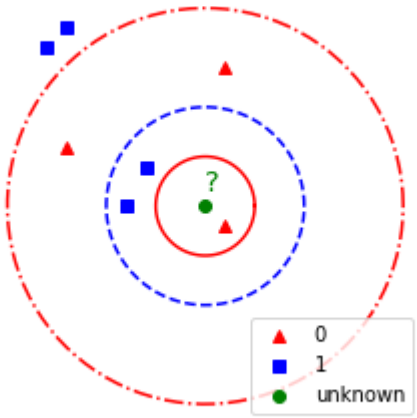
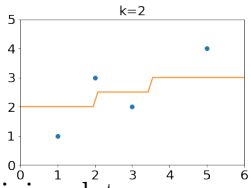
3 Fundamental Algorithms (part 5 of 5)



k-Nearest Neighbors (kNN)



Training in k-NN consists only of storing the training data.

- *k-NN classification* assigns to a new $\mathbf{x}$ the _____ *label* among its k nearest neighbors.
- *k-NN regression* assigns to a new $\mathbf{x}$ the _____ *numeric value* of its k nearest neighbors.

Distance metrics

Euclidean distance is the typical metric. Others may be worth exploring. For two vectors $\mathbf{a}$ and $\mathbf{b}$,

- *Euclidean* distance$(\mathbf{a},\mathbf{b}) = \sqrt{\sum_{i=1}^{D}\left(a^{(i)}-b^{(i)}\right)^2}$ (also called the 2-norm)
  e.g. This is the familiar length of the line segment joining two points.
- *Manhattan* distance$(\mathbf{a},\mathbf{b}) = \sum_{i=1}^{D}\left|a^{(i)}-b^{(i)}\right|$ (also called the 1-norm or absolute-value norm or taxicab distance)
  e.g. This is the _____ in blocks between two points on a square grid street layout.
- *Minkowski* distance$(\mathbf{a},\mathbf{b}) = \left(\sum_{i=1}^{D}\left|a^{(i)}-b^{(i)}\right|^p\right)^{\frac{1}{p}}$ for integer p. $p =$ _____: Manhattan; $p =$ _____: Euclidean; $p =$ _____: $\max(\{|a_i - b_i|\})$; $p =$ _____: $\min(\{|a_i - b_i|\})$.
- *Negative cosine similarity*[1] distance$(\mathbf{a},\mathbf{b}) = -\cos\angle(\mathbf{a},\mathbf{b}) = -\dfrac{\mathbf{a}\cdot\mathbf{b}}{||\mathbf{a}||\cdot||\mathbf{b}||} = -\dfrac{\sum_{i=1}^{D}a^{(i)}b^{(i)}}{\sqrt{\sum_{i=1}^{D}\left(a^{(i)}\right)^2}\sqrt{\sum_{i=1}^{D}\left(b^{(i)}\right)^2}}$

  $-\cos\angle(\mathbf{a},\mathbf{b}) \in [-1,1]$ and $-\cos\angle(\mathbf{a},\mathbf{b}) = \begin{cases} -1 \implies \mathbf{a} \text{ and } \mathbf{b} \text{ are } \_\_\_\_\_ \\ 0 \implies \mathbf{a} \text{ and } \mathbf{b} \text{ are orthogonal (perpendicular)} \\ 1 \implies \mathbf{a} \text{ and } \mathbf{b} \text{ are } \_\_\_\_\_ \end{cases}$

  e.g. In information retrieval, give each word in an n-word dictionary its own coordinate in nD space. Make a vector of word counts for each document. Then $\cos\angle(\mathbf{a},\mathbf{b})$ for documents $\mathbf{a}$ and $\mathbf{b}$ measures _____ without regard for document length, so $-\cos\angle(\mathbf{a},\mathbf{b})$ measures topical "distance".
- *Hamming* distance$(\mathbf{a},\mathbf{b})$, for two equal-length strings $\mathbf{a}$ and $\mathbf{b}$, is the is the _____ at which the corresponding characters are different.
  e.g. Hamming distance could be used in a spell-checker.
  e.g. In information theory, Hamming distance is the minimum number of errors that could account for transmitting bit sequence $\mathbf{a}$ but receiving $\mathbf{b}$.

Both k and the choice of metric are hyperparameters set before running k-NN.

[1] Replacing $\mathbf{a}$ and $\mathbf{b}$ with $\mathbf{a}-\bar{a}$ and $\mathbf{b}-\bar{b}$ yields the *negative centered cosine similarity*, which is equivalent to $-r$.

Normalization

Normalization or rescaling is necessary if the features have different units or scales (coming in §5).

e.g. Consider the distance of points from $(0, 0)$. If x and y are each uniformly distributed, x in $[0, 1]$ and y in $[0, 0.01]$ (draw _), then the y values would hardly influence the distance. They could matter if we rescaled them (e.g. by $y \mapsto y \times 100$ so that they would span $[0, 1]$).

Weighted k-NN

e.g. Weighting each of a new point's k nearest neighbors by _____ , where d_i is the distance to the ith nearest neighbor, would make near neighbors _____than distant ones.

Python

- `from sklearn.neighbors import KNeighborsClassifier`
- `from sklearn.neighbors import KNeighborsRegressor`
- `clf = KNeighborsClassifier(n_neighbors=5, weights='uniform', p=2, metric='minkowski')`
  The default `p=2, metric='minkowski'` give Euclidean distance. `metric` options include `'euclidean'`, `'manhattan'`, and `'minkowski'` for vectors in $\mathbb{R}^D$; `'hamming'` for vectors in $\mathbb{Z}^D$; and a user-defined function that takes two 1D NumPy arrays and returns a distance.
  `weights='uniform'` gives unweighted k-NN. `weights='distance'` uses weights $\left\{\frac{1}{d_i}\right\}$ (above).
- `clf = KNeighborsRegressor(n_neighbors=5)`
- `clf.fit(X, y)` fits the model to array $\texttt{X}_{N\times D}$ and $\texttt{y}_{N\times 1}$
- `clf.predict(X)` does classification or regression on examples in `X`
- classification:
  - `clf.predict_proba(X)[:, 1]` gives $\{P(y_i = 1)\}$ (`[:, 0]` gives $\{P(y_i = 0)\}$)
  - `clf.score(X, y)` gives the average accuracy on `X` with respect to `y`
- regression: `clf.score(X, y)` gives R^2, the coefficient of determination

To learn more:

- User guide: `https://scikit-learn.org/stable/modules/neighbors.html`
- Reference manual:
  - Classification:
    `https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsClassifier.html`
  - Regression:
    `https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsRegressor.html`
  - Distance metrics:
    `https://scikit-learn.org/stable/modules/generated/sklearn.metrics.DistanceMetric.html`