GPU-Accelerated Machine Learning with RAPIDS

CSCS-USI Summer School

Young-Jun Ko (NVIDIA)

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About me

- Young-Jun ($\approx$ Young - "not old", Jun - "like the month of June")
- Past:
    - SW Developer (IBM, SAP)
    - MSc at Saarland University, PhD at EPFL
    - ML Engineer at "big data" startup
- Since Nov 2018:
    - AI DevTech Engineer at NVIDIA, based in Zurich
        - Briefly looked into HPC+AI
        - Worked on GLMs for RAPIDS' `cuml` library
        - Currently: Optimizing Neural Network inference performance for NLP
- About you?

Thanks to the Organizers

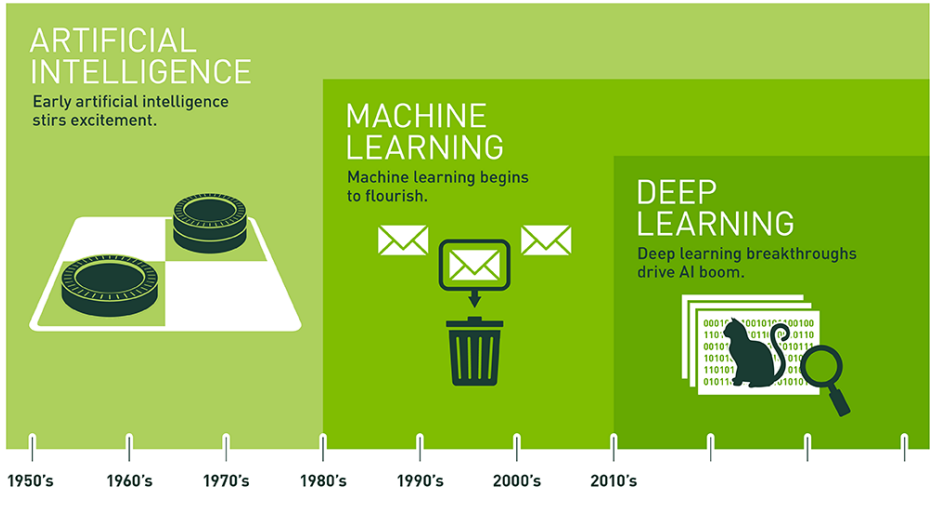
Course Overview and Organization

- Benefits of being "data-driven" lead to more and more data being collected and stored
- Processing all this data becomes a challenge
- GPU accelerators can be a viable solution
- Requirements for broad adoption: software
    - familiar, high-level APIs
    - open-source
    - integration into existing workflows
- Part 1 (motivational): what is RAPIDS, and why it could be useful to know about
- Part 2 (conceptual): taking a look at the algorithms behind the high-level APIs
- New format: Interleave with small exercises (Notebooks in the Summerschool repository)
    - Presentation of a topic
    - Small exercise
    - Time for exercises might not be well calibrated
    - Goal is not to finish everything, but to briefly recap the concepts for yourself

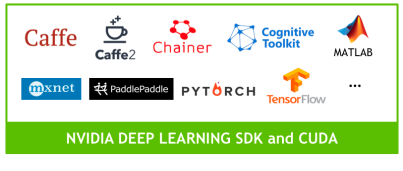
Outline

- The RAPIDS data science stack and the case for "Classical" ML
- Supervised learning
    - Recap of Fundamental Concepts
    - Generalized linear models (GLMs)
    - Gradient-boosted decision trees, XGBoost
- Unsupervised learning
    - Dimensionality reduction
    - Principal component analysis (PCA)
    - Non-linear techniques

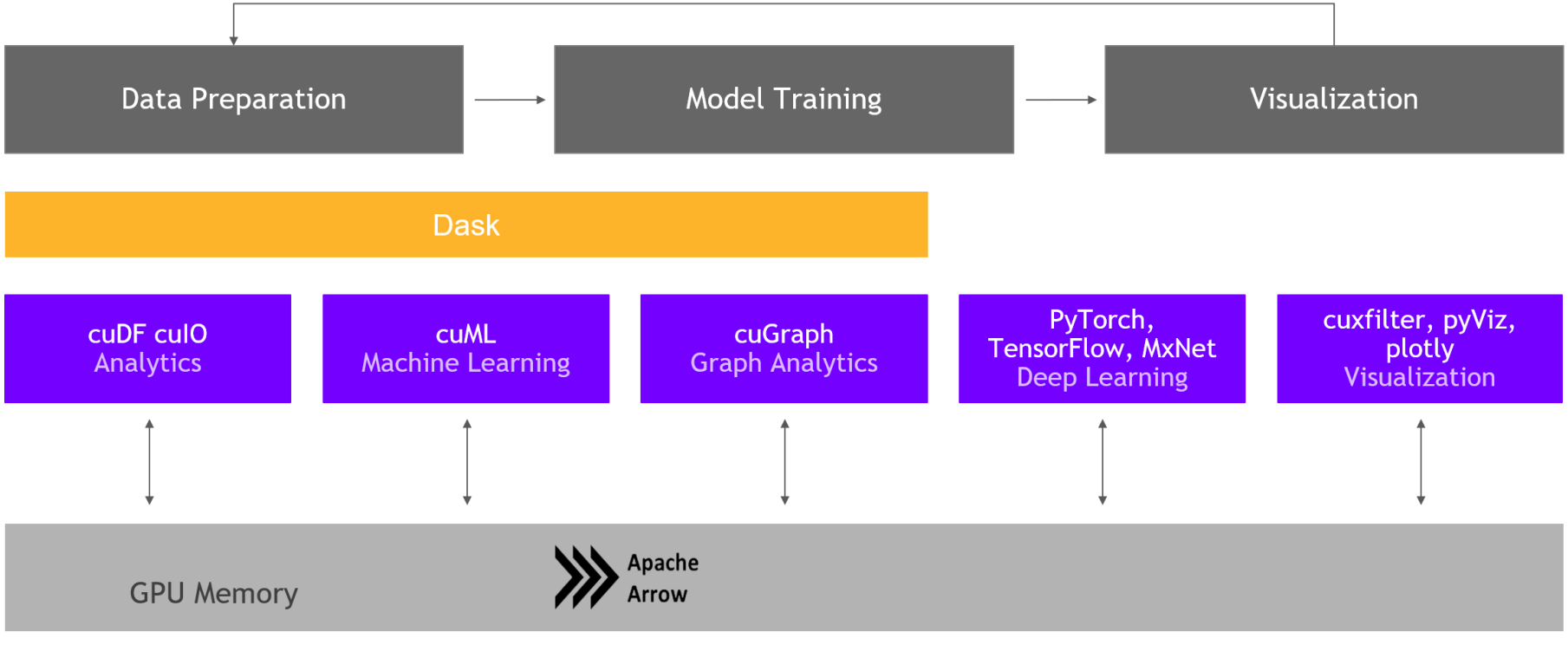
ML and Libraries at NVIDIA



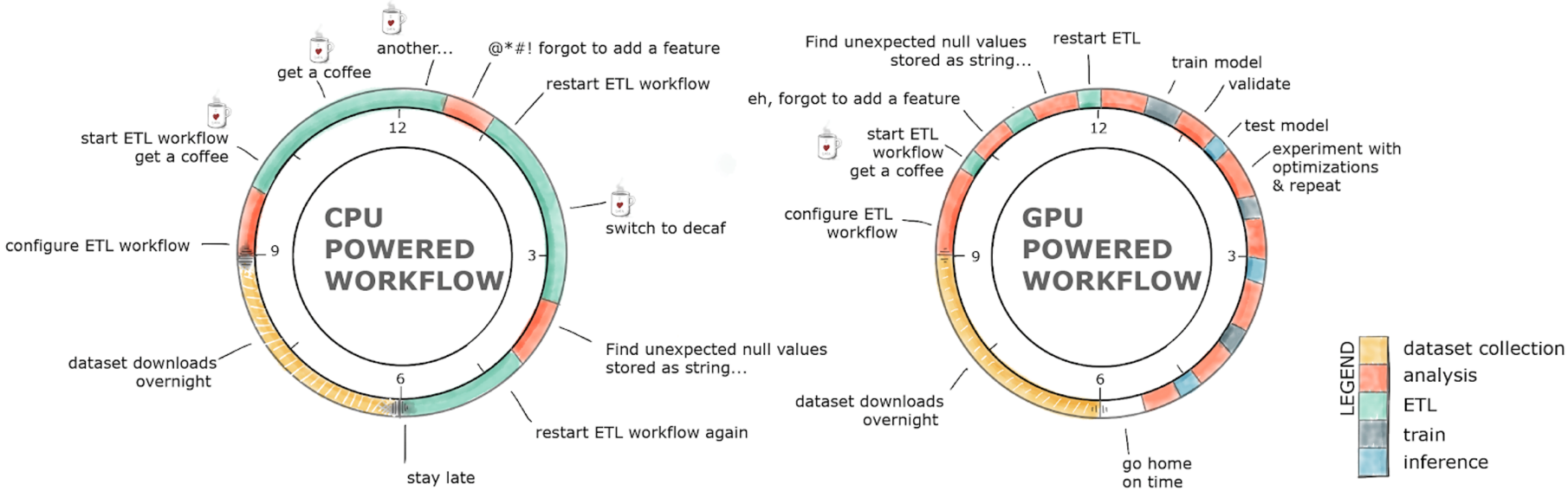
Since an early flush of optimism in the 1950s, smaller subsets of artificial intelligence – first machine learning, then deep learning, a subset of machine learning – have created ever larger disruptions.



RAPIDS Overview: End-to-end Datascience Platform



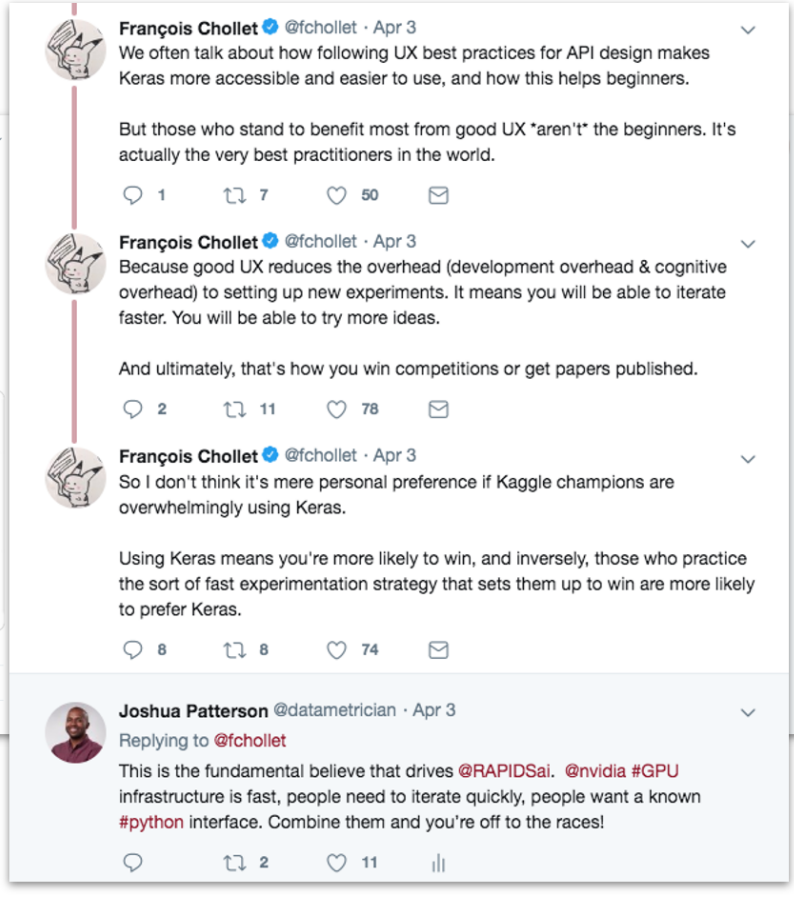
RAPIDS Value Proposition

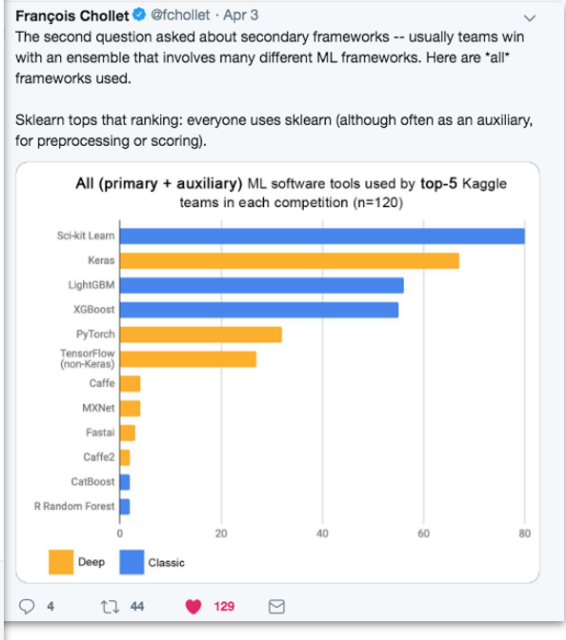


RAPIDS Details

Slides (https://docs.rapids.ai/overview/latest.pdf)

Classical ML Libraries: Workhorses of Data Science





kaggle

Move Faster with Familiar APIs

In many cases:

```
# ML on the CPU
from scikit import Model
model = Model()
model.fit(train_data)
preds = model.predict(test_data)
```

becomes:

```
# ML on the GPU with RAPIDS
from cuml import Model
model = Model()
model.fit(train_data)
preds = model.predict(test_data)
```

RAPIDS: Familiar APIs

Pandas/Scikit-learn

Take the first 20,000 rows and standardize to zero-mean and unit variance.

```
import numpy as np
pdf_http = pdf_http.head(20000)
for col in pdf_http.columns:
    series = pdf_http[col].astype('float32')
    mean = series.mean()
    var = series.var()
    pdf_http[col] = (series - mean) / (1 if var == 0 else np.sqrt(var))
```

```
from sklearn.cluster import DBSCAN
clustering = DBSCAN(eps=4, min_samples=100, n_jobs=-1)
```

```
%%time
clustering.fit(pdf_http)
```

```
CPU times: user 7min 7s, sys: 3.55 s, total: 7min 10s
Wall time: 8.8 s
```

```
pd.Series(clustering.labels_).value_counts()
```

```
 0    19196
 1      576
-1      228
dtype: int64
```

RAPDS cuDF/cuML

Take the first 20,000 rows and standardize to zero-mean and unit variance.

```
import numpy as np
gdf_http = gdf_http.head(20000)
for col in gdf_http:
    series = gdf_http[col].astype('float32')
    mean, var = series.mean_var()
    gdf_http[col] = (series - mean) / (1 if var == 0 else np.sqrt(var))
```

```
import cuml
clustering = cuml.DBSCAN(eps=4, min_samples=100)
```

```
%%time
clustering.fit(gdf_http)
```

```
CPU times: user 204 ms, sys: 40 ms, total: 244 ms
Wall time: 242 ms
<cuml.cluster.dbscan.DBSCAN at 0x7f4f7c03d978>
```

```
print(clustering.labels_.value_counts())
```

```
0    19563
1      303
-1      134
dtype: int64
```

Classic ML Algorithms (cuML Library)

- Let us not forget about classic ML (i.e. not deep learning)

What you need: Classic Machine Learning - cheap, realiable, well-understood

What you want: Deep Learning - powerful, resource-hungry, cutting-edge

Summary

- Datascience has become an important work load in many areas
- "Classic", i.e. non-DL methods, still very much alive and well
    - Methods like XGBoost extremely successful for modeling real-world data
    - Simple methods, like linear models, well-understood, scalable, robust
- GPU-Acceleration of non-DL ML methods lagging behind
    - But: data procesing time increasing everywhere (end of Moore's law, "data deluge")!
    - Virtuous cycle: faster results => more experiments => better results => better exeriments
    - Optimize for most valuable resource: scientists'/engineers', i.e. your, time!

Summary

- RAPIDS: open-source, integrating into the python eco-system
    - Goal: seamless, "drop-in" replacement using familiar APIs
    - `cuDF`: columnar data storage and manipulation, like pandas
    - `cuML`: toolbox of ML algorithms, like scikit-learn
    - `cuGraph`: toolbox of graph mining algorithms
    - `cuSignal`: toolbox of graph mining algorithms
    - `cuSpatial`: toolbox of graph mining algorithms
    - `DASK` and `Spark` integration for distributed dataframes and algorithms
    - Both, ML and DL workflows can benefit
    - More info at `rapids.ai`

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- Unsupervised learning
    - Dimensionality reduction
    - Principal component analysis (PCA)
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Recap of ML Fundamentals

- Disclaimer: mild notational abuse and a lot of hand-waving ahead!
- Conceptual intuition > mathematical rigour

Checklist of Concepts

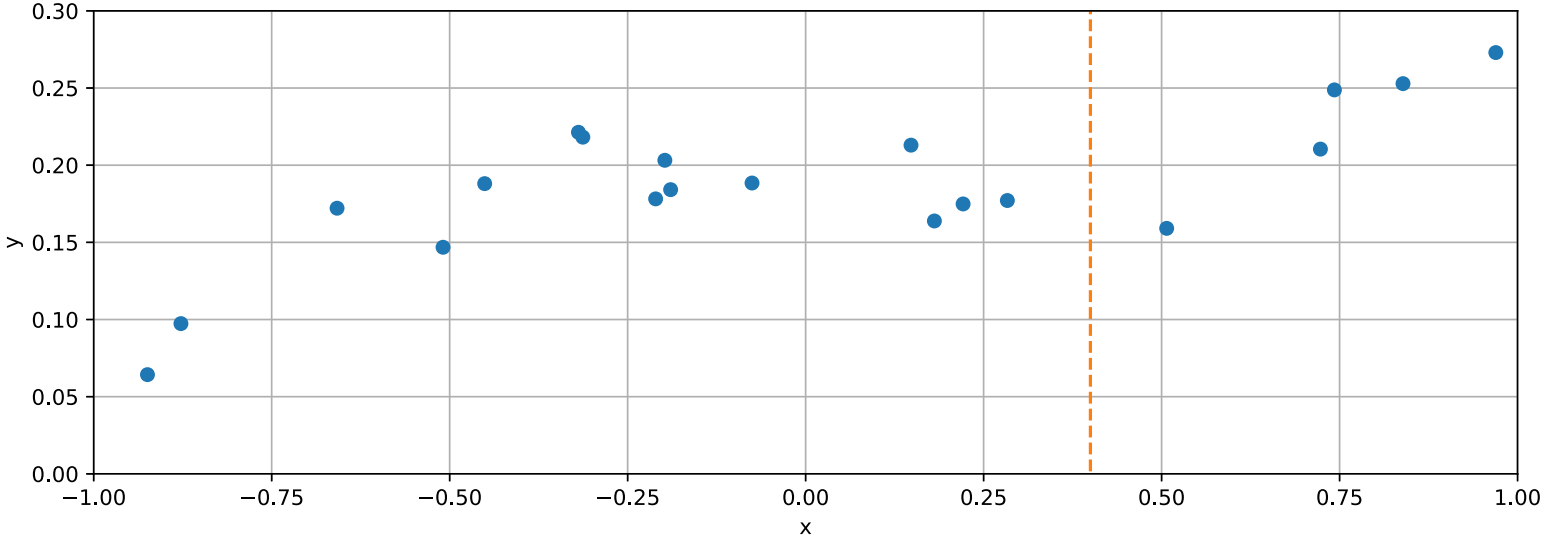
- Supervised learning
- Families of functions as models, learning algorithms, and loss functions
- Generalization, risk, and the bias-variance tradeoff

Supervised Learning

- The most common/successful paradigm
- The setup:
    - Input/feature space: $\mathcal{X}$, e.g. $\mathbb{R}^d$
    - Output/target space: $\mathcal{Y}$, e.g. $\mathbb{R}$ (regression), $\{\pm 1\}$ (classification)
- Hidden relationship: $P(X, Y)$
    - Probabilistic perspective useful for acknowledging noise
    - P is unknown (but we'll encounter it again in a moment)
    - But, we have access to N i.i.d. samples $(x_i, y_i) \sim P(X, Y)$
- Goal:
    - In practice: $P(Y \mid X)$
    - Find a "good" predictor, i.e. a deterministic $f : \mathcal{X} \mapsto \mathcal{Y}$

Example: Regression in 1D

- $\mathcal{X} = \mathbb{R}$
- $\mathcal{Y} = \mathbb{R}$
- find $f : \mathbb{R} \mapsto \mathbb{R}$, that can answer queries like "What is y at $x = 0.4$?"
- Learnt from previous "experience", i.e. pairs of (x_i, y_i)



Checklist of Concepts

- Supervised learning: $\mathcal{X}, \mathcal{Y}, P(X, Y), f$
- Families of functions as models, learning algorithms, and loss functions
- Generalization, risk, and the bias-variance tradeoff

Models, Learning Algorithms and Loss Functions

- We choose a family of functions $\mathcal{F}$ from which we choose the predictor: $f \in \mathcal{F}$
    - We will see families of linear and piece-wise constant functions
- Here, we assume that f is parameterized by a fixed-sized set of parameters θ, which we can use to index elements in $\mathcal{F}$
    - So called "parametric" models
- I.e. we can identify $f_\theta \in \mathcal{F}$ by their parameters θ
- A learning algorithm would then be a function that takes a sample and returns a set of parameters:

$$\mathcal{A}_{\mathcal{F}}(\{(x_i, y_i)\}) = \hat{\theta}$$

- It "fits the model to the data", which implies a way of quantifying "good" and "bad" (but there might be multiple notions involved!)
- Loss function:

$$l : \mathcal{Y} \times \mathcal{Y} \mapsto \mathbb{R}$$

    - Compares a true $y \in \mathcal{Y}$ to a predicted $\hat{y} = f(x)$
    - Encodes the cost we assign to errors
    - Examples:
        - squared loss: outliers cost a lot - avoid

$$l(y, \hat{y}) = (y - \hat{y})^2$$

        - absolute-error: outliers cost less - tolerate

$$l(y, \hat{y}) = |y - \hat{y}|$$

Example: The family of order-k polynomials

- Functions of this form: $f_\theta(x) = \sum_{i=0}^{k} w_i x^i$ ($k+1$ terms including bias)
- Parameters $\theta = \{w_0, \ldots, w_k\}$
- Family $\mathcal{F} = \{f_\theta\}$

- Learning algorithm and loss: e.g. least-squares regression when using squared error

$$\min_\theta \frac{1}{2}\|y - f_\theta(x)\|^2 = \min_\theta \frac{1}{2}\|y - \Phi(x)w\|^2 \qquad \mathcal{A}_\mathcal{F}(x, y) = (\Phi^T\Phi)^{-1}\Phi^T y$$

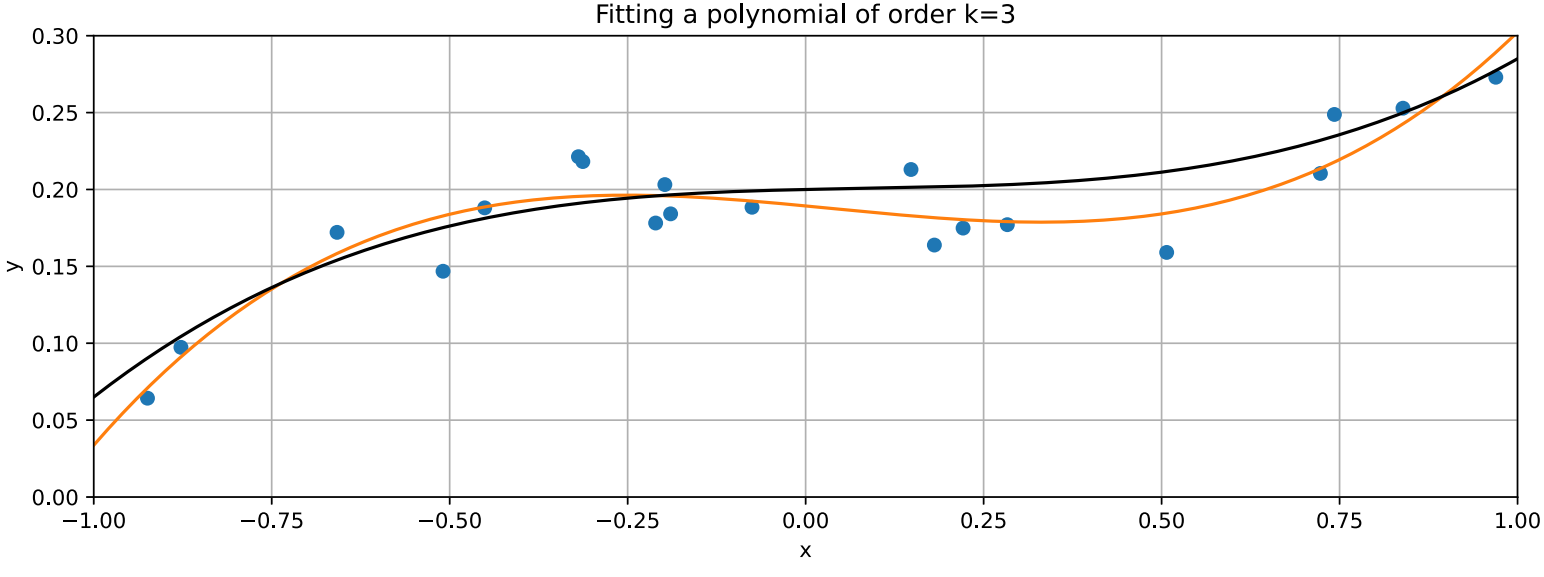
- Side note: linear in the parameters θ, but non-linear feature transform $\phi_i(x) = x^i$
    - Neural networks can be thought of as making the feature map trainable!

- In code:

```
def phi(x, order):
    Phi = np.concatenate([x ** k  for k in range(order+1) ], axis=1 )
    return Phi

def lsq(X, y):
    A = np.dot(X.T, X)
    b = np.dot(X.T, y)
    return np.linalg.solve(A,b)
```

Example of fitted Model



Exercise 1 (15 min)

Checklist of Concepts

- Supervised learning: $\mathcal{X}, \mathcal{Y}, P(X, Y), f$
- Families of functions as models, learning algorithms and loss functions: $f_\theta \in \mathcal{F}, \mathcal{A}_\mathcal{F}$, $l(y, \hat{y})$
- Generalization, risk, and the bias-variance tradeoff

The True Risk

- If we knew P (and could deal with it), for any predictor, we would want to compute the expected loss on the whole population to understand generalization

$$R(f) := \mathbb{E}_P[l(Y, f(X))]$$

- The risk is the ideal objective

$$f^* = \arg\min_f R(f) \qquad \text{or at least} \qquad f^*_{\mathcal{F}} := \arg\min_{f \in \mathcal{F}} R(f)$$

- Unfortunately, we can only *approximate* R statistically using our sample, i.e. calculate the *emprirical* risk

$$\hat{R}(f) := \frac{1}{N} \sum_{i=1}^{N} l(y_i, f(x_i))$$

- And in practice, *empirical risk minimization*:

$$f_N := \arg\min_{f \in \mathcal{F}} \hat{R}(f)$$

- We have:

$$R(f^*) < R(f^*_{\mathcal{F}}) < R(f_N)$$

Empirical Risk and Generalization

- More importantly, $R(f_N)$ and $\hat{R}(f_N)$ can be completely independent of each other
    - $\hat{R}$ is *not* a useful estimate of the generalization of f_N (could be 0!)
    - We "used up" the sample for fitting the model
- I.e. the empirical risk will not tell us anything about the generalization error (the error on the whole population)
- However, generalization is all we care about
- Need another dedicated test sample, to estimate $R(f_N)$!
    - Check if fitting the model captured something useful or mostly noise

Decomposing the Error

- Studying these quantities can give us some insights into what we can do about this
- We can compare our estimate f_N with the best possible predictor f^*, and consider the (positive) risk difference:

$$\mathbb{E}[R(f_N) - R(f^*)]$$

- The expectation is taken over the samples (f_N is a random quantity, if we don't condition on the training data)

$$\begin{aligned}
\mathbb{E}[R(f_N) - R(f^*)] &= \mathbb{E}[R(f_N) - R(f^*) + R(f^*_{\mathcal{F}}) - R(f^*_{\mathcal{F}})] \\
&= \mathbb{E}[R(f^*_{\mathcal{F}}) - R(f^*) + R(f_N) - R(f^*_{\mathcal{F}})] \\
&= (R(f^*_{\mathcal{F}}) - R(f^*)) + (\mathbb{E}[R(f_N)] - R(f^*_{\mathcal{F}})) \\
&= \text{Approximation Error} + \text{Estimation Error} \\
&\rightarrow \text{"Bias"} + \text{"Variance"}
\end{aligned}$$

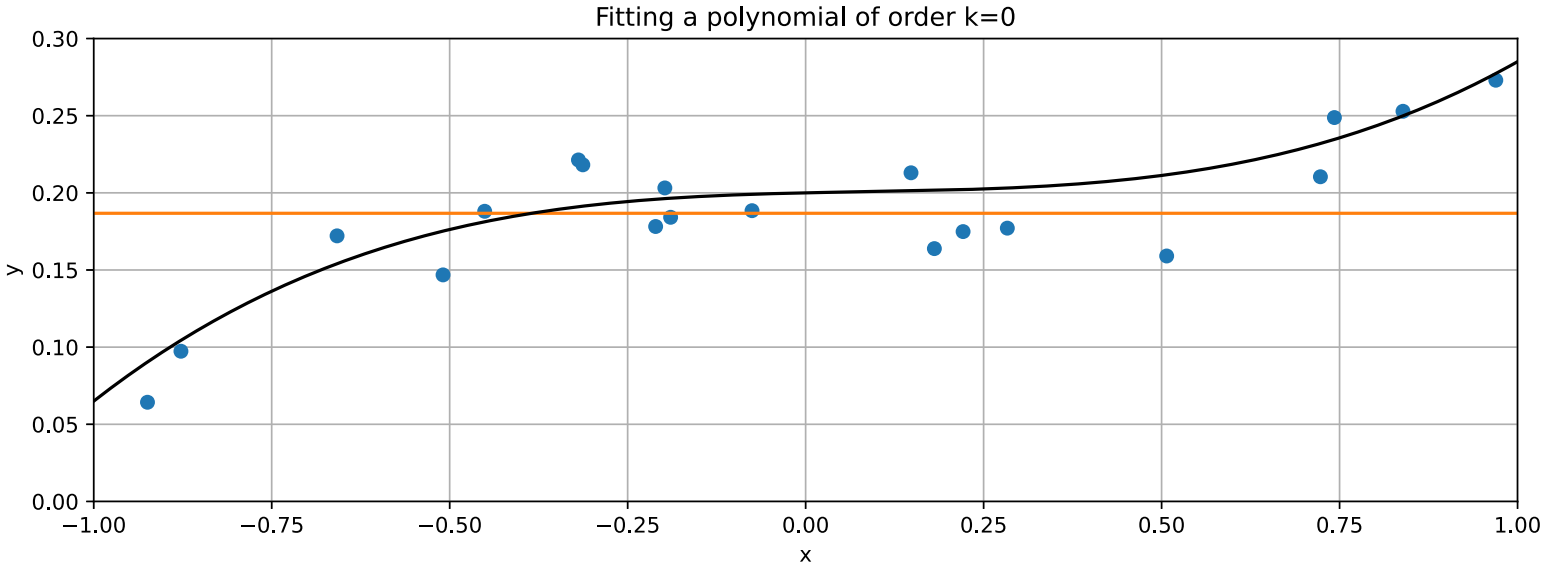
Decomposing the Error

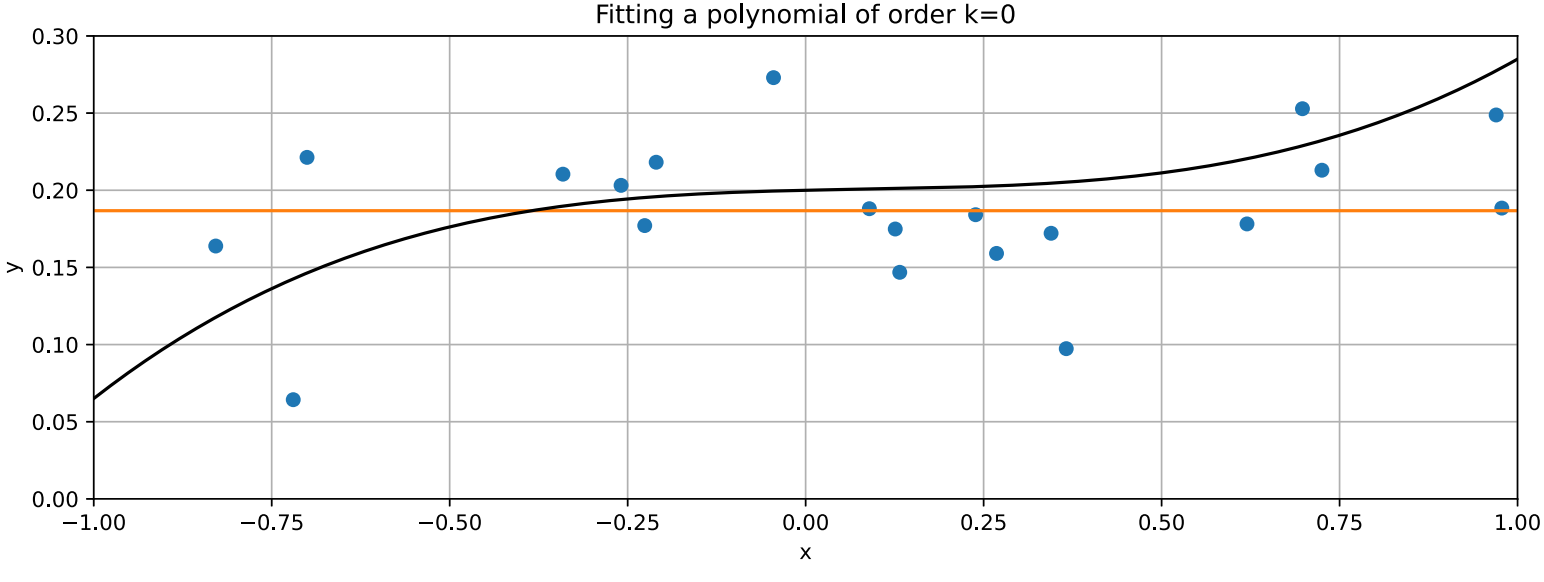
- Approximation error $R(f^*_{\mathcal{F}}) - R(f^*)$
    - How much do we loose because of our choice of $\mathcal{F}$?
    - The more different functions $\mathcal{F}$ offers, the smaller this term can be
- Estimation error $\mathbb{E}[R(f_N)] - R(f^*_{\mathcal{F}})$
    - How much do we loose by fitting on a limited, possibly very noisy sample?
    - The more samples we have, the closer the two terms will be
    - BUT: for a large function class, f_N fitted on different samples can look *dramatically* different
        - f_N has high variance
        - Most of them will be wrong, i.e. very different from $f^*_{\mathcal{F}}$
        - $\Rightarrow$ large estmation error
- For a limited amount of data (as in practice), we cannot "afford" a low approximation error because the estimation error will blow up
- Whereas for a large amount of data, we need a "sufficiently" large function class

Model Selection

- The main object, we have control over: $\mathcal{F}$
    - allow less functions explicitely (e.g. restrict k)
    - add regularization that penalizes complexity
- Very "small" $\mathcal{F}$, i.e. low model complexity: high bias, low variance - we underfit
- Very "large" $\mathcal{F}$, i.e. high model complexity: low bias, high variance - we overfit
- Have different models in your toolkit
- Beware of optimistic risk estimate

Extreme Underfitting: High Bias - Low Variance


Fitting a polynomial of order k=0
0.30
0.25
0.20
0.15
0.10
0.05
0.00
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x


Fitting a polynomial of order k=0
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0.00
y
−1.00
−0.75
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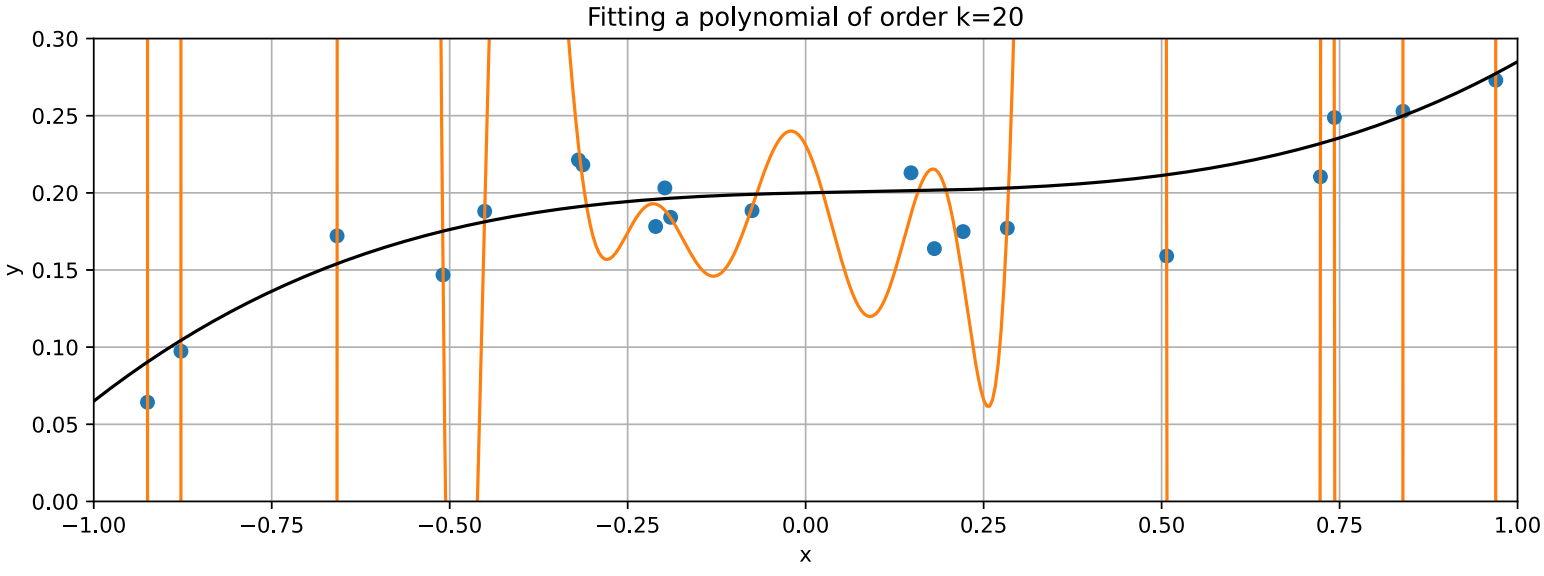
−0.25
0.00
0.25
0.50
0.75
1.00
x

Extreme Overfitting: Low Bias but Arbitrarily High Error


Fitting a polynomial of order k=20
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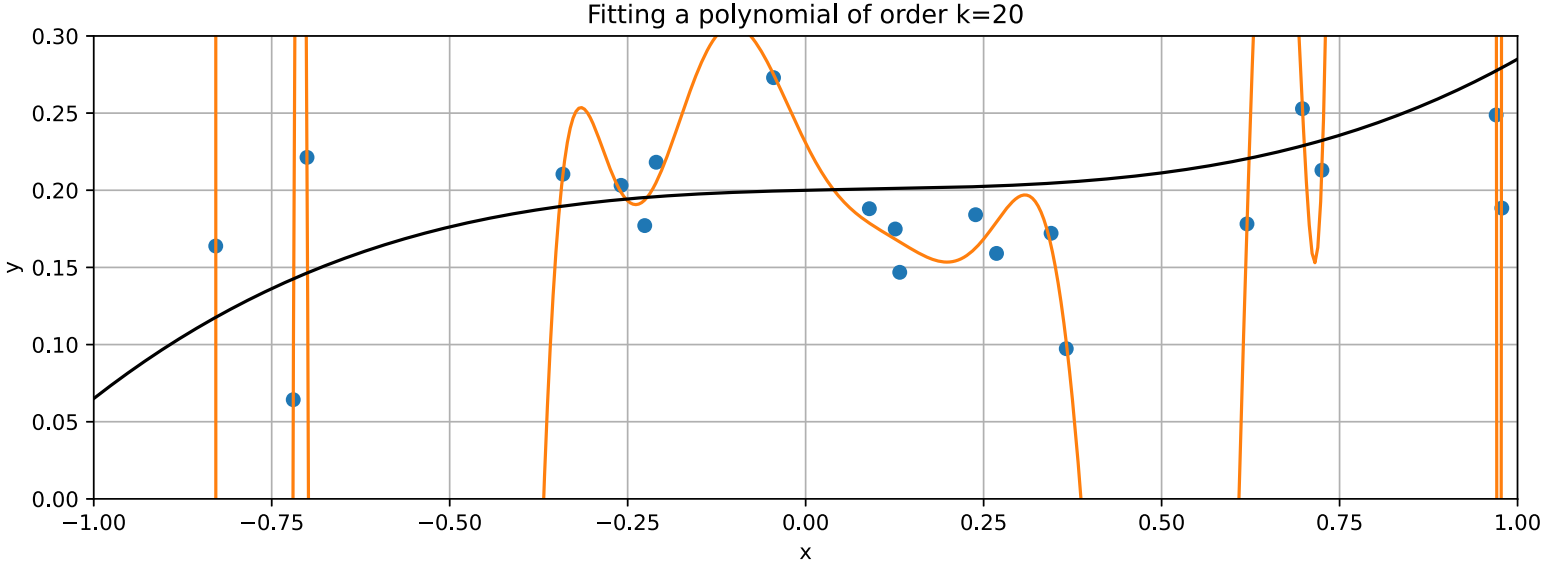
x


Fitting a polynomial of order k=20
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0.75
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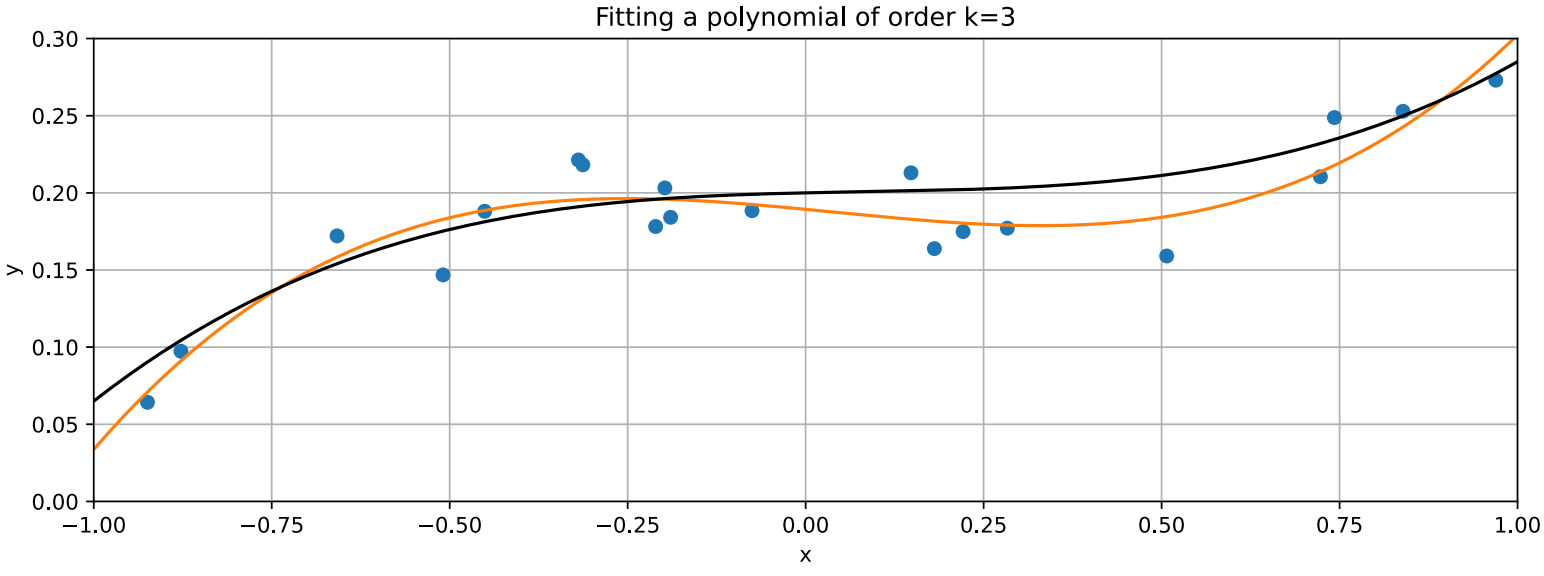
x

Correct Order


Fitting a polynomial of order k=3
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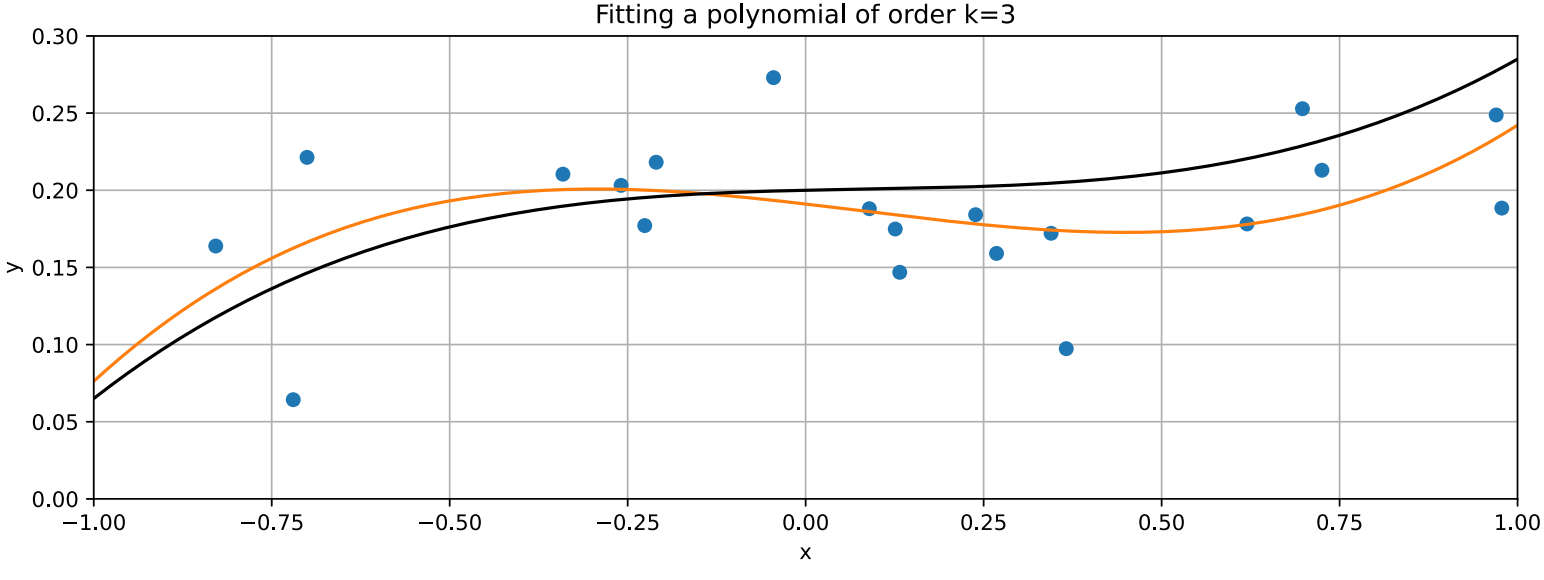
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Checklist of Concepts

- Supervised learning: $\mathcal{X}, \mathcal{Y}, P(X, Y), f$
- Families of functions as models, and learning algorithms: $f_\theta \in \mathcal{F}, \mathcal{A}_\mathcal{F}, l$
- Generalization, risk, and the bias-variance tradeoff: R, over-/under-fitting

Summary

- What Machine Learning is all about:
    - Choose an appropriate model (e.g. add regularization)
    - Come up with an efficient learning algorithm
    - Measuring Generalization is itself difficult: often estimates are optimistic (e.g. cross validation)
- Practical ML is by necessity very experimental (we don't have control over some key objects)
- Need tools to iterate quickly:
    - Wide selection of models: software matters
    - It's a computational discipline: performance matters

Exercise 2 (30 min)

Outline

- The RAPIDS data science stack and the case for "Classical" ML
- Supervised learning
    - Recap of Fundamental Concepts
    - Generalized linear models (GLMs)
    - Gradient-boosted decision trees, XGBoost
- Unsupervised learning
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    - Principal component analysis (PCA)
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Logistic Regression - A Generalized Linear Model

- Linear models have been in the toolbox of statisticians for ages
- We've seen linear models for regression
- What about classification, i.e. $\mathcal{Y} = \{\pm 1\}$?
    - we could assume $\mathcal{Y}$ is just $\mathbb{R}$ and fit to the discrete labels. Better way?
- A probabilistic perspective: generative models and maximum likelihood estimation

GLM Perspective on Least-Squares

- Least squares typically derived from an white additive noise model:
$$y = f_\theta(x) + \epsilon, \epsilon \sim N(0, 1)$$
- Implies a Gaussian data likelihood
$$P(Y \mid X = x) = N(Y \mid f_\theta(x), 1)$$
- A Gaussian is appropriate since we are dealing with real values, i.e. regression
- In GLMs, we go the other way around:
    - Depending on the data *type* we would like to model, choose it's likelihood, e.g.:
        - Binary outcomes: Bernoulli
        - Counts: Poisson
    - Model the mean by transforming a linear function, or *linear predictor*
$$\mathbb{E}[Y \mid X] = g^{-1}(f_\theta(x))$$
    - Using the inverse of g from statistics
    - Think of it as mapping the real-valued output of f to the domain of the mean

GLM Perspective on Least-Squares

- For least squares, $\mu = f_\theta(x)$, i.e. $g(x) = x$:

$$P(Y \mid X = x) = N(Y \mid \mu(x), 1) \propto \exp(-\frac{1}{2}(Y - \mu(x))^2)$$

- The likelihood of the data is the probability of the dataset (conditioned on the parameters):

$$P(Y = y \mid X = x, \theta) = \prod_{i=1}^{N} P(Y = y_i \mid X = x_i, \theta)$$

- Maximizing the likelihood is equvalent to minimizing the negative log-likelihood:

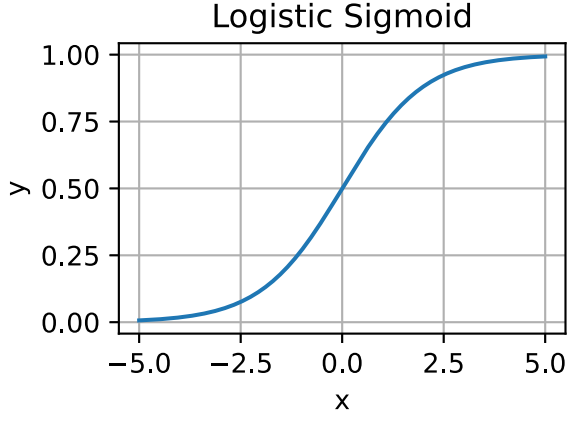
$$\begin{aligned} -\log P(Y = y \mid X = x, \theta) &= -\sum_{i=1}^{N} \log P(Y = y_i \mid X = x_i, \theta) \\ &= \sum_{i=1}^{N} \frac{1}{2}(y_i - \mu(x_i))^2 \\ &= \frac{1}{2}\|y - f_\theta(x)\|^2 \end{aligned}$$

Logistic Regression

- no-one prevents us to model other distributions/data types for y, just need to find the right distribution and parameterization in terms of the predictor
- Now consider a binary RV $Y \in \{0, 1\}$
- Bernoulli distribution: $P(Y = 1 \mid p) = p$ and $P(Y = 0 \mid p) = 1 - p$, can be written as:

$$P(Y = y \mid p) = p^y (1 - p)^{1-y}$$

- The parameter $p \in [0, 1]$ and $\mathbb{E}[Y] = p$
- In logistic regression, we model the mean of Y as $\mu(x) = p(x) = \sigma(f_\theta(x))$
- Logistc sigmoid $\sigma : \mathbb{R} \mapsto [0, 1]$ for a valid probability, with $\sigma(x) = 1/(1 + \exp(-x))$
- Interpretation:
    - Large positive values: we're sure about $Y = 1$
    - Small negative values: we're sure about $Y = 0$
    - Zero: uncertain about the outcome (close to the decision boundary)



Logistic Regresion: Likelihood

- Bernoulli distribution:

$$P(Y = y \mid p) = p^y (1-p)^{1-y} \text{ where } p(x) = \sigma(f_\theta(x))$$

- Neg.log-likelihood:

$$\begin{aligned} -\log P(Y = y \mid X = x, \theta) &= -\log \prod_{i=1}^{N} \sigma(f_\theta(x_i))^{y_i} (1 - \sigma(f_\theta(x_i)))^{1-y_i} \\ &= -\sum_{i=1}^{N} y_i \log \sigma(f_\theta(x_i)) + (1-y_i) \log(1 - \sigma(f_\theta(x_i))) \\ &= \sum_{i=1}^{N} l_\sigma(y_i, f_\theta(x_i)) \end{aligned}$$

- Simplifies a lot when expressed in $Y = \pm 1$
- Key point: l_σ differentiable, we have $\frac{\partial}{\partial f} l_\sigma(y, f)$ and even $\frac{\partial^2}{\partial f^2} l_\sigma(y, f)$

Logistic Regression: Learning Algorithms

- No closed form solution. Iterative, gradient based optimization needed
- For most regularizers a convex problem, well behaved, well studied (can be important in practice/production!)
- Vast literature (primal/primal-dual/dual, stochastic/batch, ...)
- Key ingredient: $\nabla_\theta \sum_{i=1}^N l_\sigma(y_i, f_\theta(x_i))$
- We know what to do - Let's do (shallow) back-propagation
- Forward pass: let $f_\theta(x) = x^T w$
    - MVM: $f = Xw$
    - loss vector: $l = l(y, f)$ (scalar operation)
    - loss value: $L = \sum_i l_i$ (reduction)
- Backward pass: compute $\sum_{i=1}^N \nabla_\theta l_\sigma(y_i, f_\theta(x_i))$ as $\sum_i \frac{\partial}{\partial f_i} l_\sigma(y, f_i) \cdot \nabla_\theta x_i^T w$
    - loss derivative vector: $d_i = \frac{\partial}{\partial f_i} l_\sigma(y, f_i)$ (scalar operation)
    - MVM: $\nabla_\theta L(\theta) = X^T d$

Summary

- A probabilistic view allows us to generalize to other output spaces
- Differentiable objective: gradient based
- We can apply the same framework and the same learning algorithms, as long as we have differentiable log-likelihood terms
    - Counts: Poisson, Neg.-Binomial
    - Multi-class: categorical distribution, ("softmax")
    - etc.

Exercise 3 (30 min)

Decision Trees and XGBoost

- One of the most successful methods used on Kaggle
- Not directly part of RAPIDS
- XGBoost
    - has great out of the box performance
    - interpretable by examining the structure
    - has a fast, high-quality implementation (same people behind MxNet DL lib)
- Function class:
    - binary decision trees (think axis-aligned space partitioning)
    - each tree represents a piece-wise constant function
    - each node n either
        - is a leaf node: contains the function value
        - is a split node: has a condition on a single input dimension of the form $x_j < s_n$
    - We map an input (vector) to an output (scalar) by traversing the tree until we hit a leaf and report the value stored there
    - functions now look very different: non-linear

Decision Tree: 1D-Example

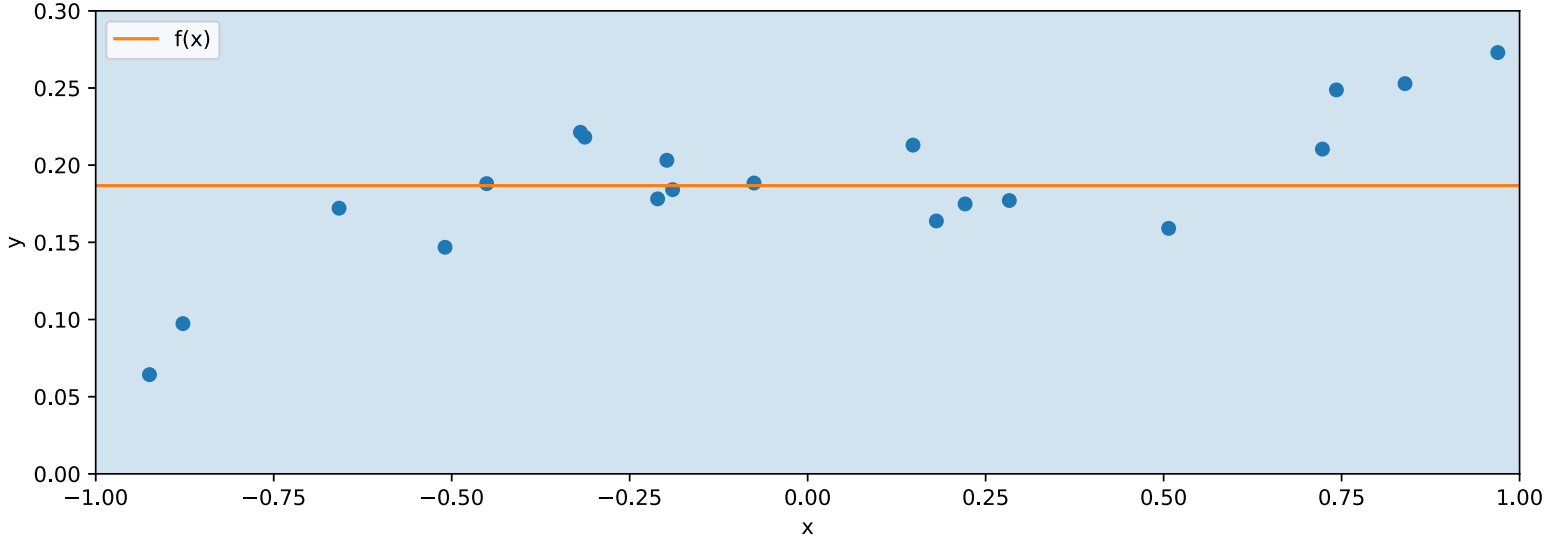
```
class Node:
    def __init__(self):
        self.split = None # split position
        self.left  = None # region left of the split
        self.right = None # region right of the split
        self.value = None # value of the node

def eval1d(node, x):              #traverse the tree to evaluate the function
    if node.split is None:        # no split: it's a leaf
        return n.value            #           report the function value
    if x < node.split:            # the point falls into the left region
        return eval1d(node.left, x)
    return eval1d(node.right, x) # the point falls into the right region
```

- Next:
  - First, some examples
  - How to build the tree

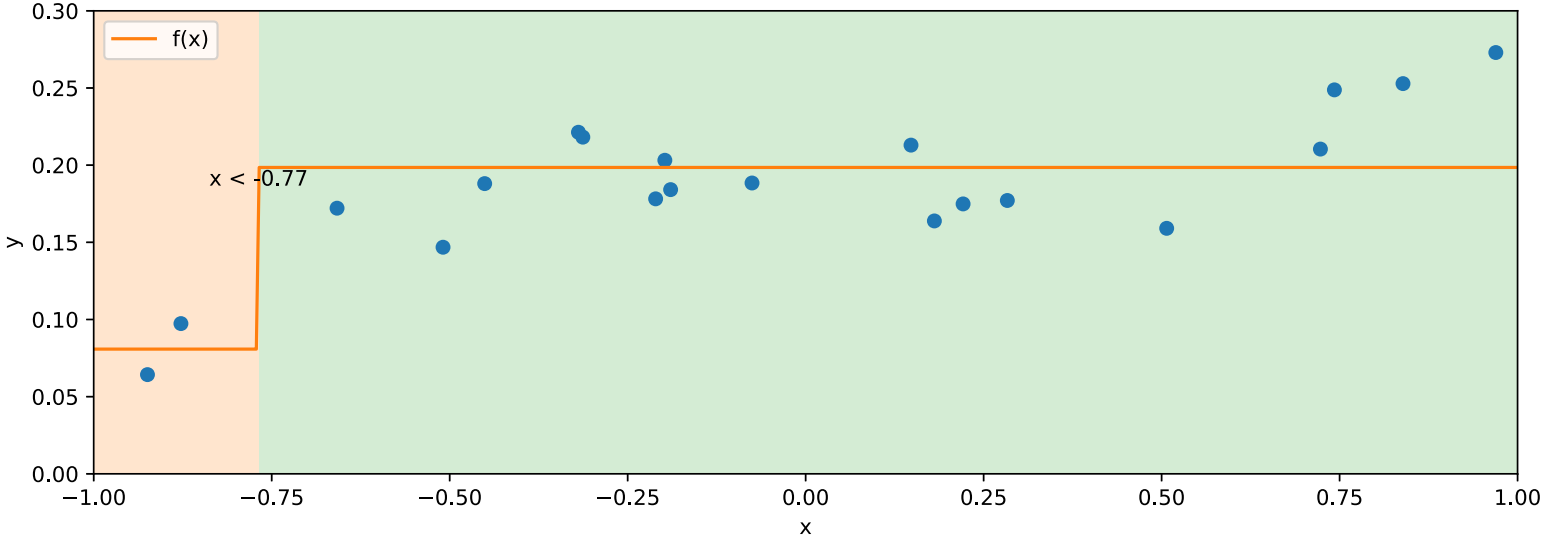
Depth 0

- No split
- A single leaf
- All points assigned
- Constant function value



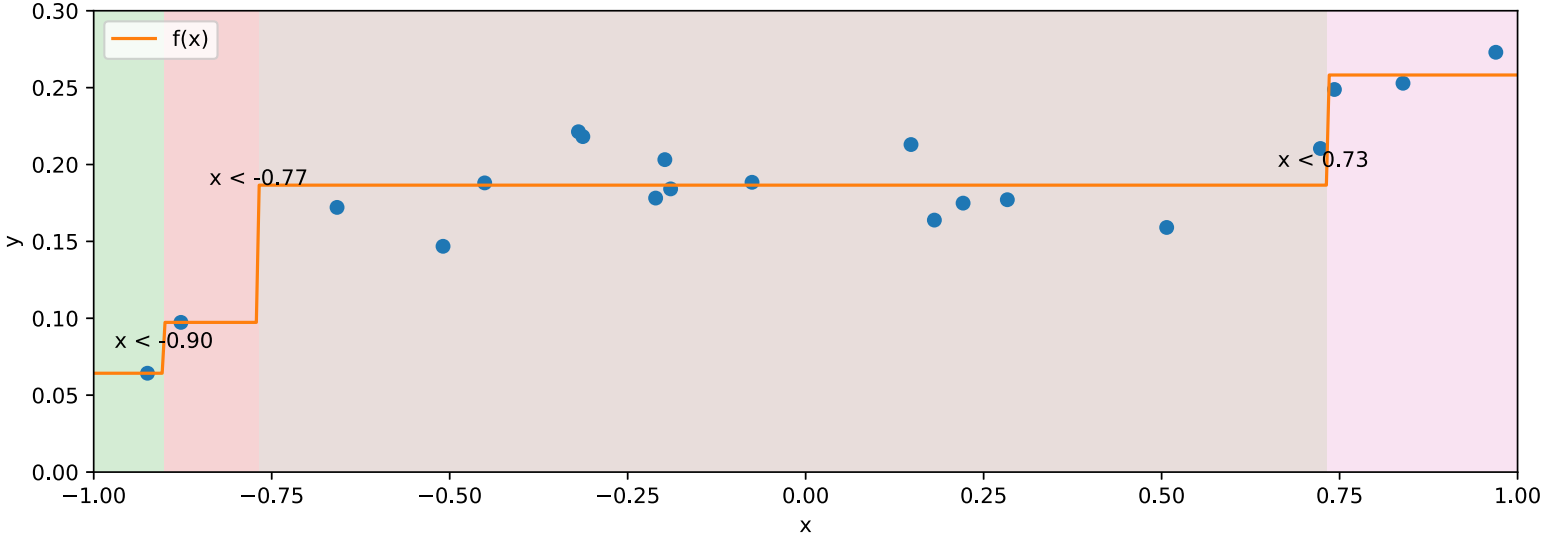
Depth 1

- One split
- Two leafs
- Two constant regions



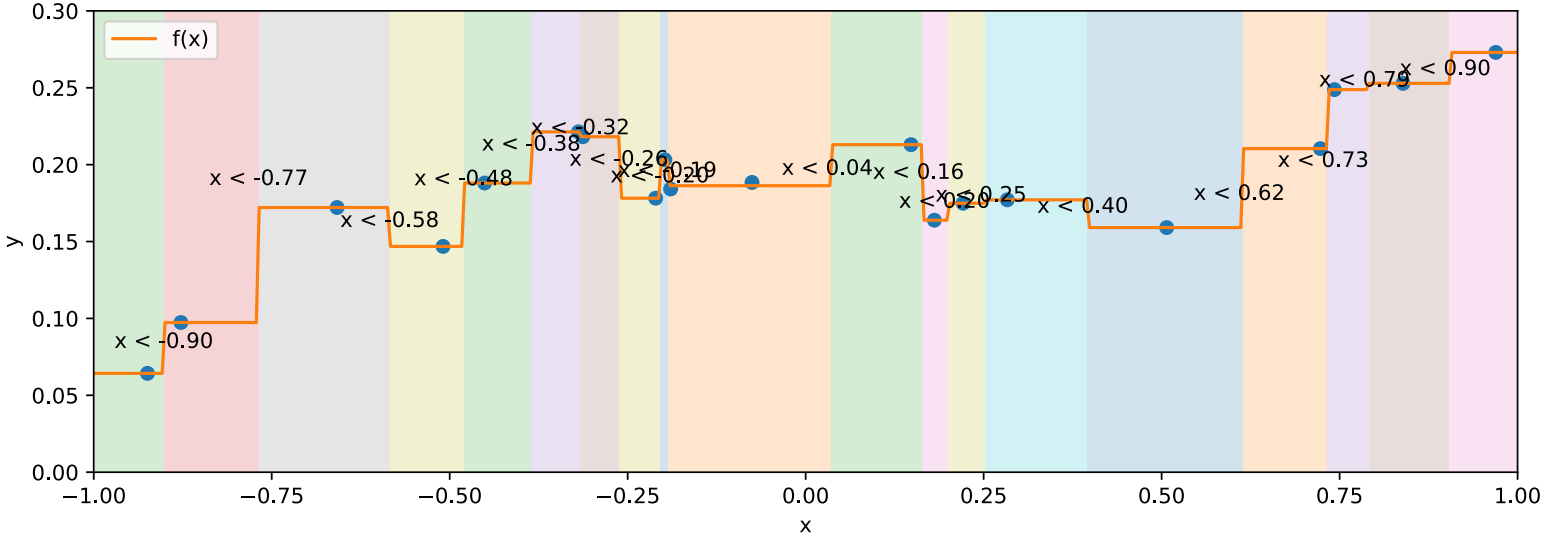
Depth 2

- Three splits
- Four leaves - four regions



Depth 8

- Etc.
- Unique mappings:
    - point to value (because function)
    - point to leaf (remember for later)
- So given a function represented by a tree $t(x)$, we can decompose it into two parts:
    - Map points to one of the L leaves: $q : \mathbb{R} \mapsto \{0, \ldots, L-1\}$
    - A vector $w \in \mathbb{R}^L$ of L weights: the constant values at the leaves
    - Then, $t(x) = w_{q(x)}$



Exercise 4

Challenges Learning Decision Trees

- Tree is discrete: no gradient-based training
    - optimization over discrete objects often result in combinatorial explosion
- A single tree is highly non-linear:
    - small changes in the data might dramatically affect the structure
- Techniques:
    - Discrete optimization: use greedy heuristic
    - High-variance of single tree: use an ensemble of many trees
- Simplest tree ensemble method: bagging/random forrest (also available in `cuml`)
    - Sub-sample the dataset and fit a different tree on each
    - Performs often worse than XGBoost

Learning Algorithm: XGBoost

- Goals:
  - high-level understand how the algorithm works
  - gain familiarity with notation and terminology to understand the API
- A few crucial details omitted, like regularization. But easy to add them, once the algorithm is clear
  - More details the excellent official intro: https://xgboost.readthedocs.io/en/latest/tutorials/model.html (https://xgboost.readthedocs.io/en/latest/tutorials/model.html)
- Notation:
  - $f_\theta(x)$: the function, represented by an ensemble of trees
  - $t_\theta(x)$: a single binary tree
    - L: the number of *leaves* in the tree
    - w: a L-vector, containing the *values* of the piece-wise constant regions
    - $q : \mathcal{X} \mapsto 1, \ldots, L$: mapping of input (e.g. training) points to leaves
    - $\mathcal{L}_n := \{i \mid q(x_i) = n\}$: set of training points assigned to leaf node n

Exercise 5

Learning Algorithm: XGBoost

- Boosting: stage-wise (greedy!) additive model of T trees defines the function f_θ as

$$f_\theta^{(T)}(x) = \sum_{k=1}^{T} t_\theta^{(k)}(x)$$

  - or recursively, which reflects, how we will learn the ensemble

$$f_\theta^{(T)}(x) = f_\theta^{(T-1)}(x) + t_\theta^{(T)}(x)$$

- The algorithm progresses sequentially, performing T rounds
- Implication: $t^{(k)}$ should not be trained on the original labels y but the *residual* $y - f^{(k)}$ (in regression)
  - the k-th tree tries to "fix" the errors, the model at the previous round made
  - But: *without* revisiting their parameters (greedy)
- Need two ingredients, that are related
  - Criterion to optimize to set the function values
  - Scoring structures to decide where to make a split

XGBoost: Loss Function

- Similar to GLMs, the trees in XGBoost are functions into the Reals, hence we can use the same objective functions/likelihood terms (but we will see again, that the details can be abstracted away as well)
    - regression: $l_{sq}(y, f_\theta(x)) = \frac{1}{2}(y - f_\theta(x))^2$
    - classification: $l_\sigma(y, f_\theta(x)) = \log \sigma(y f_\theta(x))$
- The optimization problem at each stage k is to add a tree such that the error is reduced, i.e.

$$E(t_\theta^{(k)}) = \sum_{i=1}^{N} l(y_i, f_\theta(x_i)^{(k-1)} + t_\theta^{(k)}(x_i))$$

XGBoost Loss: Quadratic Approximation

- Instead of considering E directly, the first approximation the XGBoost method introduces, is to approximate this error with it's *second order Taylor expansion*, i.e. with a quadratic function (which is of course exact for the squared loss)
- We treat the existing model as the point and the new tree as the perturbation, with g_i, h_i the first and second derivatives of the loss

$$E(t_\theta^{(k)}) = \sum_{i=1}^{N} l(y_i, f_\theta(x_i)^{(k-1)} + t_\theta^{(k)}(x_i))$$

$$\sum_{i=1}^{N} l(y_i, f_i + t_i) \approx \sum_{i=1}^{N} l(y_i, f_i) + g_i t_i + \frac{1}{2} h_i t_i^2 \doteq \sum_{i=1}^{N} g_i t_i + \frac{1}{2} h_i t_i^2$$

- Just like GLMs! Again, from the loss, we only need derivatives to drive the algorithm!
  - $g = \frac{\partial}{\partial f} l(y, f), g_i = g(y_i, f(x_i))$
  - $h = \frac{\partial^2}{\partial f^2} l(y, f), h_i = g(y_i, f(x_i))$
- Of course, for $l_{sq}(y, f)$ this is exact and $g = (f - y), h = 1$

XGBoost: Making w explicit

- Remember our view on trees:
  - A vector $w \in \mathbb{R}^L$ of L weights: the constant values at the leaves
  - Then, $t(x) = w_{q(x)}$
- Given a tree, i.e. w and q, we can find all training samples in a leaf node n
  - We can find the set $\mathcal{L}_n = \{i \mid q(x_i) = n\}$
  - Note: $t(x_i) = w_n$ for all x_i s.t. $i \in \mathcal{L}_n$
- Now for any given tree, with L the number of leaves , we can re-write $E(t) = \sum_{i=1}^{N} g_i t_i + \frac{1}{2} h_i t_i^2$ in terms of w and $\mathcal{L}$:

$$E(t) = \sum_{i=1}^{N} g_i t_i + \frac{1}{2} h_i t_i^2 = \sum_{n=1}^{L} (\sum_{i \in \mathcal{L}_n} g_i) w_n + \frac{1}{2} (\sum_{i \in \mathcal{L}_n} h_i) w_n^2$$

$$= \sum_{n=1}^{L} G_n w_n + \frac{1}{2} H_n w_n^2$$

- Nicely decomposes over the parameters of the tree

XGBoost: Summary

- Find the minimizer w^* of $E(t) = \sum_{n=1}^{L} G_n w_n + \frac{1}{2} H_n w_n^2$ analytically
  - Assumption: the loss is twice differentiable, (strongly) convex: $h > 0$

$$w_n^* = -\frac{G_n}{H_n} \qquad E(w^* \mid q) = -\frac{1}{2} \sum_{n=1}^{L} \frac{G_n^2}{H_n}$$

- We still assume that we are given some particular tree *structure*, i.e. the point to leaf mapping q
- Now: contribution of leaf n to the loss: $\propto \frac{G_n^2}{H_n} = \frac{\left(\sum_{i \in \mathcal{L}_n} g_i\right)^2}{\sum_{i \in \mathcal{L}_n} h_i}$ - is it worth breaking up the points in leaf n, i.e. $\mathcal{L}_n$ into two? What's the "gain"?
- Gain of new split into n_{left}, n_{right}: "contrib. $\mathcal{L}_{n_{left}}$ + contrib. $\mathcal{L}_{n_{right}}$ - contrib. $\mathcal{L}_n$"

$$\text{Gain} = \frac{G_{n_{left}}^2}{H_{n_{left}}} + \frac{G_{n_{right}}^2}{H_{n_{right}}} - \frac{G_n^2}{H_n}$$

XGBoost: Greedy Tree Building Algorithm

- Given a set of N training points:
    - for each feature:
        - sort the points by feature value
        - for each possible $N-1$ split positions find the split with the best gain
    - partition the points according to the split
    - recurse left of the split and right of the split

Tree Building Algorithm in 1D

- Does not take into account searching over features

```
def gain(g,h,it):
    Gl, Gr = sum(g[:it+1]), sum(g[it+1:])
    Hl, Hr = sum(h[:it+1]), sum(h[it+1:])
    return  Gl**2 / Hl # contrib. left
          + Gr**2 / Hr # contrib. right
          - (Gl+Gr)**2 / (Hl+Hr) # cost of removing current leaf

def build1d(x, g, h, d, max_depth):
    n = Node()
    n.value = -sum(g) / sum(h) # determine current function value E, i.e. the constant w
    # check stopping criterion:
    if d == max_depth or len(x) == 1:
        return n
    # evaluate splits and maximize gain
    max_score, split = max([(gain(g,h,it) , it) for it in range(len(x) - 1)])
    n.split = 0.5*(x[split] + x[split+1]) # split in the middle
    # divide points and recurse on the split
    n.left = build1d(x[:split+1], g[:split+1], h[:split+1], d+1, max_depth)
    n.right = build1d(x[split+1:], g[split+1:], h[split+1:], d+1, max_depth)
    return n
```

Toy XGBoost Algorithm for Regression

```
def xgboost1d(xs, ys, rounds, depth): #single input feature is already sorted
    forrest = []                      #we're growing a forrest
    yprev = np.zeros_like(ys)         #initial predictions are constant 0
    h = np.ones(len(ys))              #for squared loss, h is constant 1
    for r in range(rounds):
        g = yprev - ys                #update g, the residual
        root = build1d(xs, g, h, 0, depth) #tree
        yprev += np.array([eval1d(root, x_) for x_ in xs]) #update the prediction of the whole model
        forrest.append(root)          #add to the forrest
    return forrest

def pred1d(forrest, x):
    pred = np.zeros_like(x.flatten())
    for tree in forrest:              #evaluate contribution from each tree and sum up
        pred += np.array([eval1d(tree, x_) for x_ in x])
    return pred
```

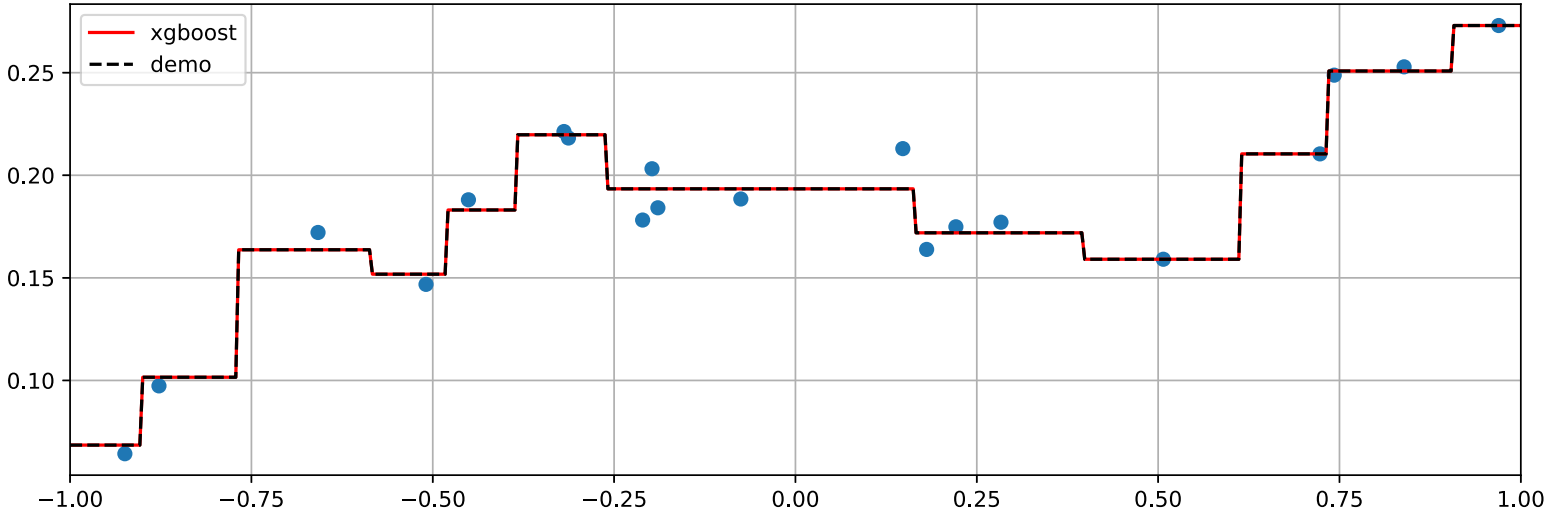
XGBoost API Example

```
import xgboost as xgb

dtrain = xgb.DMatrix(x, y)
dtest = xgb.DMatrix(xtest)
param = {'max_depth':3,                          #depth of the tree
         'eta':1,                                #shrinkage: fractional update
         'objective':'reg:squarederror',         #regression: loss function
         'reg_lambda':0}                         #l2 regularization parameter

num_round = 2                                    #number of rounds: trees in the forrest

bst = xgb.train(param, dtrain, num_round)
xgb_pred = bst.predict(dtest)
```



Exercise 6 (30 min)

Summary

- Discussed trees as a function class
- Saw the same techniques as in GLMs to model data types
- Worked through the XGBoost derivation
    - Greedy approximations
    - Taylor approximation
    - Loss-based splitting criterion (structure score)
- Looked at a toy implementation to clarify the concepts
- Important, but missing here: regularization
    - L2: penalize magnitude of weights
    - Prefer shallower trees: subtract penalty from gain of a split
    - Shrinking ("learning rate"): scale down contributions of individual trees added in each round

Outline

- The RAPIDS data science stack and the case for "Classical" ML
- Supervised learning
    - Recap of Fundamental Concepts
    - Generalized linear models (GLMs)
    - Gradient-boosted decision trees, XGBoost
- Unsupervised learning
    - Dimensionality reduction
    - Principal component analysis (PCA)
    - Non-linear techniques

Unsupervised Learning

- No labels. "Training" set consists of high-dimensional vectors $x \in \mathbb{R}^D$
- Goal: find structure in the data, e.g.
    - Find similarities (clustering)
    - Find lower-dimensional representation (dimensionality reduction)
        - more efficient, without spurious dimensions
        - can be initial step of a ML pipeline
        - 2D/3D: visualization
- Methods make strong assumptions on the structure

Principal Components Analysis

- Canonical dimensionality reduction example
- Goal: find a linear projection onto orthogonal vectors
- Criterion: preserve the maximum amount of variance in the data

Principal Component Analysis

- Dataset: N vectors $x_i \in \mathbb{R}^D$, stored in $X \in \mathbb{R}^{N \times D}$
- For simplicity, assume data is centered around the origin: $x_i \leftarrow x_i - \mu$
- Covariance matrix: $\Sigma_X = \frac{1}{N} X^T X, \Sigma_X \in \mathbb{R}^{D \times D}$
- Find k projection vectors $u_j \in \mathbb{R}^D$, such that $u_i \perp u_j$ for $i \neq j$, stored in $U \in \mathbb{R}^{D \times k}$
- Variance for j-th projection: $\frac{1}{N} u_j^T X^T X u_j = u_j^T \Sigma_X u_j$
- Optimization problem:

$$\max_U \operatorname{tr}(U^T \Sigma_X U), \text{ s.t. } u_i \perp u_j, i \neq j$$

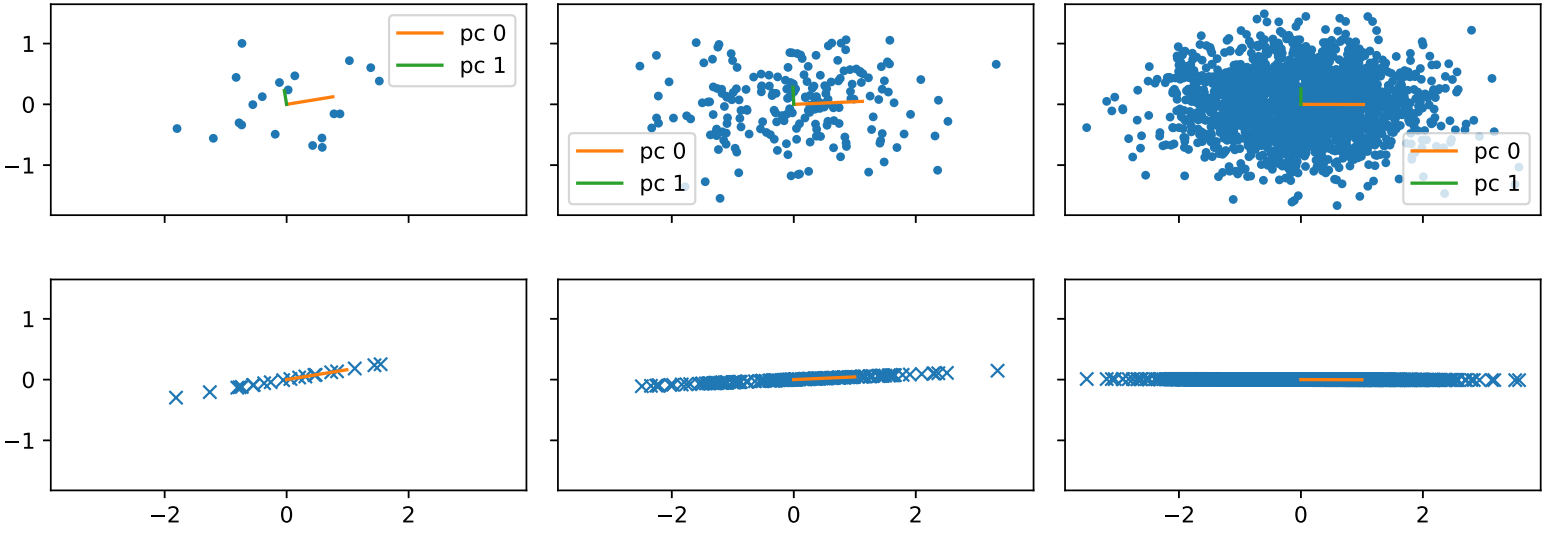
Principal Component Analysis

$$\max_U \operatorname{tr}(U^T \Sigma_X U), \text{s.t.} u_i \perp u_j$$

- Solution: k eigenvectors of Σ_X corresponding to the largest eigenvalues
- Eigenvalues of Σ_X: $\lambda_j \geq 0$. Let them be ordered such that λ_0 is the largest
- Corresponding eigenvectors q_j
- For $k = 1$: maximize $u^T \Sigma_X u = u^T \sum_j \lambda_j q_j q_j^T u^T$
- Solution: pick $u = q_0$
- In general: $U = [q_0, \ldots, q_{k-1}]$
- Variance of the j-th projection: λ_j
- Alternative view: best rank k approximation of data matrix X
    - SVD of X

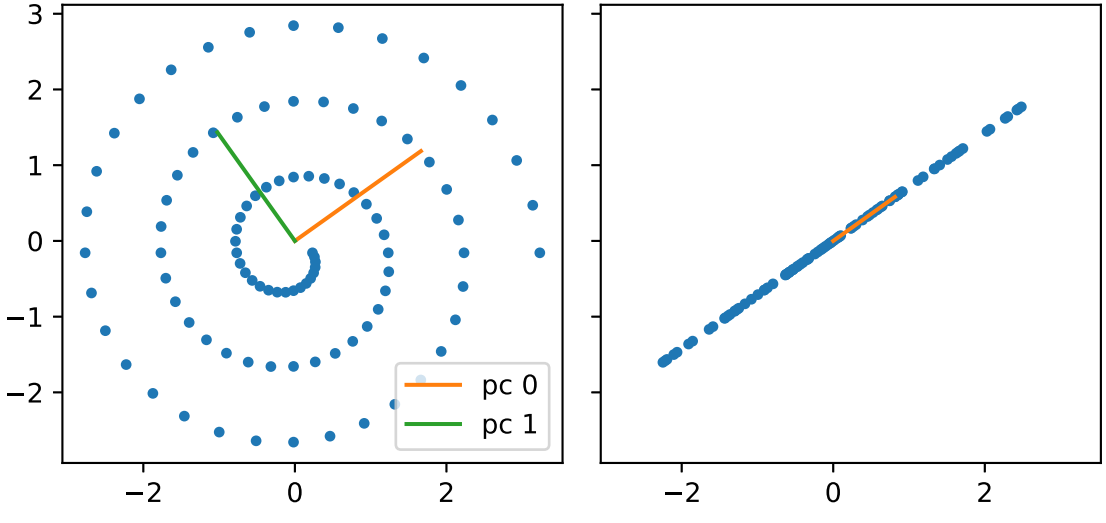
PCA: Assumed Structure

- "Pancake" model: data lives on a hyper plane with little volume around it
- Variance preservation formulation:
    - PCA prioritizes maintaining large distances
    - Small distances are rather considered noise and can be collapsed



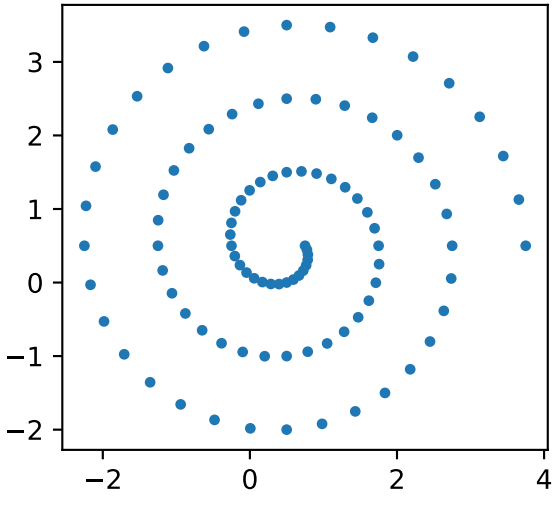
Exercise 7 (30 min)

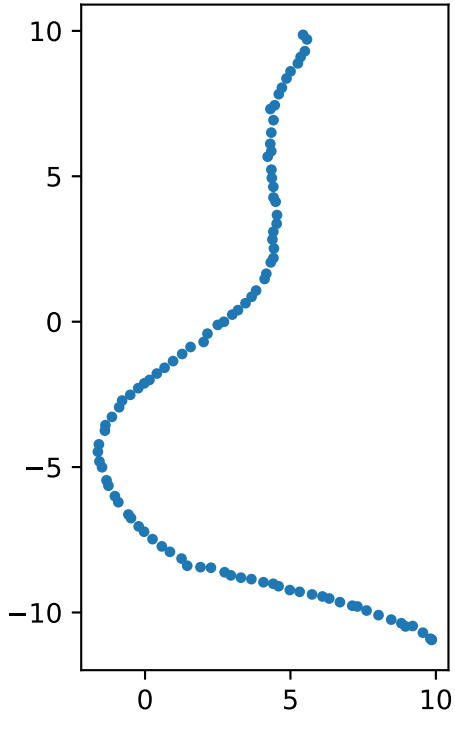
A Failure Case for PCA



Non-linear Dimensionality Reduction Techniques

- Assumption: Data lives on a low-dimensional, non-linear manifold
- This means that global distances can be very misleading for discovering structure
- Need to focus on local neighborhoods
- Close points on the manifold should also lie close in the ambient space
- Goal: use local information to "patch" together





Non-linear Dimensionality Reduction Techniques

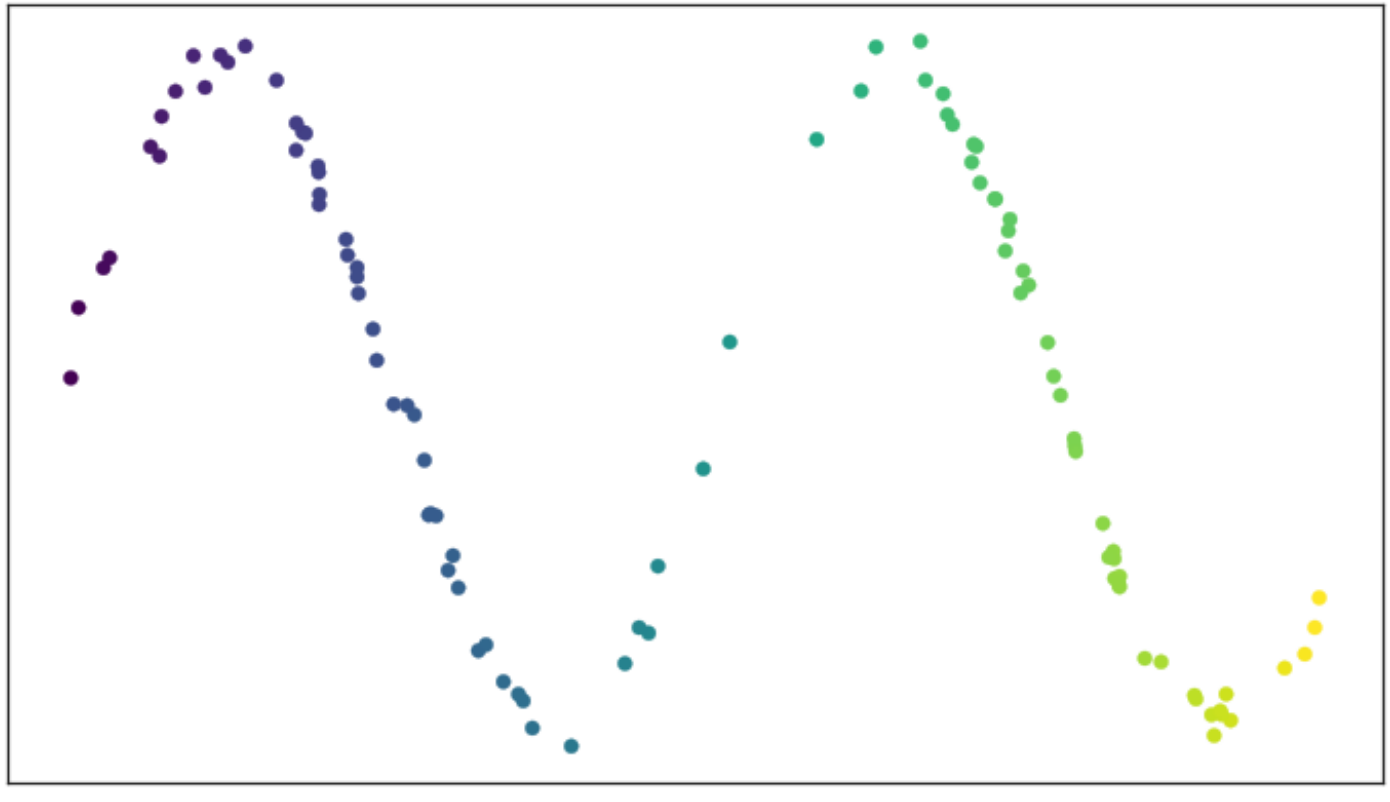
- Two most popular techniques:
    - tSNE: t-distributed Stochastic Neightborhood Embedding (van der Maarten, Hinton, 2008)
    - UMAP: Uniform Manifold Approximation and Projection (McInnes et al, 2018)
- UMAP can be seen as an evolution of tSNE
    - more rigourous mathematical foundation
    - slightly different formulation with large practical (i.e. computational) benefits
    - From a high-level, conceptually, very similar
- Both are two-step procedures:
    1. Define a weighted neighborhood graph in high-dimensions
        - based on local distances
        - weights are similarity measures: the closer two points, the higher the weight
        - probabilistic interpretation: use Gaussian density as similarity measure
    2. Fit the embeddings vectors, that can be interpreted as force-directed graph layout
        - define a similarity measure in low-dimensions as well, but use different distributions
        - more heavy tailed
        - us an information-theoretic criterion comparing these two distributions over the whole graph

UMAP

- We'll go over the high-level steps of graph construction and the optimization criterion
- Full mathematical picture is quite involved and out of scope
- Plots from official UMAP documentation (https://umap-learn.readthedocs.io/en/latest/how_umap_works.html)

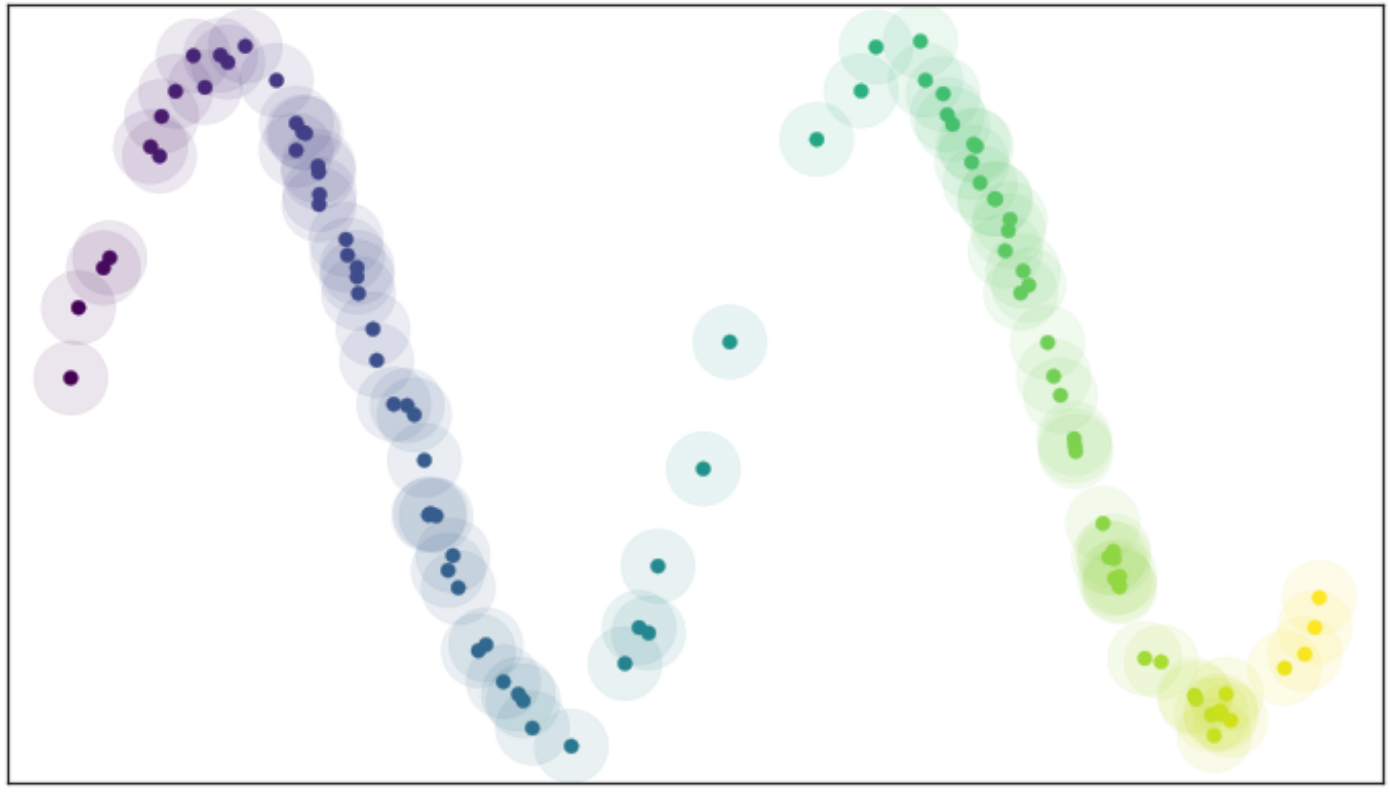
UMAP

Let's start with some data



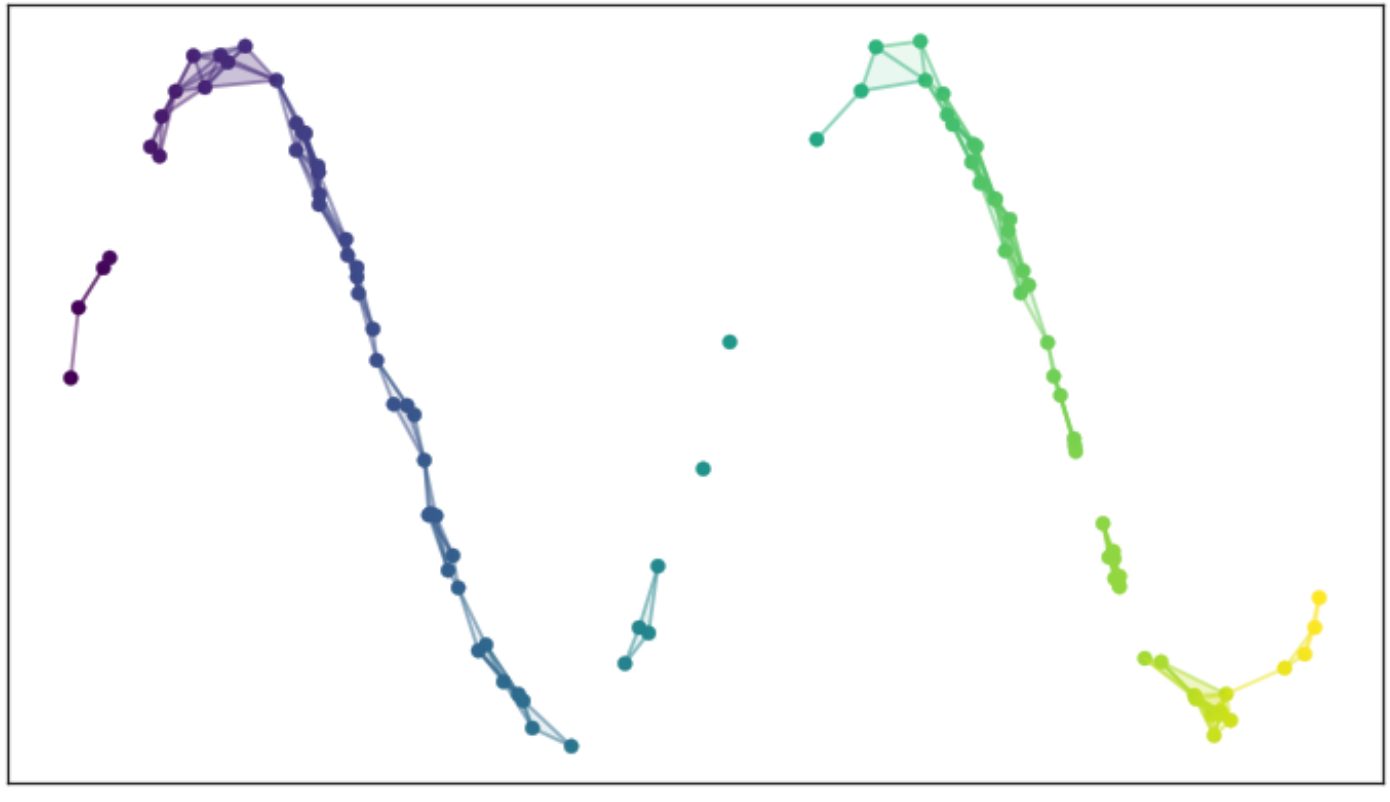
UMAP

To find and connect locally similar points, we could look inside balls around each point and connect two points if the balls overlap.



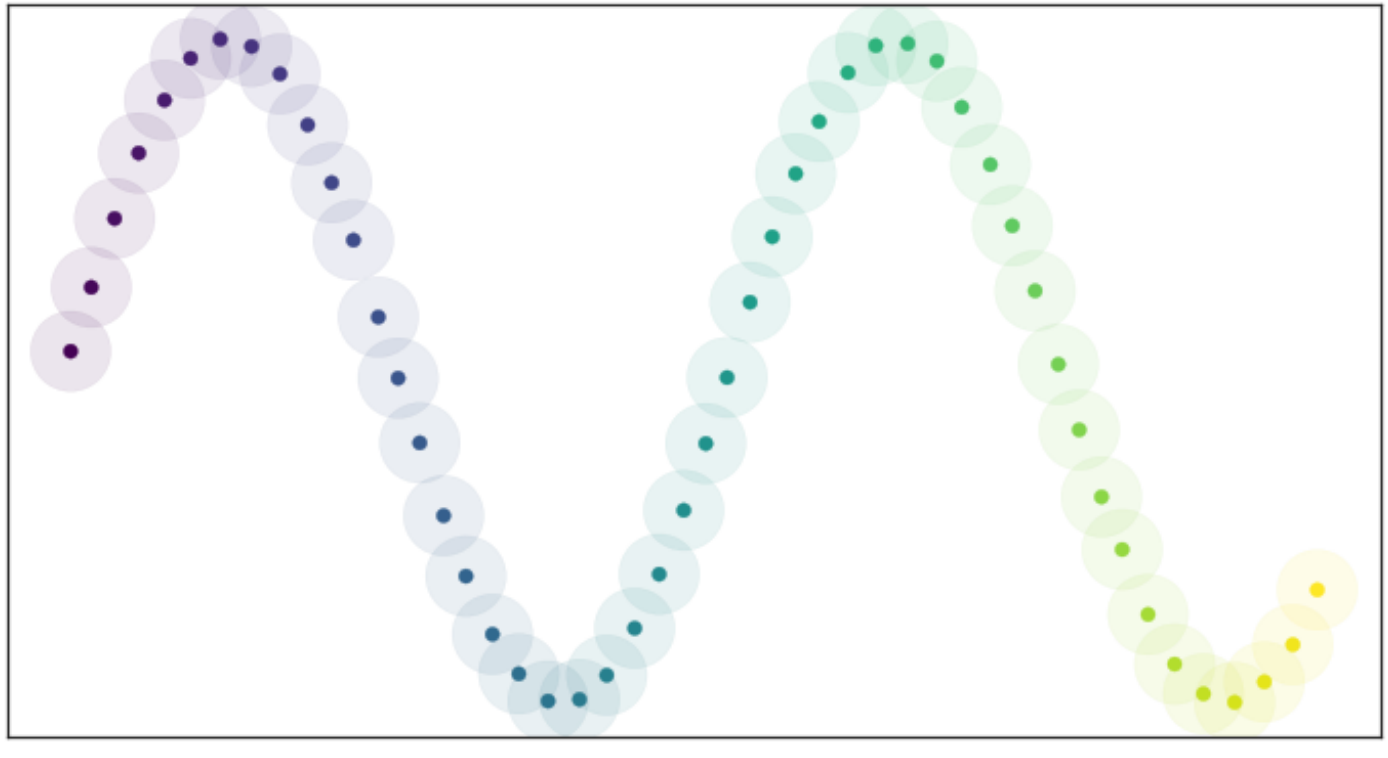
UMAP

Some points would be isolated



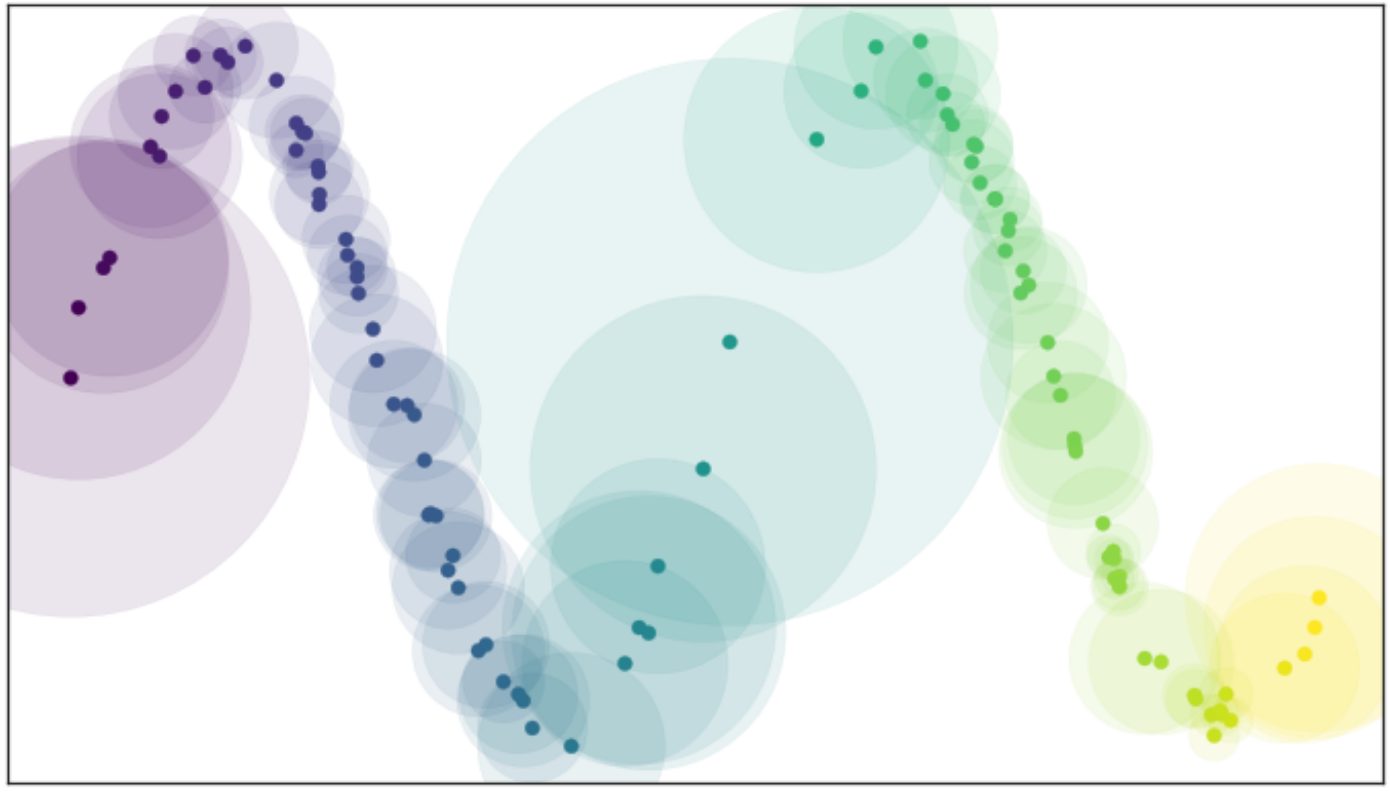
UMAP

This would be a much less severe problem, if our sampling were more uniform



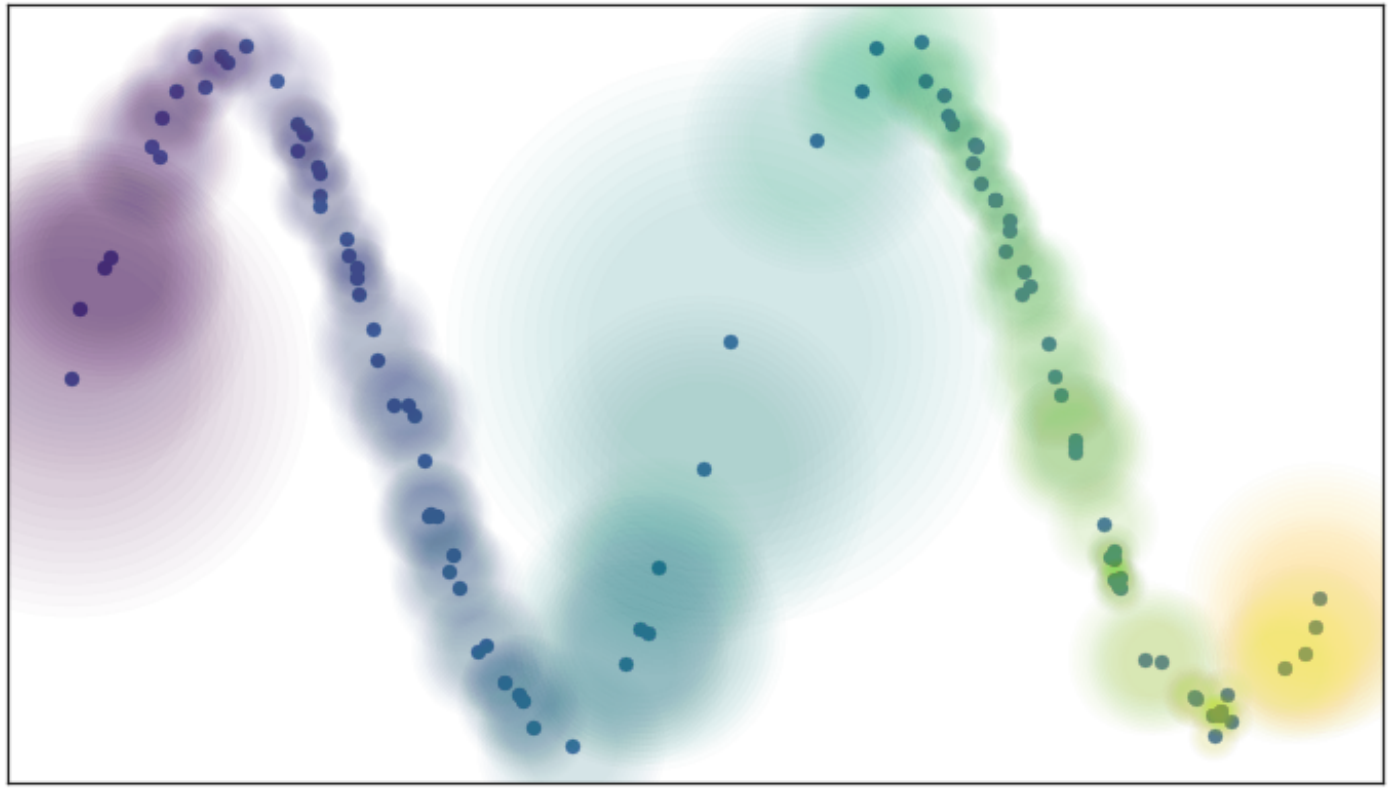
UMAP

Get around this by allowing locally adaptive radii.



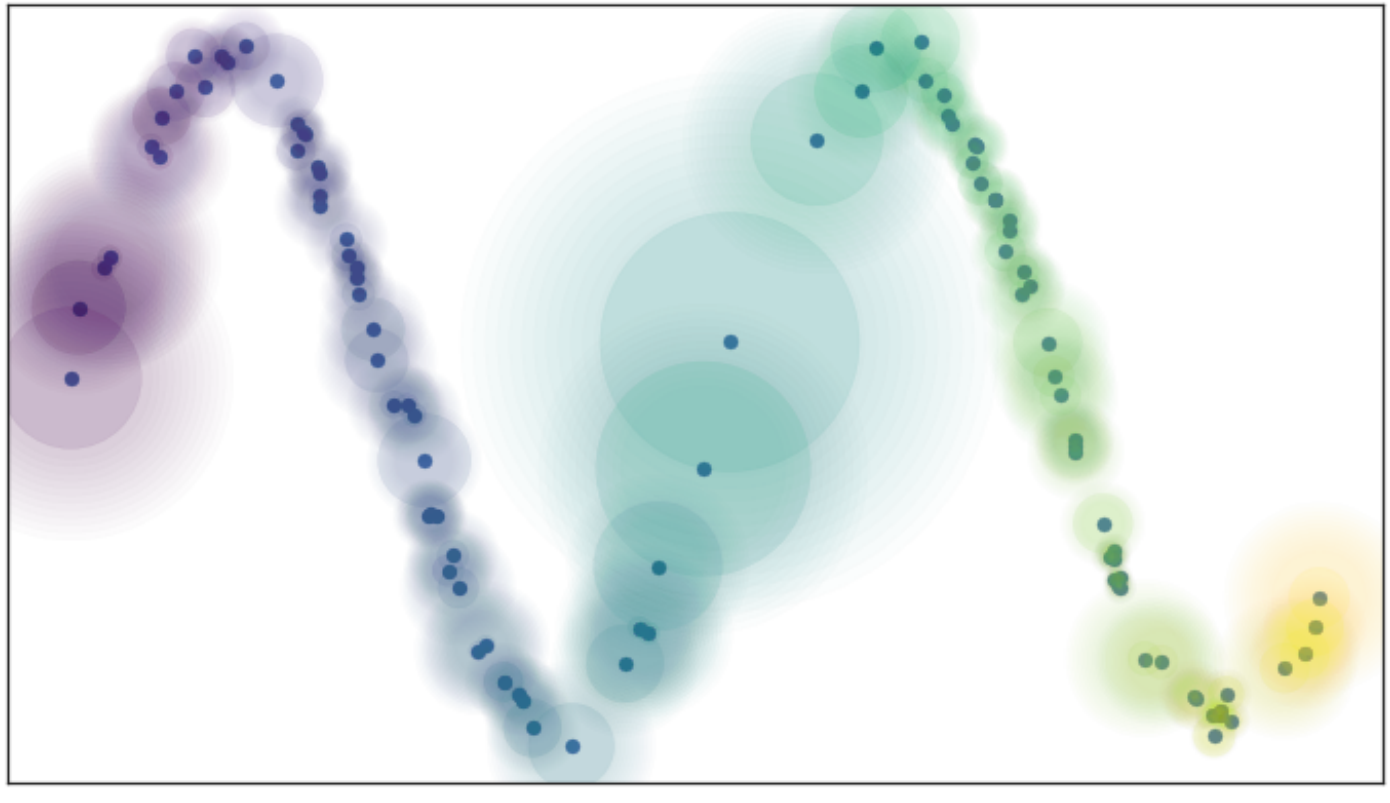
UMAP

Instead of solid balls, make them fuzzy with a distance dependent decay.



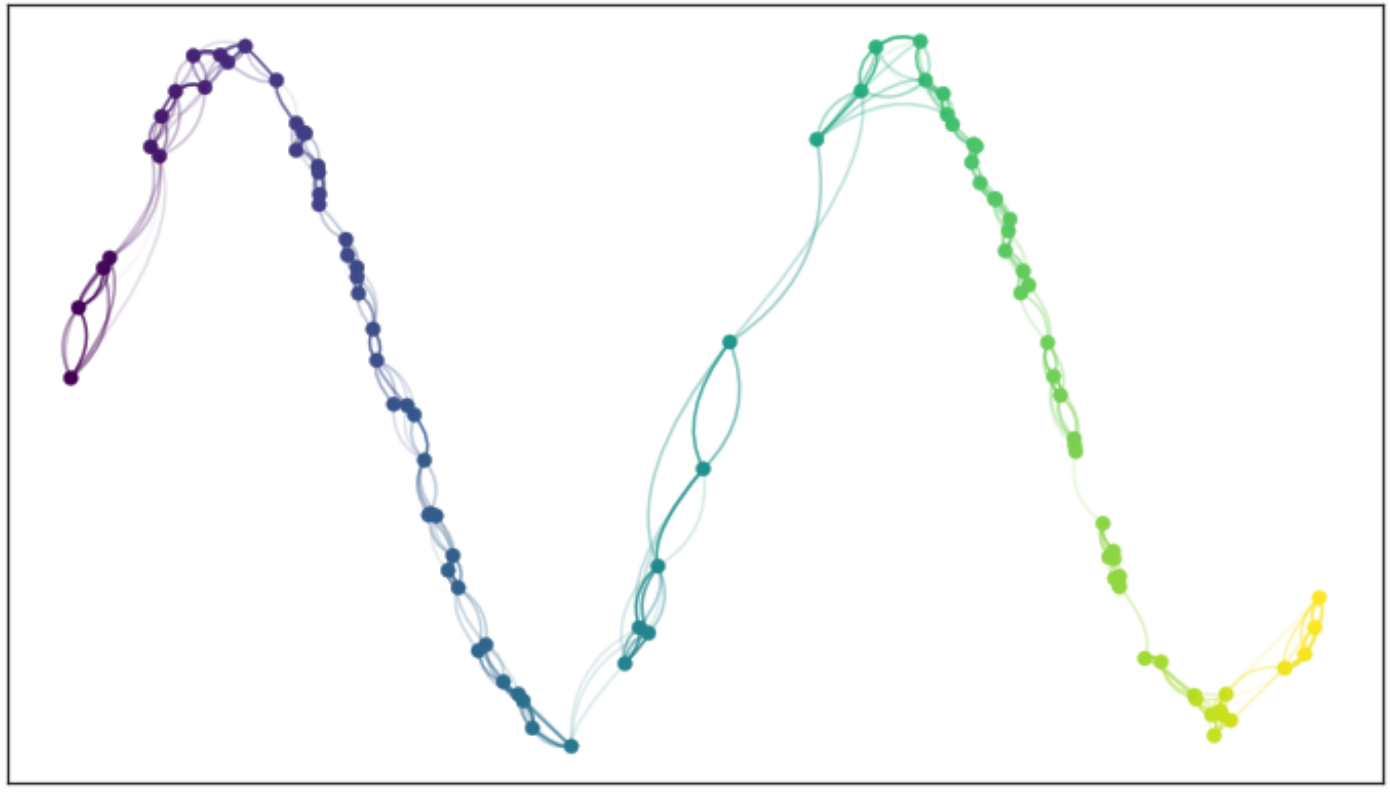
UMAP

To avoid the issue of isolated points, the authors introduce the assumption of local connectivity: each point has at least one neighbour. Distances are expressed relative to the nearest neighbour.

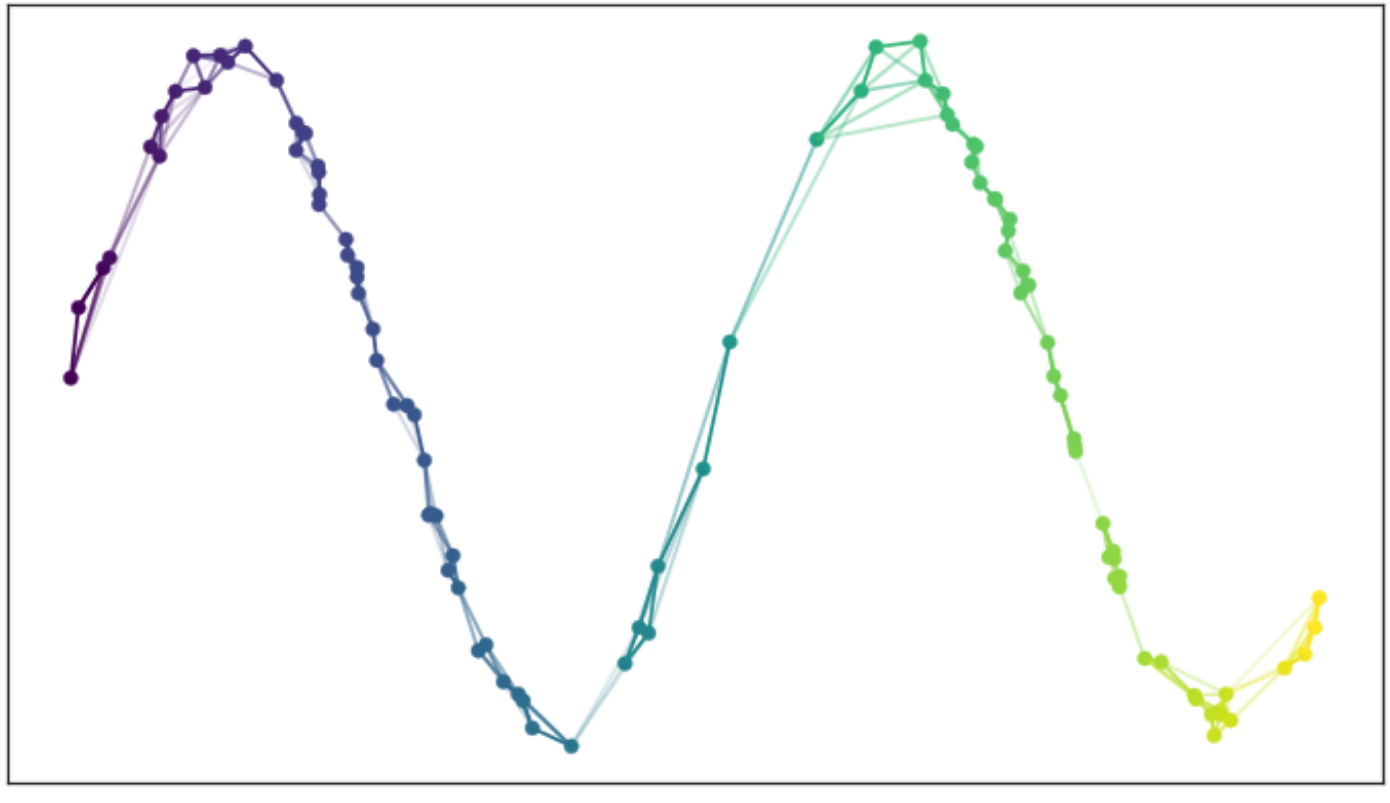


UMAP

The resulting weighted graph might not be symmetric: nodes can disagree on the strenght of the connection. Make symmetric using the probabilistic interpretation.



UMAP



UMAP Graph Construction - Take Away

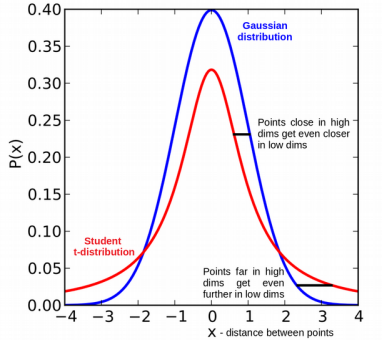
- UMAP is very particular in its graph construction
    - the authors justify each decision taken with arguments from topology
    - additional assumptions are very clearly stated
- What we end up with, given the high dimensional data matrix $X \in \mathbb{R}^{N \times D}$
    - a graph $G = (V, E)$ with weights $w_D : E \mapsto [0, 1]$
    - Vertices $V = 1, \ldots, N$ represent the N input data points
    - capturing similarities adapted to local sampling density:
        - $w_D(i, j)$ will large if $\|x_i - x_j\|_2$ is small
- Goal: "reproduce" this information in low-dimensional Euclidean space
    - UMAP defines a similarity funcition $w_d : E \mapsto [0, 1]$ in low dimensions as well
    - Similarly, $w_d(i, j)$ will large if $\|y_i - y_j\|_2$ is small
    - find the embedding matrix $Y \in \mathbb{R}^{N \times d}$, e.g. $d = 2$

UMAP Opimtization Criterion

- UMAP minimizes the following cross-entropy objective

$$\begin{aligned}\mathcal{L}(Y) &= \sum_{e \in E} w_D(e) \log \frac{w_D(e)}{w_d(e)} + (1 - w_D(e)) \log \frac{1 - w_D(e)}{1 - w_d(e)} \\ &= -\sum_{e \in E} w_D(e) \log w_d(e) - (1 - w_D(e)) \log(1 - w_d(e))\end{aligned}$$

- Encourages Y such that w_d values match w_D values
- We can bias the preference for first or second term by the choices of distributions used in w_D and w_d



Exercise 8

Summary

- Dimensionality reduction useful for data visualization, exploration, ...
- Linear projections of PCA often a good starting point
- Exciting to see powerful non-linear techniques developed to address PCA's short comings
- Can be tricky to develop a good intuition for them

Conclusion

- The RAPIDS data science stack and the case for "Classical" ML
- Supervised learning
    - Recap of Fundamental Concepts
    - Generalized linear models (GLMs)
    - Gradient-boosted decision trees, XGBoost
- Unsupervised learning
    - Dimensionality reduction
    - Principal component analysis (PCA)
    - Non-linear techniques