CS-UY 4563: Lecture 12
k-Nearest Neighbors, Kernel Methods

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COURSE ADMIN

- Lab 4 due on **Friday, at 11:59pm**. Requires correct solution to HW3, Problem 2. I will post this after class.
- Short lab on Gradient Descent will be released soon and due after break.
- Upcoming labs involve image data and require more programming. Made up with lighter written homework.

COURSE PROJECT

Break is a great time to start mulling over ideas for your course project! Details in `project_guidelines.pdf`.

1. Find or collect a data set.
2. Ask a question (or two) about the data set which can possibly be answered with machine learning.
3. Apply tools and techniques learned in the class to answering that question.

COURSE PROJECT

- Must work in **groups of 2**. Coordinate over Piazza if looking for a partner.
- Any data set or topic is allowed, but youo should not reproduce an analysis that has already been done! Ask a new question or take a new approach.
- Talk to me or the TA's early if you are stuck on coming up with an idea, or need help narrowing down options.

COURSE PROJECT

4/1, Choose Project Partner and Topic. Email me.

4/2,4/6-4/8, Schedule Mandatory Meeting. Claim a time-slot in the Google Doc linked in the project information document.

4/13, Project Proposal Due. 2 Pages. Need to have dataset finalized!

5/6, 5/11, Project Presentations in Class. 5 Minutes.

5/11, Final Report Due 4+ Pages.

PROJECT TIPS

Look at your data! Plot features, examine full examples, look for missing data or inconsistencies.

Start small. Test and debug code on a small subset of your data before running on the whole thing.

Start simple. Try the simplest methods first. Linear regression, naive Bayes, etc. Even simpler: for regression, predict using mean($\vec{y}$). For classification predict using max $\vec{y}$ (the most common label). **You need to develop a baseline to compare your methods against.**

k-NEAREST NEIGHBOR METHOD

k-NN algorithm: a simple but powerful baseline for classification.

Training data: $(\vec{x}_1, y_1), \ldots, (\vec{x}_n, y_n)$ where $y_1, \ldots, y_n \in \{1, \ldots, q\}$.

Classification algorithm:

Given new input $\vec{x}_{new}$,

- Compute $sim(\vec{x}_{new}, \vec{x}_1), \ldots, sim(\vec{x}_{new}, \vec{x}_n)$.[1]
- Let $\vec{x}_{j_1}, \ldots, \vec{x}_{j_k}$ be the training data vectors with highest similarity to $\vec{x}_{new}$.
- Predict y_{new} as $majority(y_{j_1}, \ldots, y_{j_k})$.

[1] $sim(\vec{x}_{new}, \vec{x}_i)$ is any chosen similarity function, like $1 - \|\vec{x}_{new} - \vec{x}_i\|_2$.

k-NEAREST NEIGHBOR METHOD

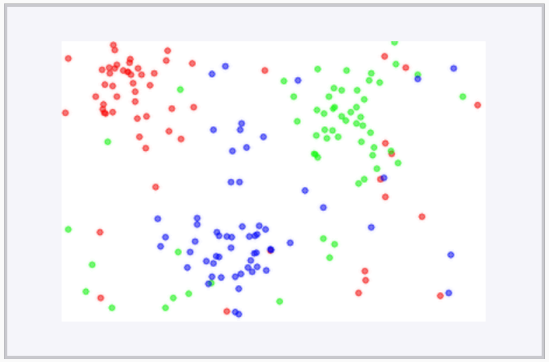


Fig. 1. The dataset.

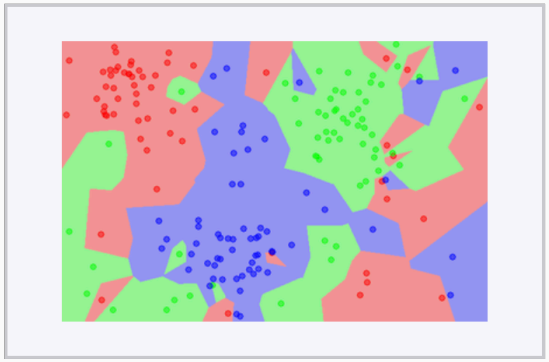


Fig. 2. The 1NN classification map.

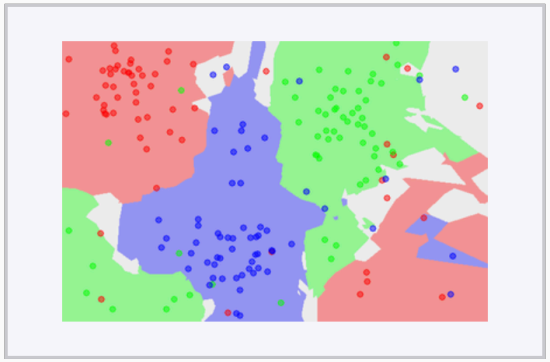


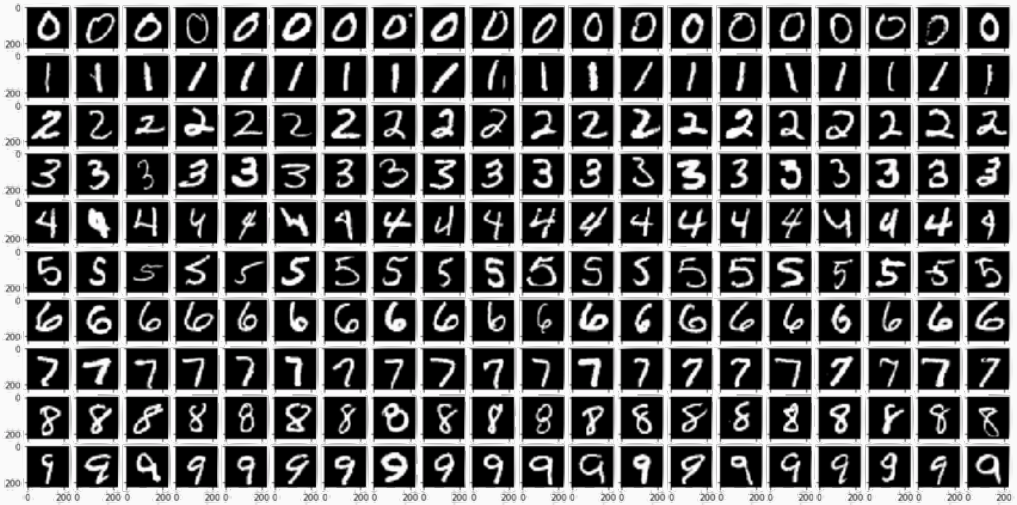
Fig. 3. The 5NN classification map.

- Smaller k, more complex classification function.
- Larger k, more robust to noisy labels.

Works remarkably well for many datasets.

MNIST IMAGE DATA

Especially good for large datasets with lots of repetition.
Works well on MNIST for example:



≈ 95% Accuracy out-of-the-box.[2]

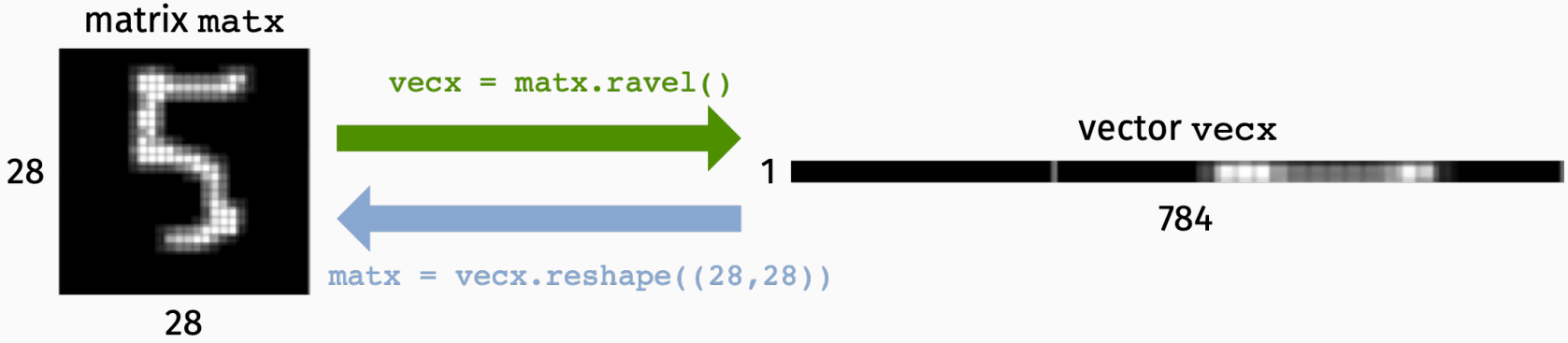
Let's look into this example a bit more...

[2] Can be improved to 99.5% with some simple tricks!

MNIST IMAGE DATA

Each pixel is number from $[0, 1]$. 0 is black, 1 is white.

Represent 28×28 matrix of pixel values as a flattened vector.




```
xmat = np.array([[1,2,3],[4,5,6],[7,8,9]])
```

```
array([[1, 2, 3],
       [4, 5, 6],
       [7, 8, 9]])
```

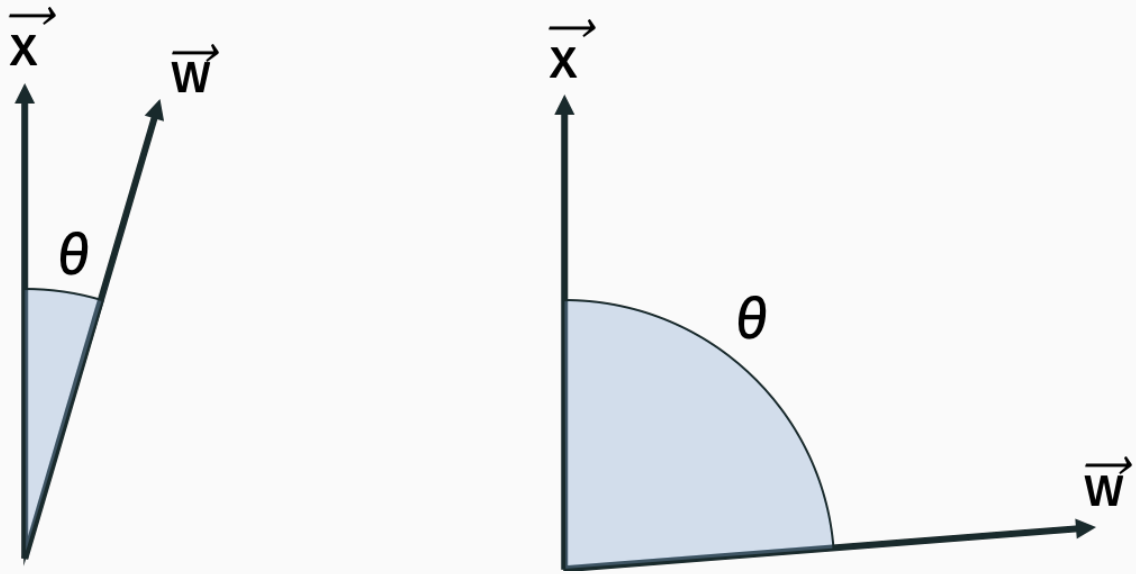
```
xvec = xmat.ravel()
```

```
array([1, 2, 3, 4, 5, 6, 7, 8, 9])
```

INNER PRODUCT SIMILARITY

Given data vectors $\vec{x}, \vec{w} \in \mathbb{R}^d$, the inner product $\langle \vec{x}, \vec{w} \rangle$ is a natural similarity measure.

$$\langle \vec{x}, \vec{w} \rangle = \sum_{i=1}^{d} \vec{x}[i]\vec{w}[i] = \cos(\theta)\|\vec{x}\|_2\|\vec{w}\|_2.$$



INNER PRODUCT SIMILARITY

Connection to Euclidean (ℓ_2) Distance:

$$\|\vec{x} - \vec{w}\|_2^2 = \|\vec{x}\|_2^2 + \|\vec{w}\|_2^2 - 2\langle \vec{x}, \vec{w} \rangle$$

For a set of vectors with the same norm, the pair of vectors with largest inner product is the pair with smallest Euclidean distance.

INNER PRODUCT FOR MNIST

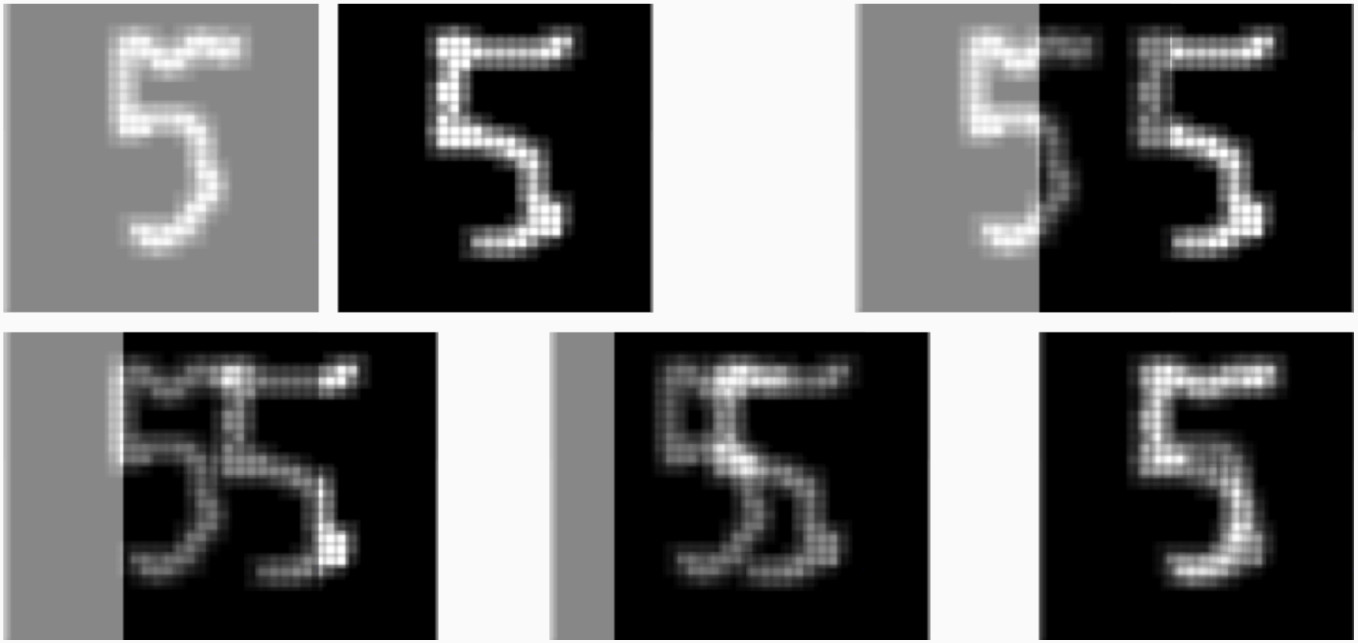
Inner product between MNIST digits:

$$\langle \vec{x}, \vec{w} \rangle = \sum_{i=1}^{28} \sum_{j=1}^{28} \texttt{matx}[i,j]\texttt{matw}[i,j].$$

Inner product similarity is higher when the images have large pixel values (close to 1) in the same locations. I.e. when they have a lot of overlapping white/light gray pixels.

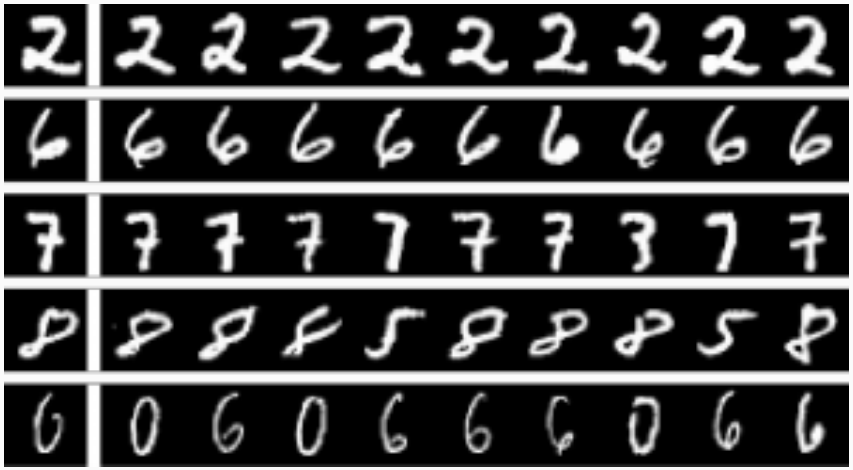
INNER PRODUCT FOR MNIST

Visualizing the inner product between two images:



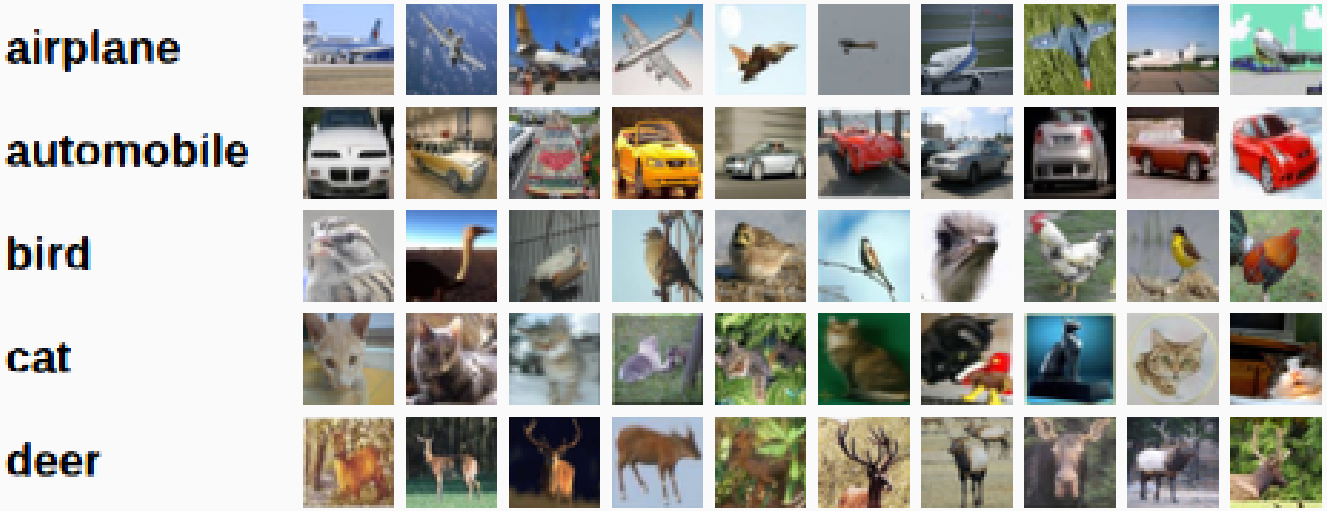
Images with high inner product have a lot of overlap.

Most similar images during k-nn search, $k = 9$:



K-NN FOR OTHER IMAGES

Does not work as well for less standardized classes of images:



CIFAR 10 Images

Even after scaling to have same size, converting to separate RGB channels, etc. something as simple as *k*-nn won't work.

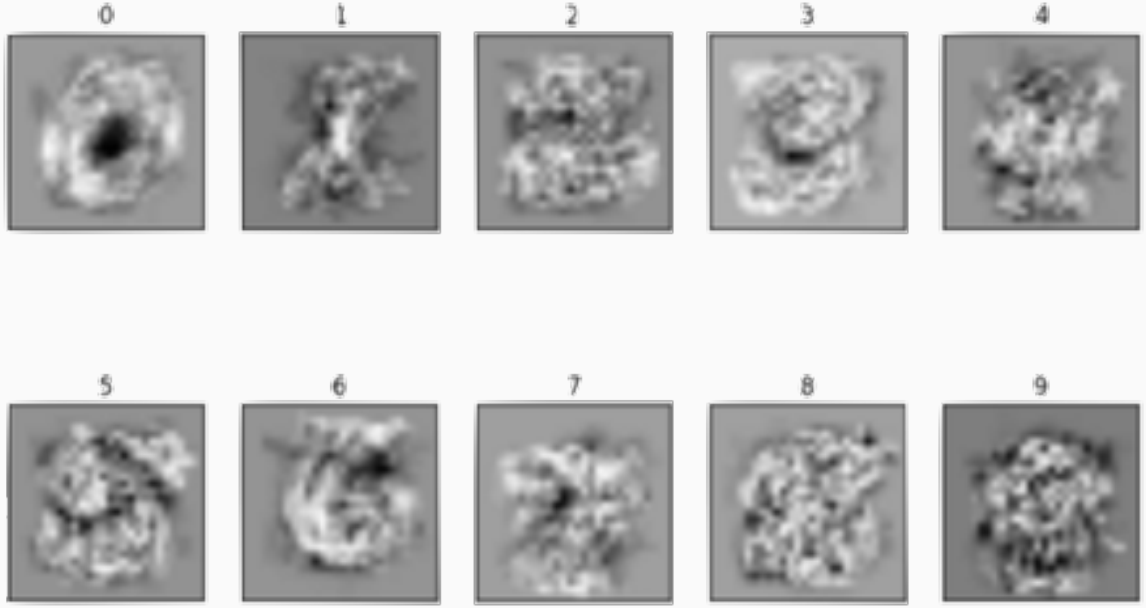
One-vs.-all Classification with Logistic Regression:

- Learn q classifiers with parameters $\vec{\beta}_1, \vec{\beta}_2, \ldots, \vec{\beta}_q$.
- Given $\vec{x}_{new}$ compute $\langle \vec{x}_{new}, \vec{\beta}_1 \rangle, \ldots, \langle \vec{x}_{new}, \vec{\beta}_q \rangle$
- Predict class $y_{new} = \arg\max_i \langle \vec{x}_{new}, \vec{\beta}_i \rangle$.

If each $\vec{x}$ is a vector with $28 \times 28 = 784$ entries than each $\vec{\beta}_i$ also has 784 entries. Each parameter vector can be viewed as a 28×28 image.

MATCHED FILTER

Visualizing $\vec{\beta}_1, \ldots, \vec{\beta}_q$:



For an input image  , compute inner product similarity with all weight matrices and choose most similar one.

In contrast to k-NN, only need to compute similarity with q items instead of n.

Logistic Regression Model:

Given data matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ (here $d = 784$) and binary label vector $\vec{y} \in \{0, 1\}^n$ for class i (1 if in class i, 0 if not), find $\vec{\beta} \in \mathbb{R}^d$ to minimize the log loss between:

$$\vec{y} \qquad \text{and} \qquad h(\mathbf{X}\vec{\beta})$$

where $h(z) = \frac{1}{1+e^{-z}}$ applies the logistic function entrywise to $\mathbf{X}\vec{\beta}$.

$$\text{Loss} = -\sum_{j=1}^{n} y_j \log(h(\mathbf{X}\vec{\beta})_j) + (1 - y_j) \log(1 - h(\mathbf{X}\vec{\beta})_j)$$

Logistic Regression Model:

Given data matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ (here $d = 784$) and binary label vector $\vec{y} \in \{0, 1\}^n$ for class i (1 if in class i, 0 if not), find $\vec{\beta} \in \mathbb{R}^d$ to minimize the log loss between:

$$\vec{y} \qquad \text{and} \qquad h(\mathbf{X}\vec{\beta})$$

Reminder from linear algebra: Without loss of generality, can assume that $\vec{\beta}$ lies in the row span of $\mathbf{X}$.

So for any $\vec{\beta} \in \mathbb{R}^d$, there exists a vector $\vec{\alpha} \in \mathbb{R}^n$ such that:

$$\vec{\beta} = \mathbf{X}^T \vec{\alpha}.$$

Logistic Regression Equivalent Formulation:

Given data matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ (here $d = 784$) and binary label vector $\vec{y} \in \{0, 1\}^n$ for class i (1 if in class i, 0 if not), find $\vec{\alpha} \in \mathbb{R}^n$ to minimize the log loss between:

$$\vec{y} \qquad \text{and} \qquad h(\mathbf{X}\mathbf{X}^T\vec{\alpha}).$$

Can still be minimized via gradient descent:

$$\nabla L(\vec{\alpha}) = \mathbf{X}\mathbf{X}^T(h(\mathbf{X}\mathbf{X}^T\vec{\alpha}) - \vec{y}).$$

What does classification for a new point $\vec{x}_{new}$ look like?

- Learn q classifiers with parameters $\vec{\alpha}_1, \vec{\alpha}_2, \ldots, \vec{\alpha}_q$.
- Given $\vec{x}_{new}$ compute $\langle \vec{x}_{new}, \mathbf{X}^T \vec{\alpha}_1 \rangle, \ldots, \langle \vec{x}_{new}, \mathbf{X}^T \vec{\alpha}_q \rangle$
- Predict class $y_{new} = \arg\max_i \langle \vec{x}_{new}, \mathbf{X}^T \vec{\alpha}_i \rangle$.

$$\langle \vec{x}_{new}, \mathbf{X}^T \vec{\alpha} \rangle = \sum_{j=1}^{n} \alpha_j \langle \vec{x}_{new}, \vec{x}_j \rangle.$$

Similar to $k - NN$ classifier but we learn a weight α_i for every $\vec{x}_i$ in our training set – can be positive or negative.

KERNEL FUNCTIONS

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