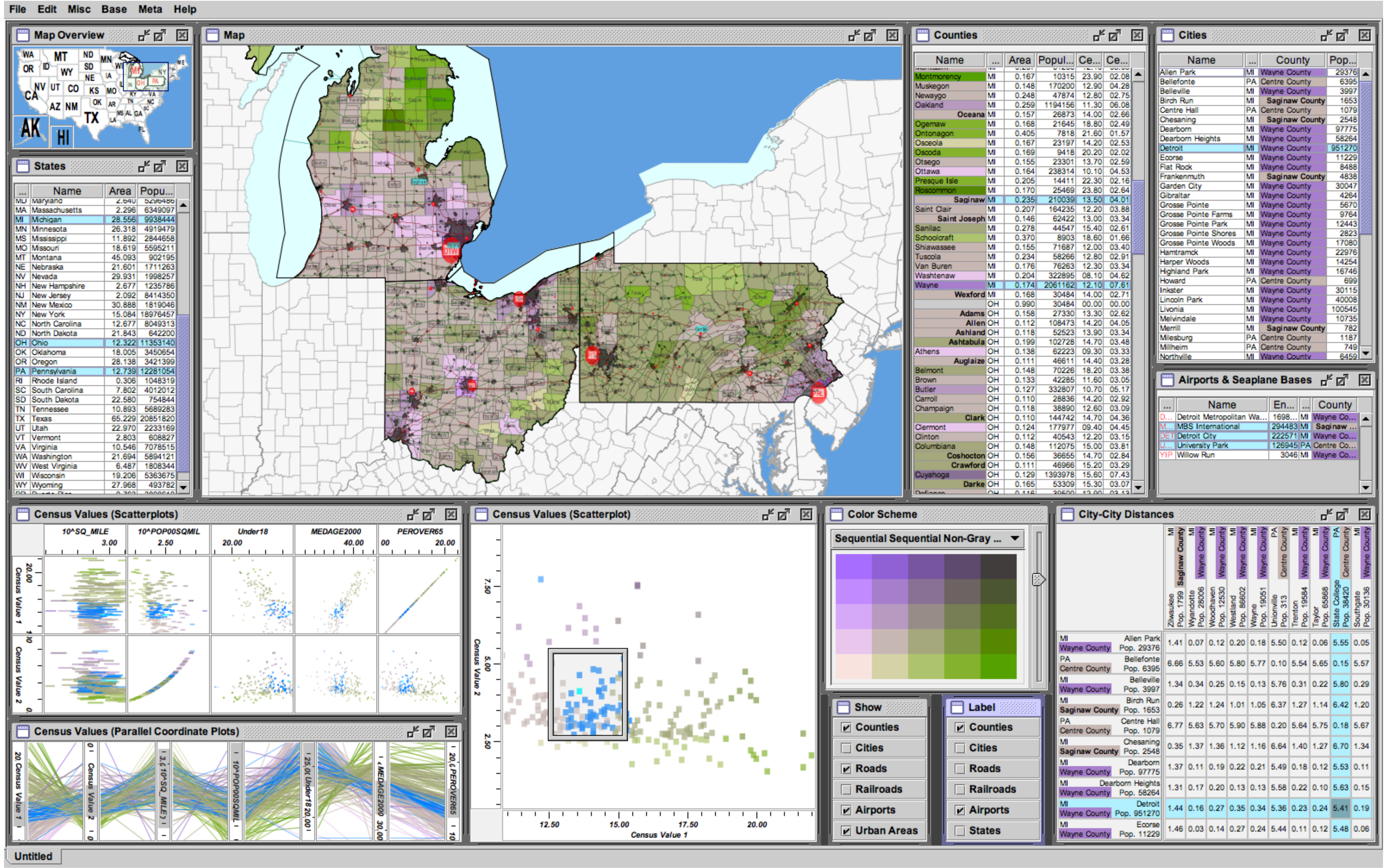
[Munzner (ill. Maguire), 2014]

Multiple Views in Visualization



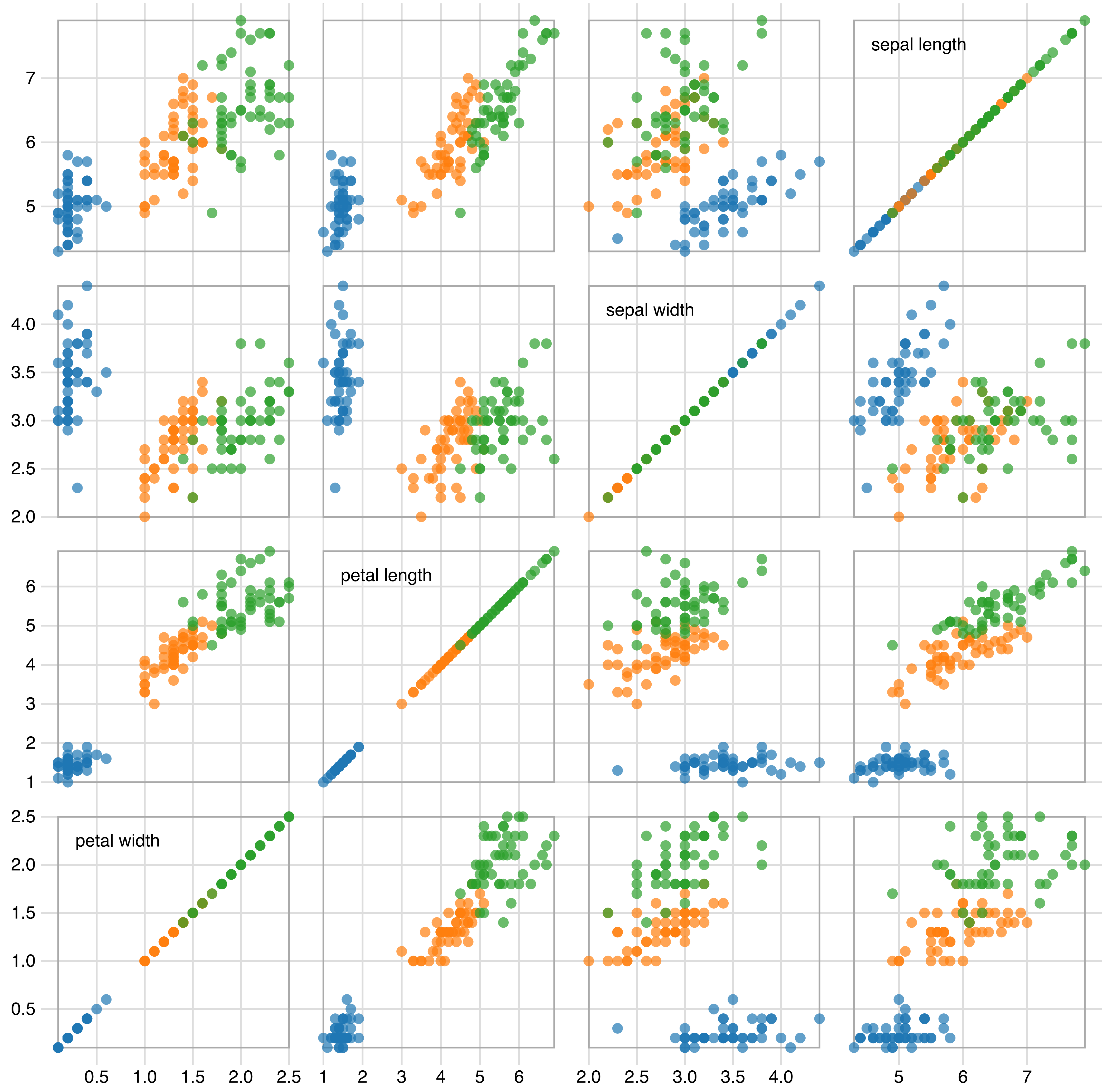
[Altair]

Multiple Views in Visualization



[Improvise, Weaver, 2004]

Multiple Views in Visualization

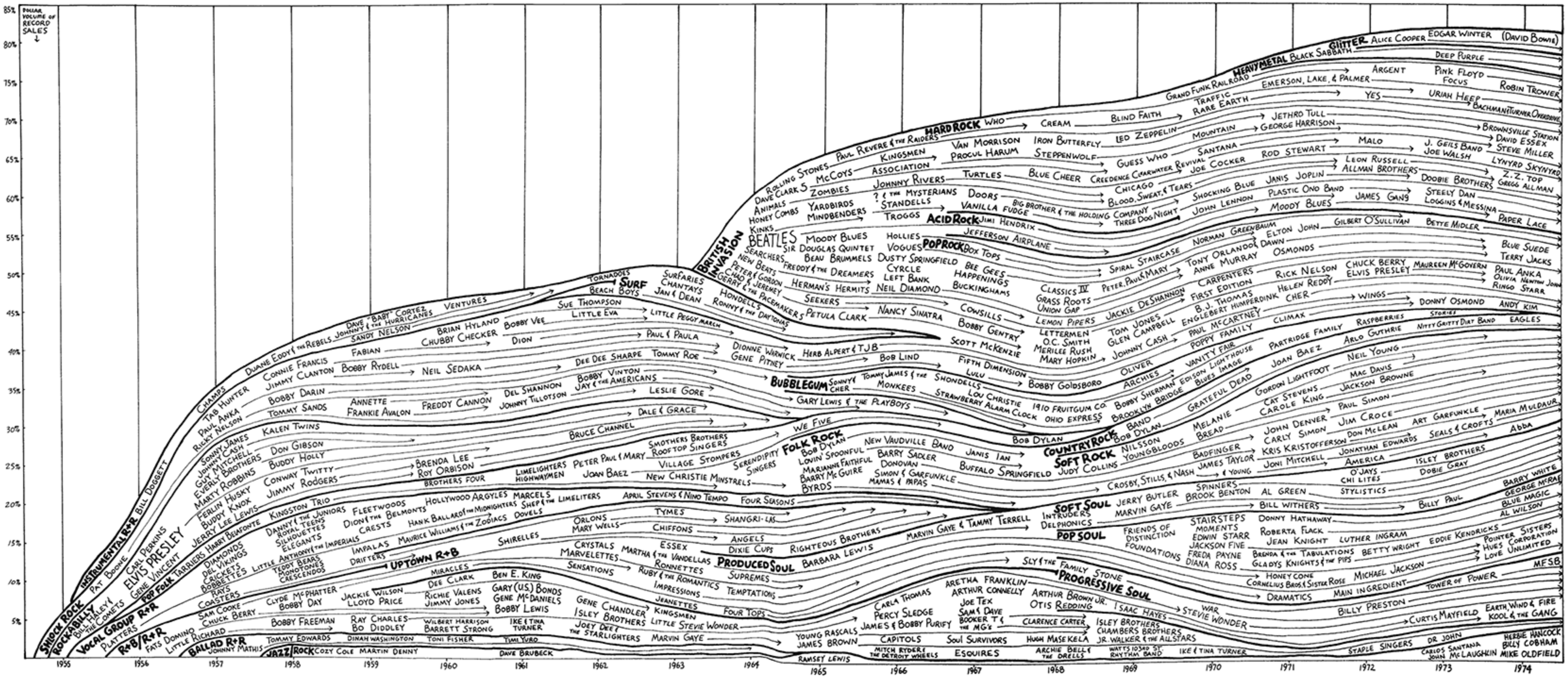


[M. Bostock]

Altair Supports Concatenation, Layering, & Repetition

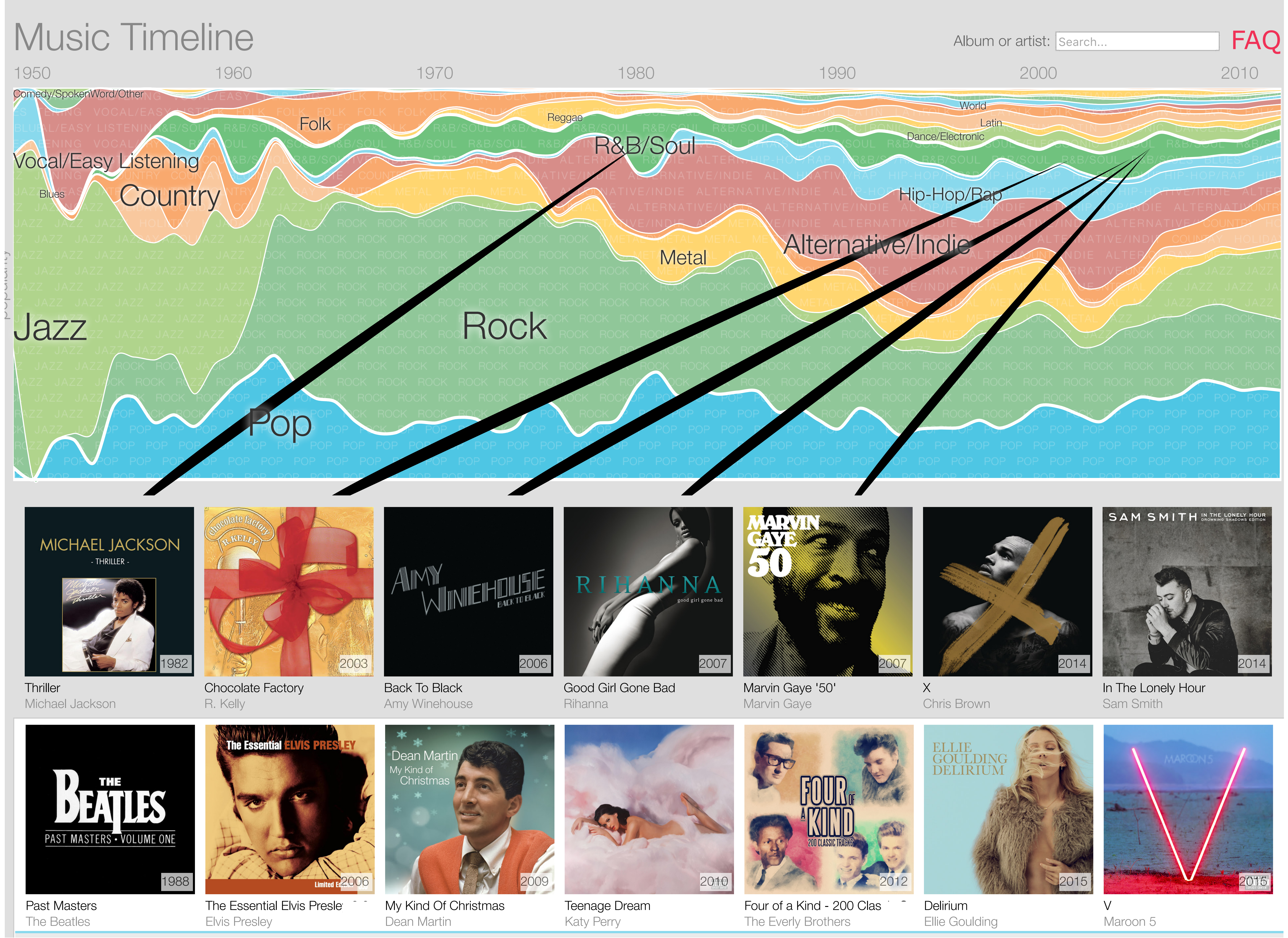
- Layering:
  - \+ Operator
- Concatenation:
  - Horizontal: | operator
  - Vertical: & operator
- Repetition
  - Use of .repeat for layout
  - Reference repeated variables in the encoding

Visualization



[Rock 'N' Roll is Here to Pay, R. Garofalo, 1977 (via Tufte)]

Also Visualization, but with Interaction



[Music Timeline, Google Research (no working version)]

Interaction

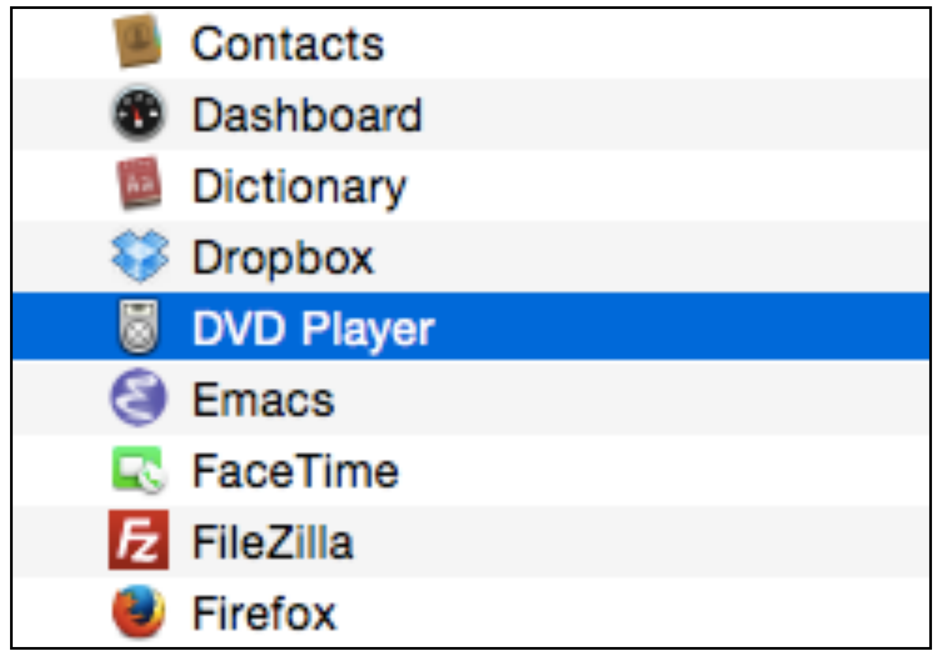
- Grammar of Graphics, why not Grammar of Interaction?
- Vega-Lite/Altair is about **interactive** graphics
- Types of Interactions:
  - Selection
  - Zoom
  - Brushing

Selection

- Selection is often used to initiate other changes
- User needs to select something to drive the next change
- What can be a selection target?
  - Items, links, attributes, (views)
- How?
  - mouse click, mouse hover, touch
  - keyboard modifiers, right/left mouse click, force
- Selection modes:
  - Single, multiple
  - Contiguous?

Highlighting

- Selection is the user action
- Feedback is important!
- How? Change selected item's visual encoding
  - Change color: want to achieve visual popout
  - Add outline mark: allows original color to be preserved
  - Change size (line width)
  - Add motion: marching ants



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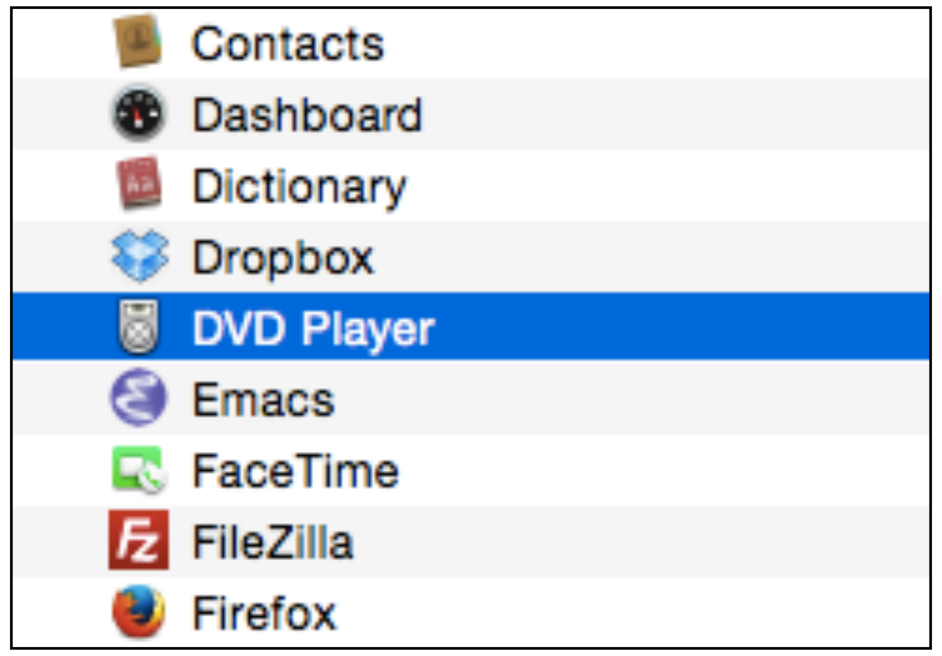
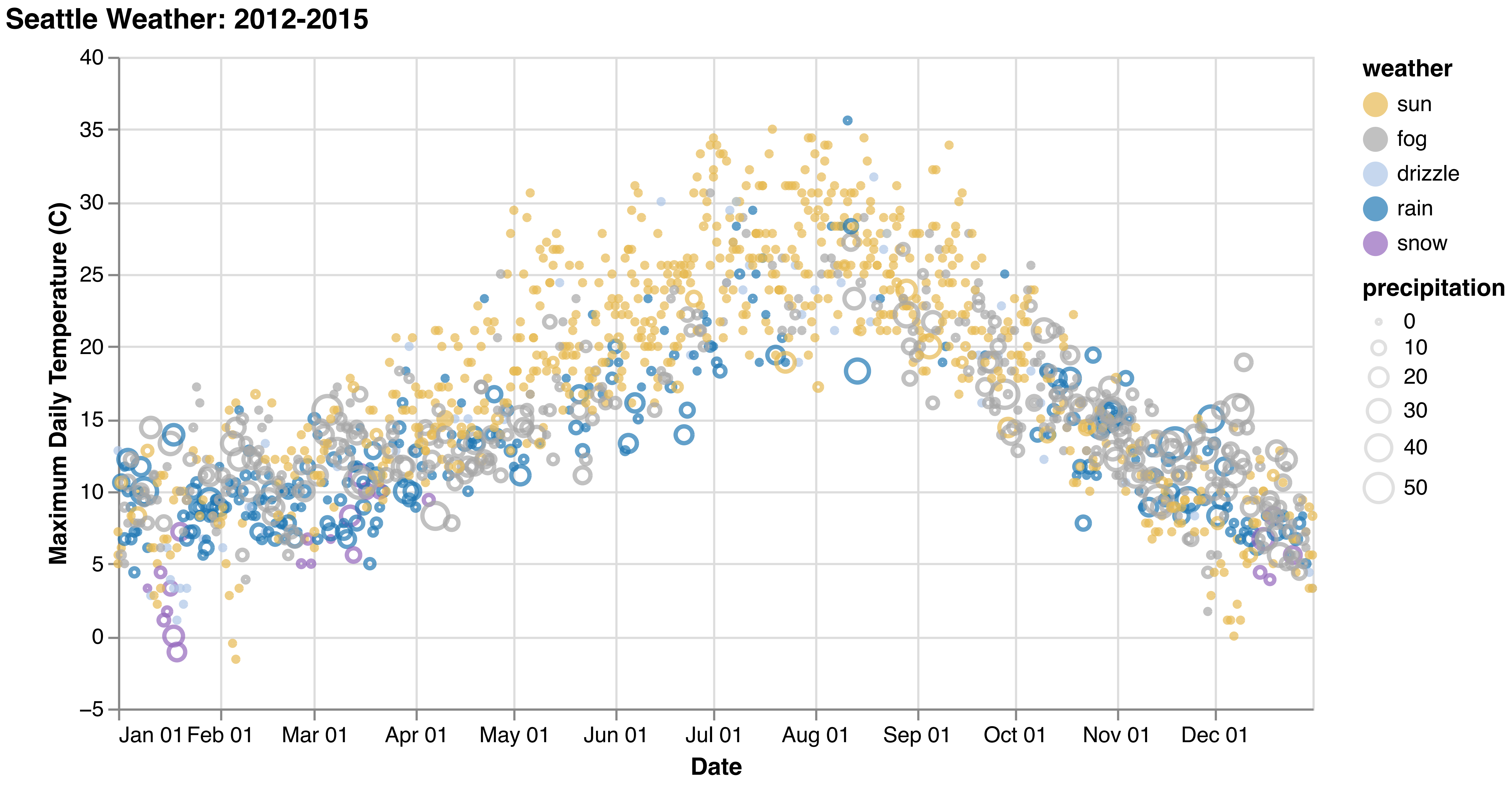
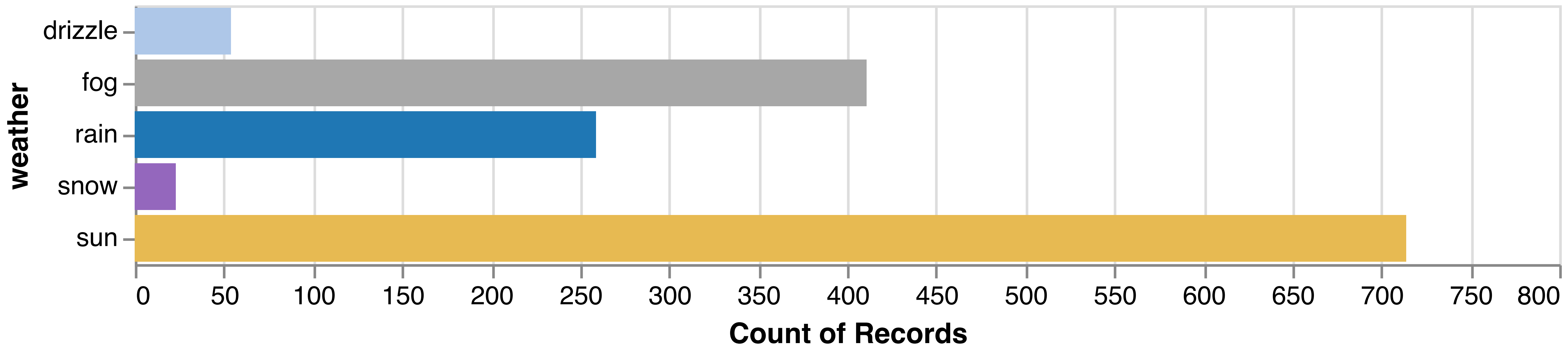


Altair's Interactive Charts

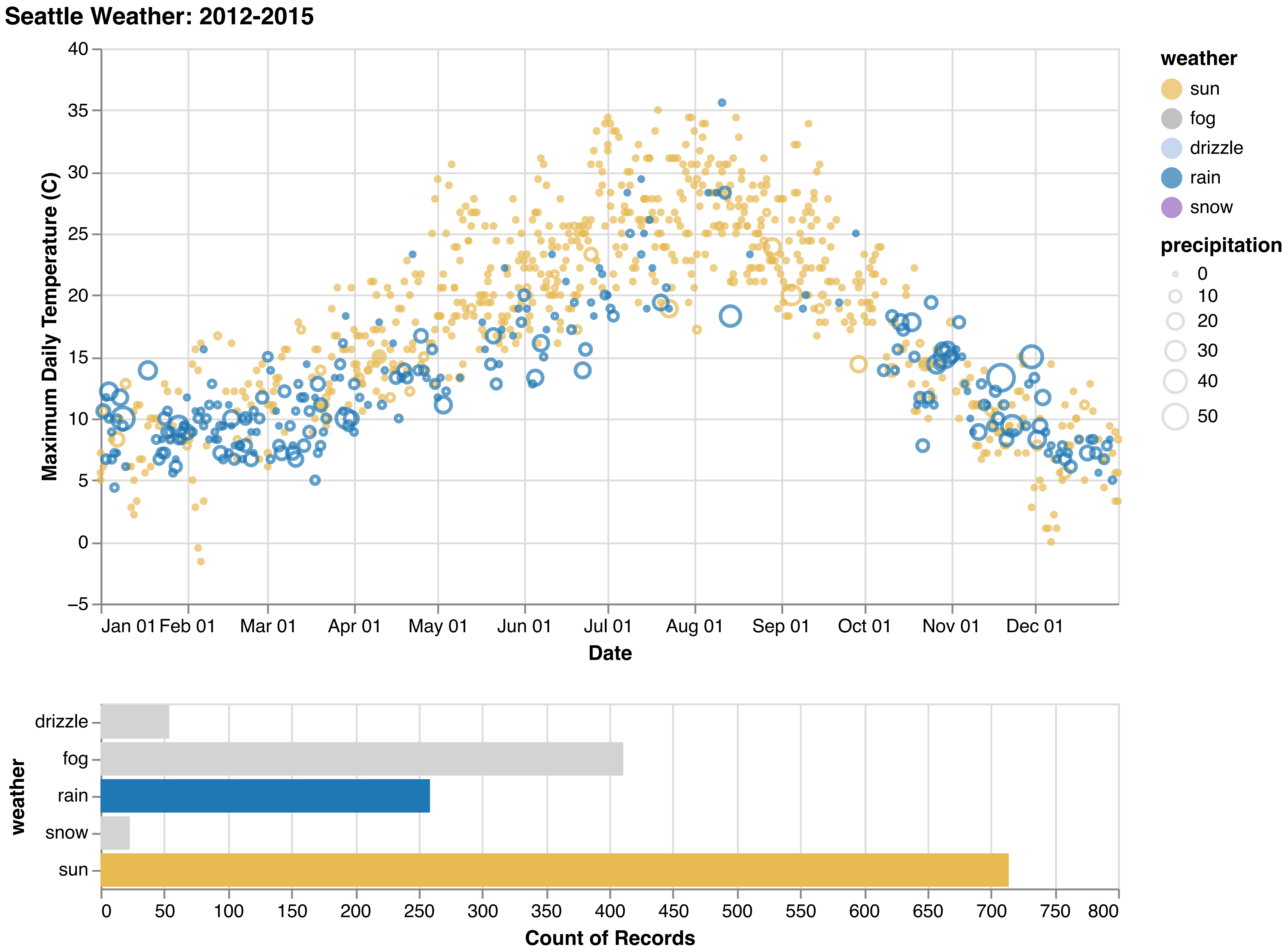
- https://altair-viz.github.io/gallery/index.html#interactive-charts

Interaction

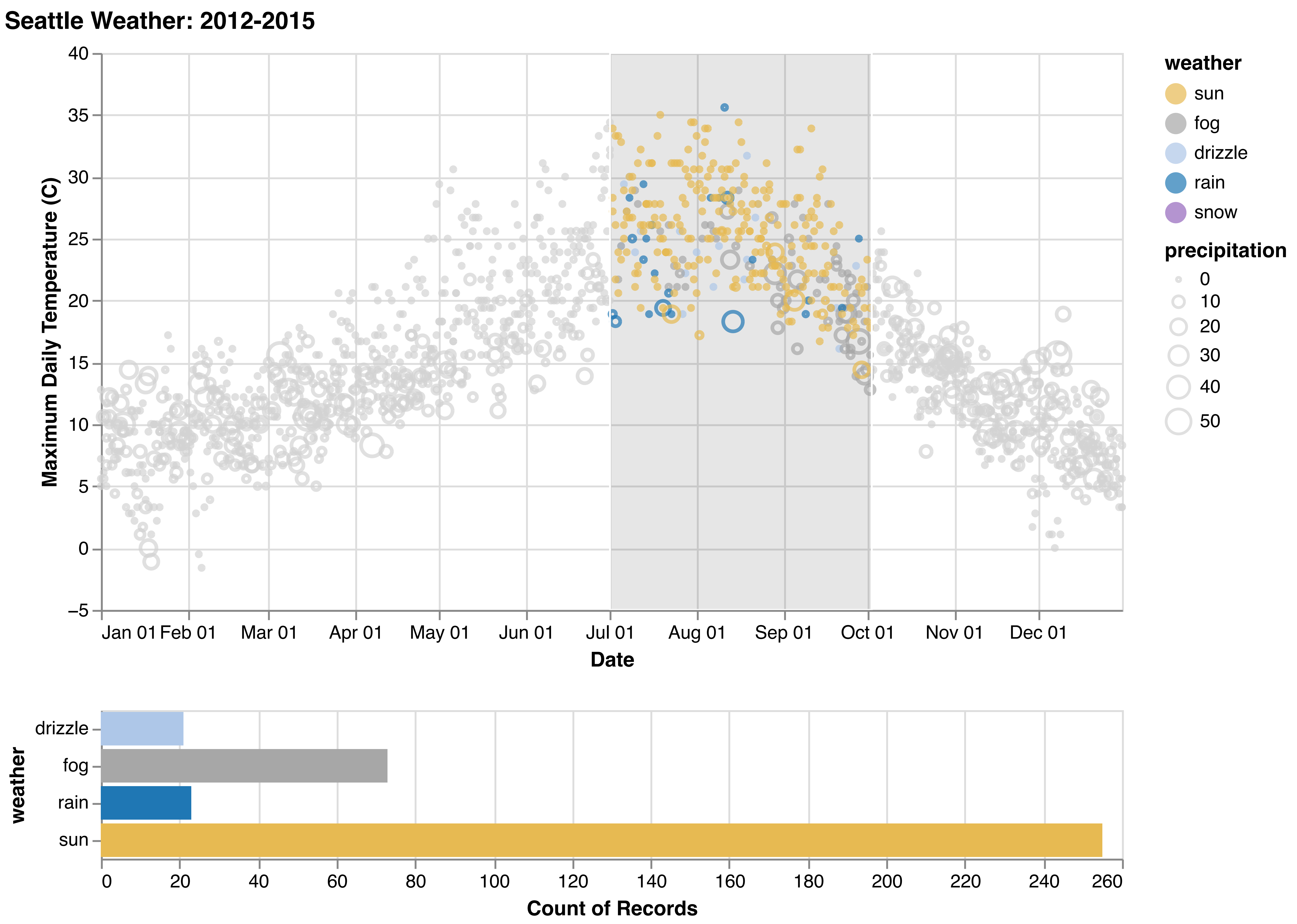




Weather Selection: Rain vs. Sun



Date Selection: July-September Sun



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]

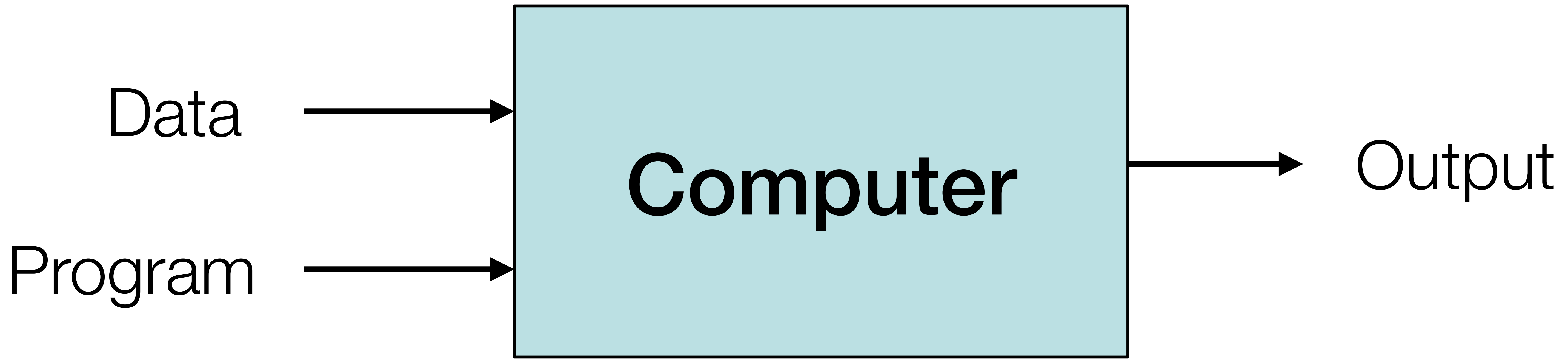
Machine Learning Workflow Overview

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).

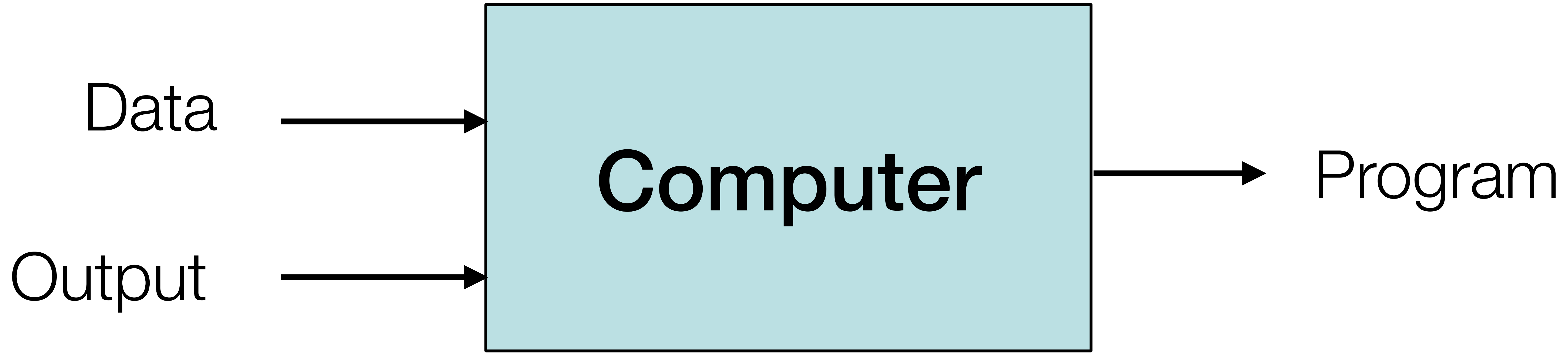
[R. Grosse et al.]

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]

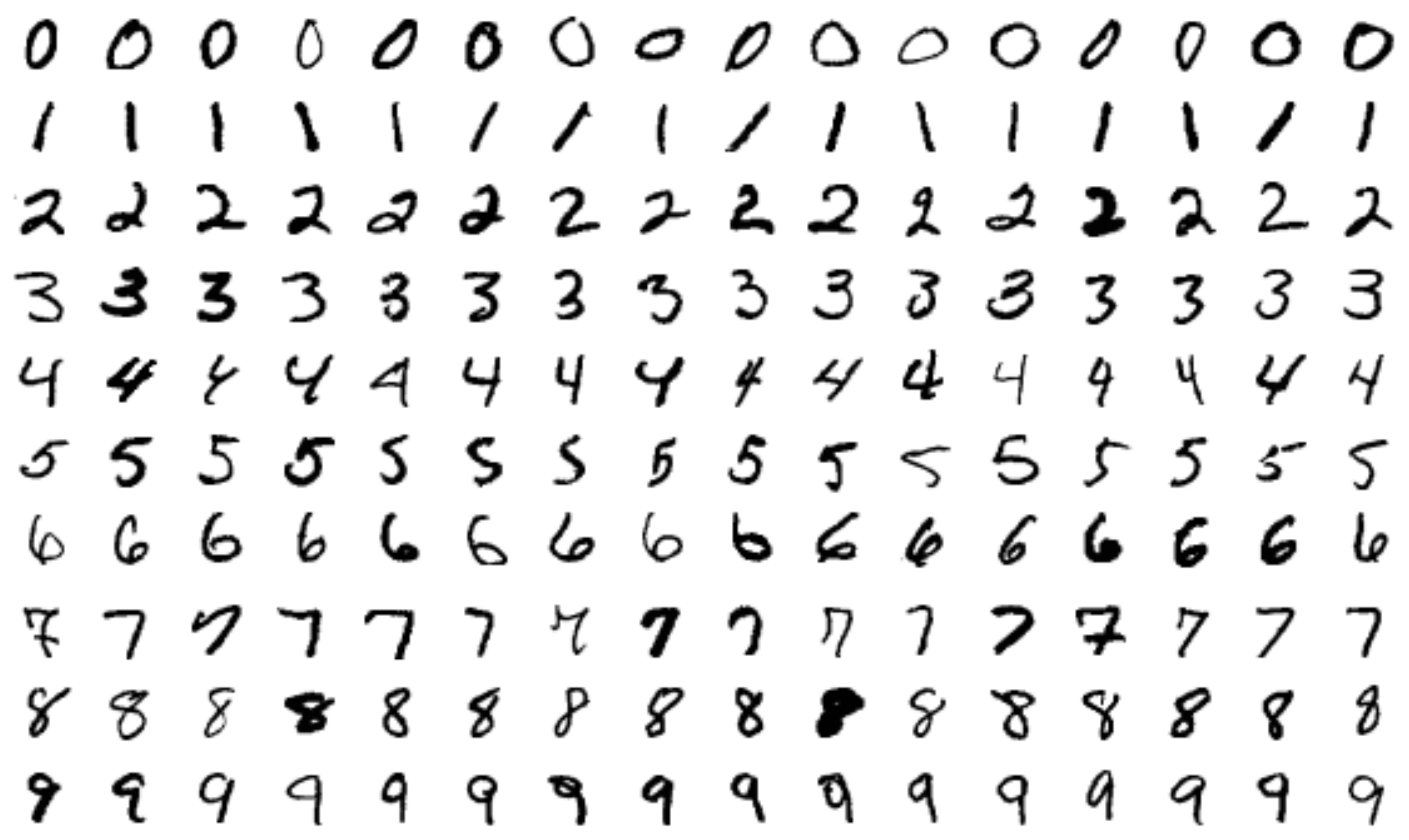
Areas of Machine Learning

- 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

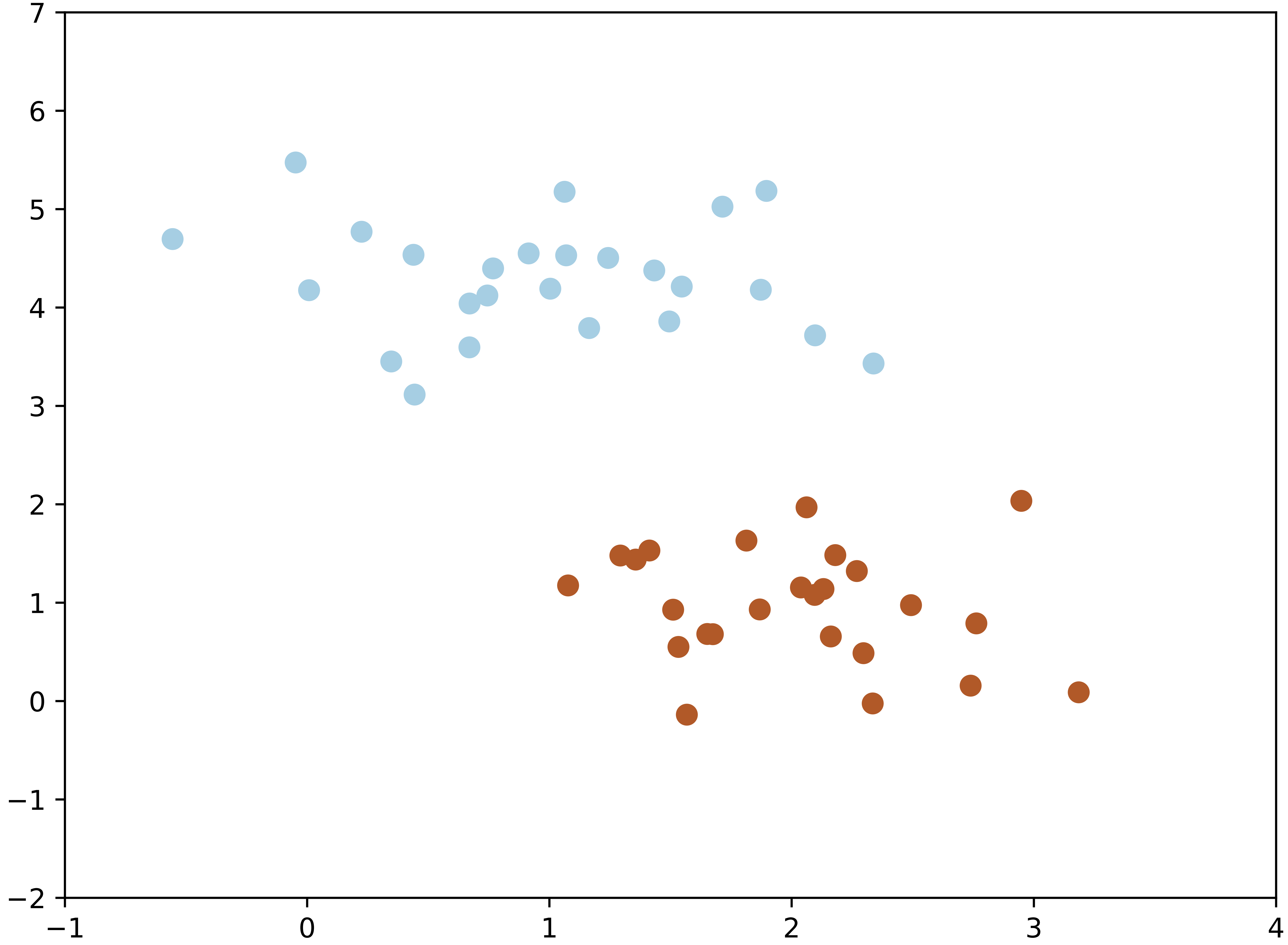
- Identifying the zip code from handwritten digits on an envelope (**supervised**)



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

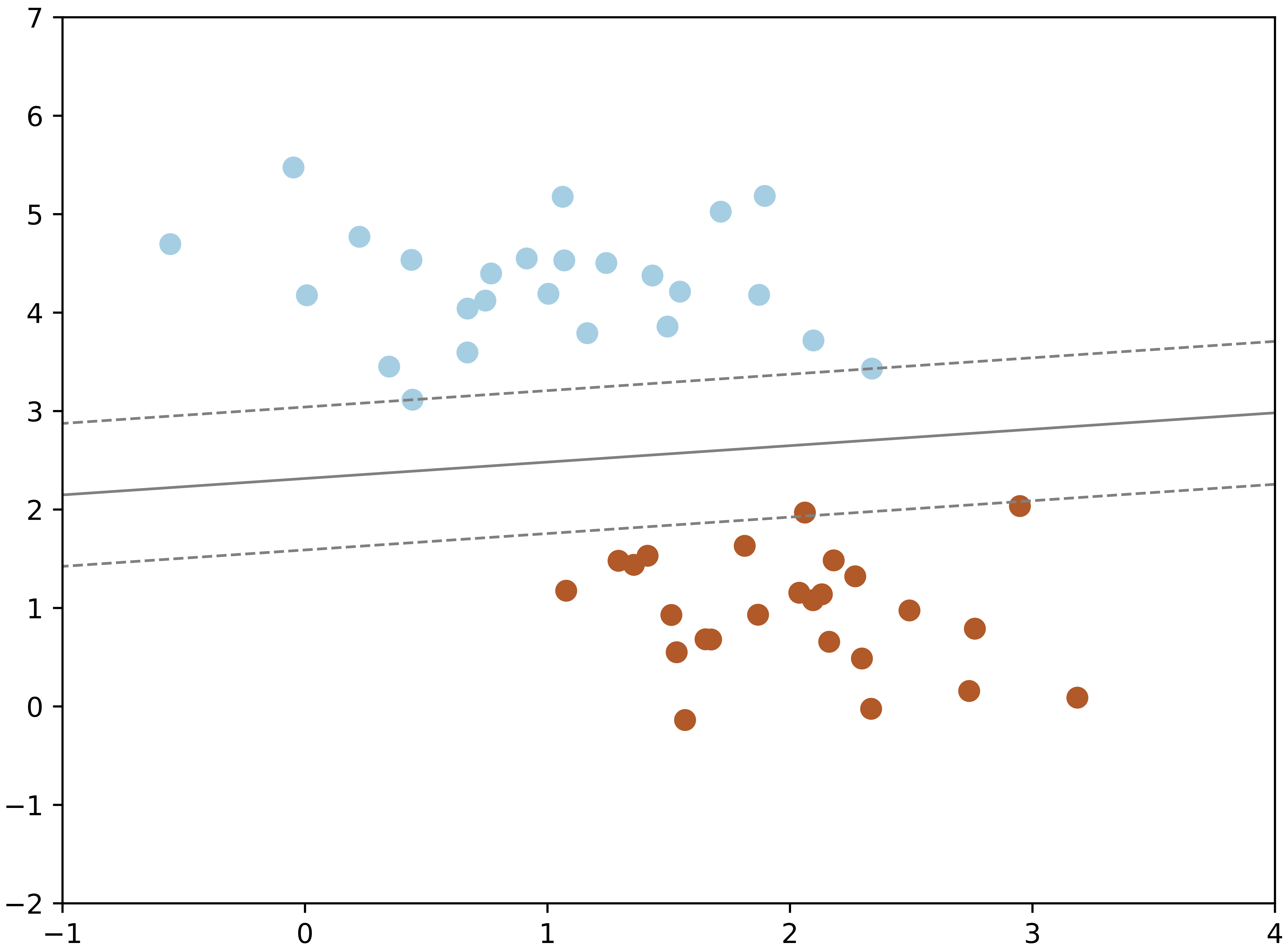
[A. Müller & S. Guido, Introduction to Machine Learning with Python, J. Steppan (MNIST image)]

Supervised Learning



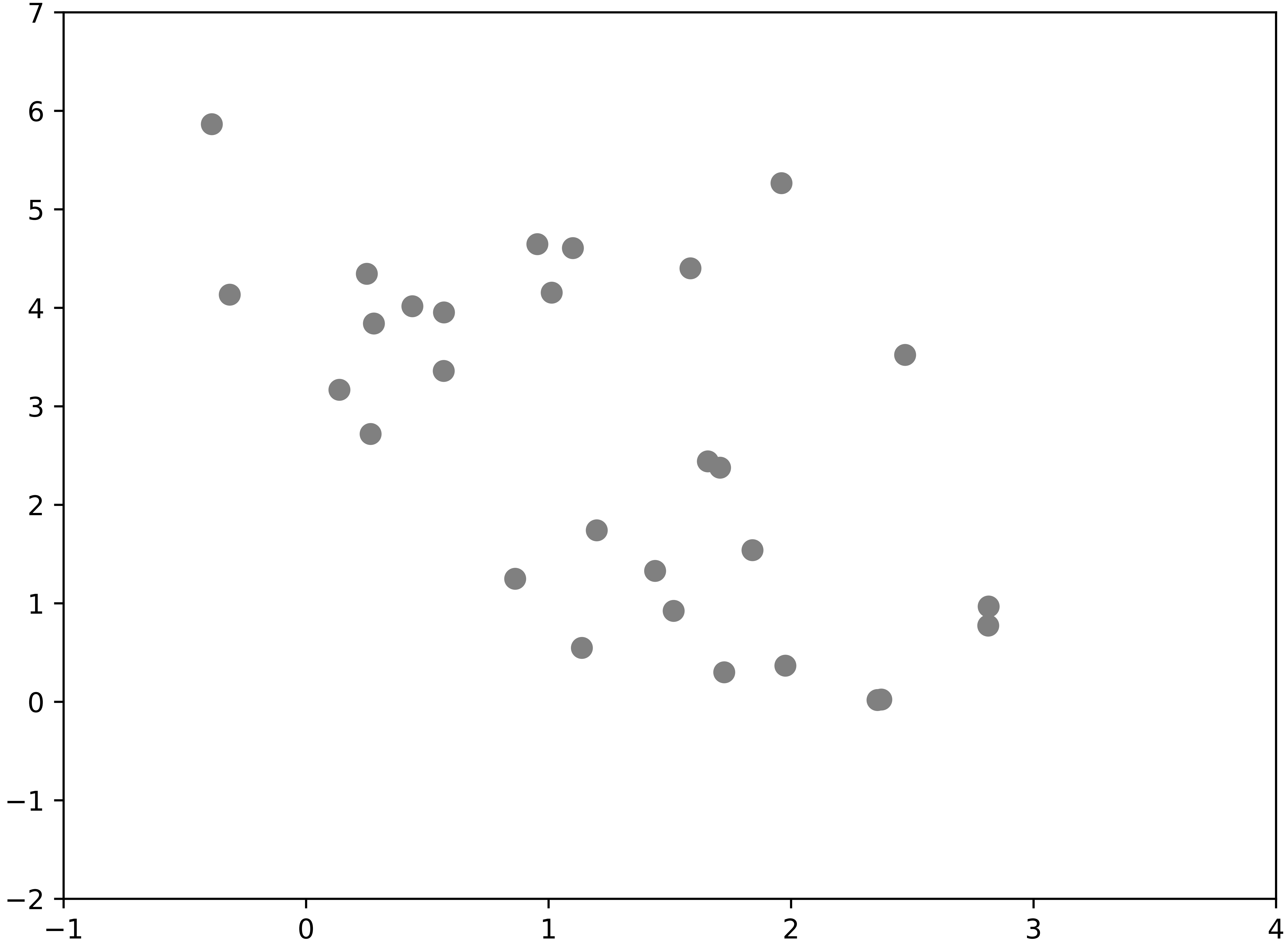
[J. VanderPlas]

Supervised Learning: Learned Algorithm (Fit)



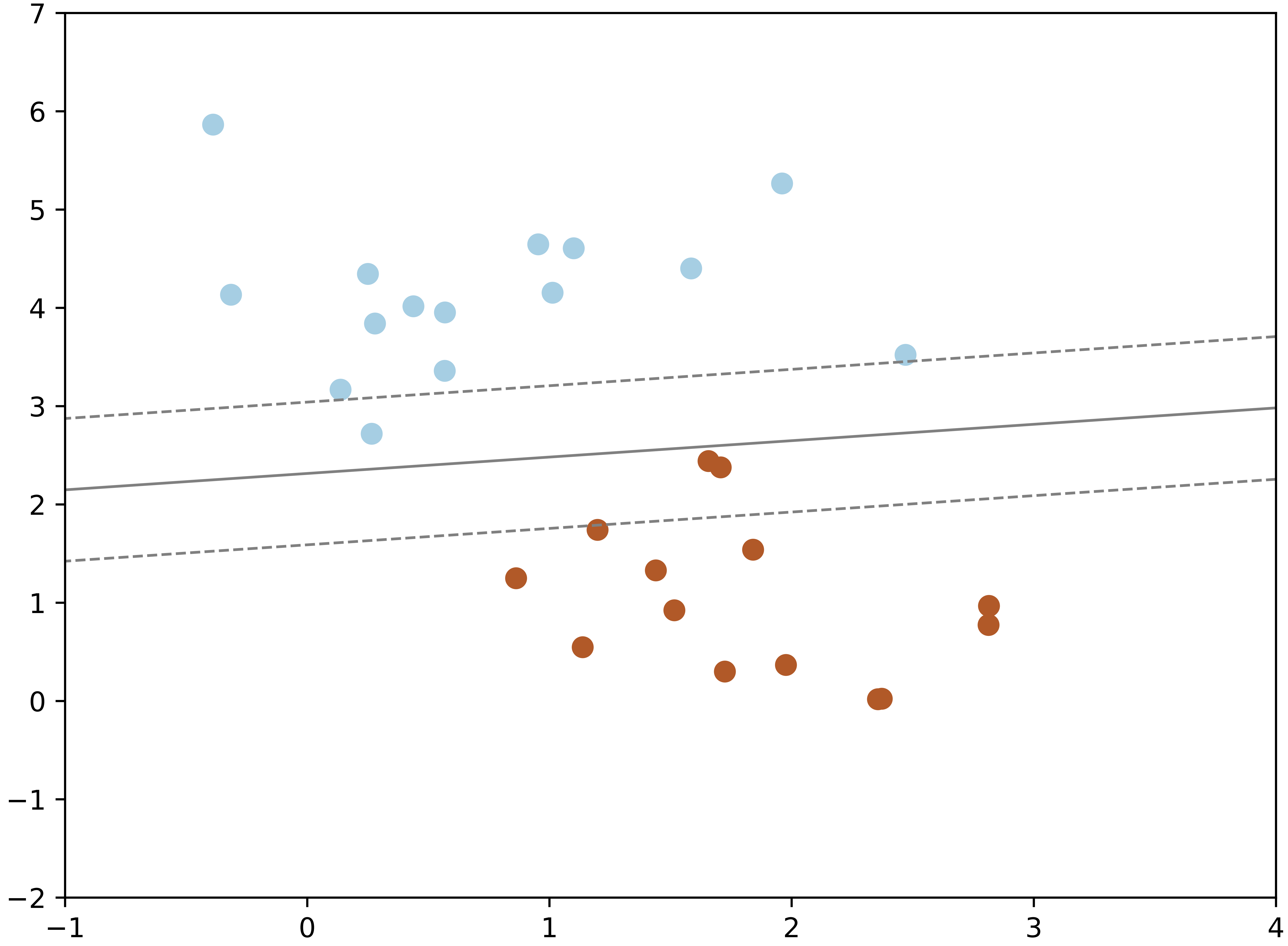
[J. VanderPlas]

Supervised Learning: Prediction



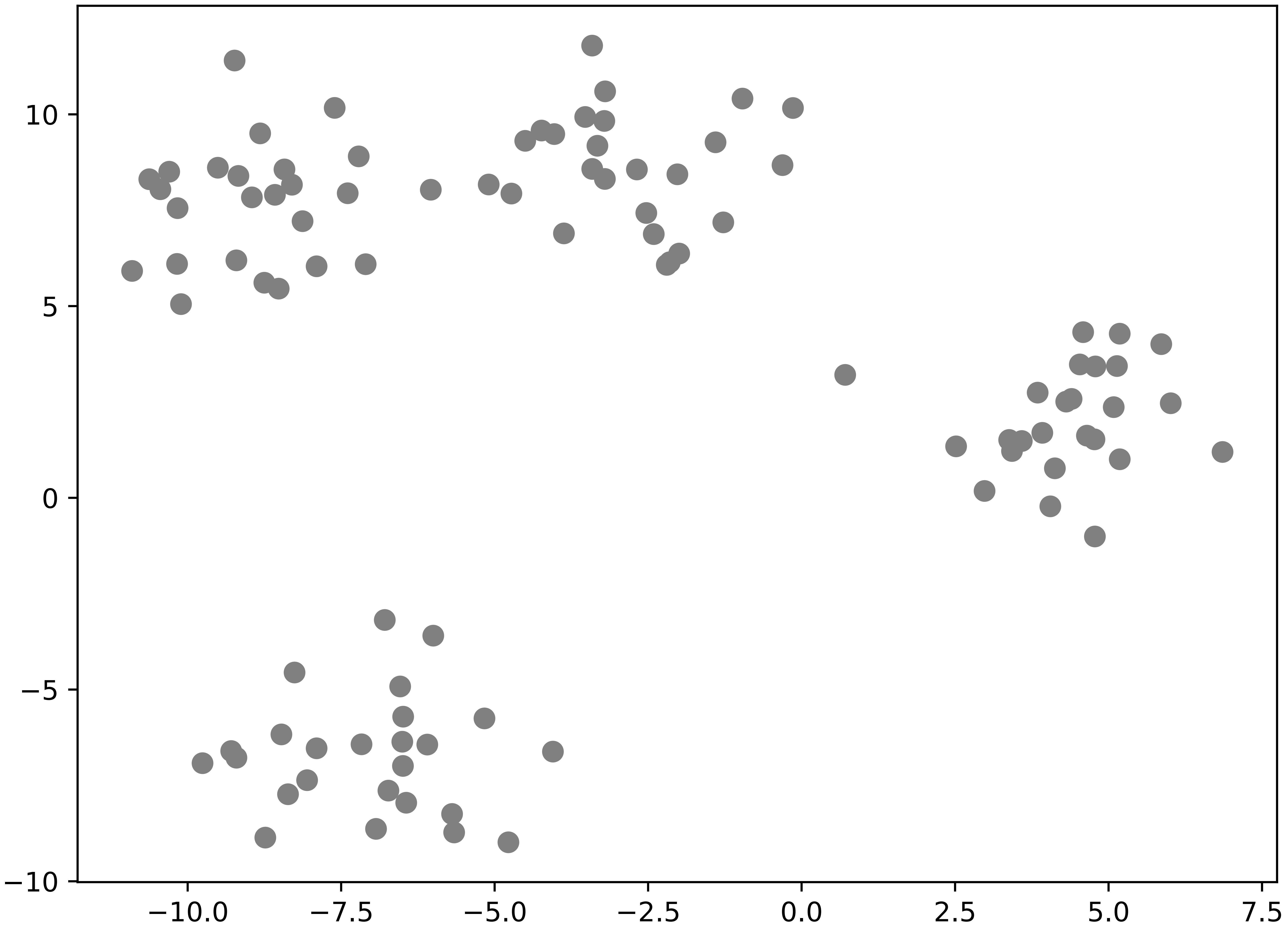
[J. VanderPlas]

Supervised Learning: Prediction



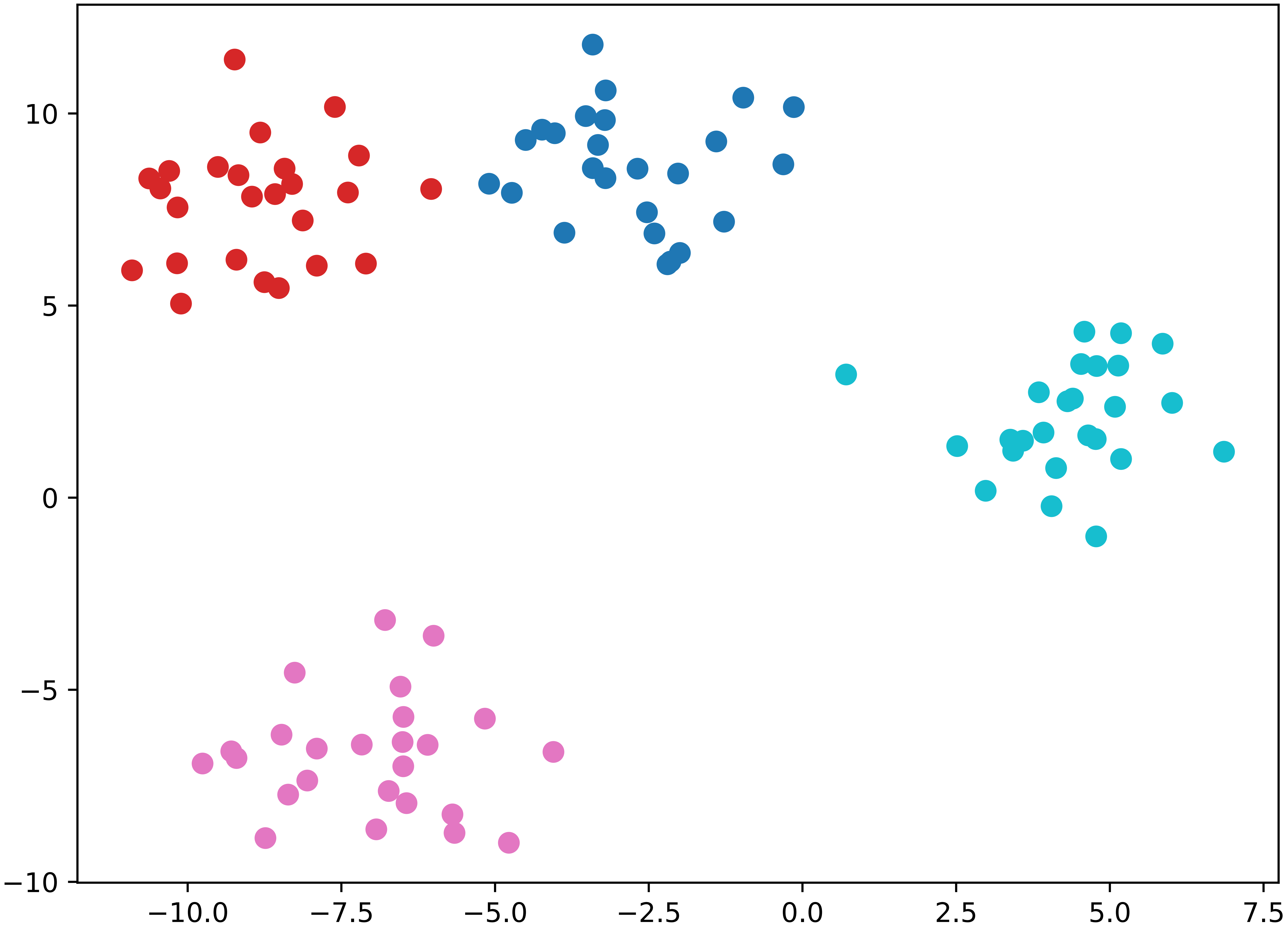
[J. VanderPlas]

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`

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Penguin Example

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