Nearest Neighbor Classification

Professor Ameet Talwalkar

Slide Credit: Professor Fei Sha

Outline

Textbook

- *Machine Learning: A Probabilistic Perspective* not currently available at the library
- I've included a second optional textbook (*Elements of Statistical Learning*) that is free online
- Course website will include readings from both books

Registering for Course

- We can currently accommodate 75 students
- 120+ students want to take the course
- I'd like to bump up enrollment; I don't know if this will happen
  - We'd need another TA and a bigger classroom
  - I expect an update shortly, and will post to Piazza
  - No updates to waitlist and no PTEs until this is resolved
- If enrollment does not go up, then priority will go to CS students who do well on the first problem set
  - Pre-req of CS180 will not be an issue

Homework 1

- I will upload it right after class to the course website
- Basic math questions, MATLAB coding assignment, Academic Integrity Form
  - Look on course website for details about getting access to MATLAB
- Due next Tuesday (10/6) at the beginning of class
  - Submission details are included in the assignment
  - Join Piazza if you haven't already

Outline

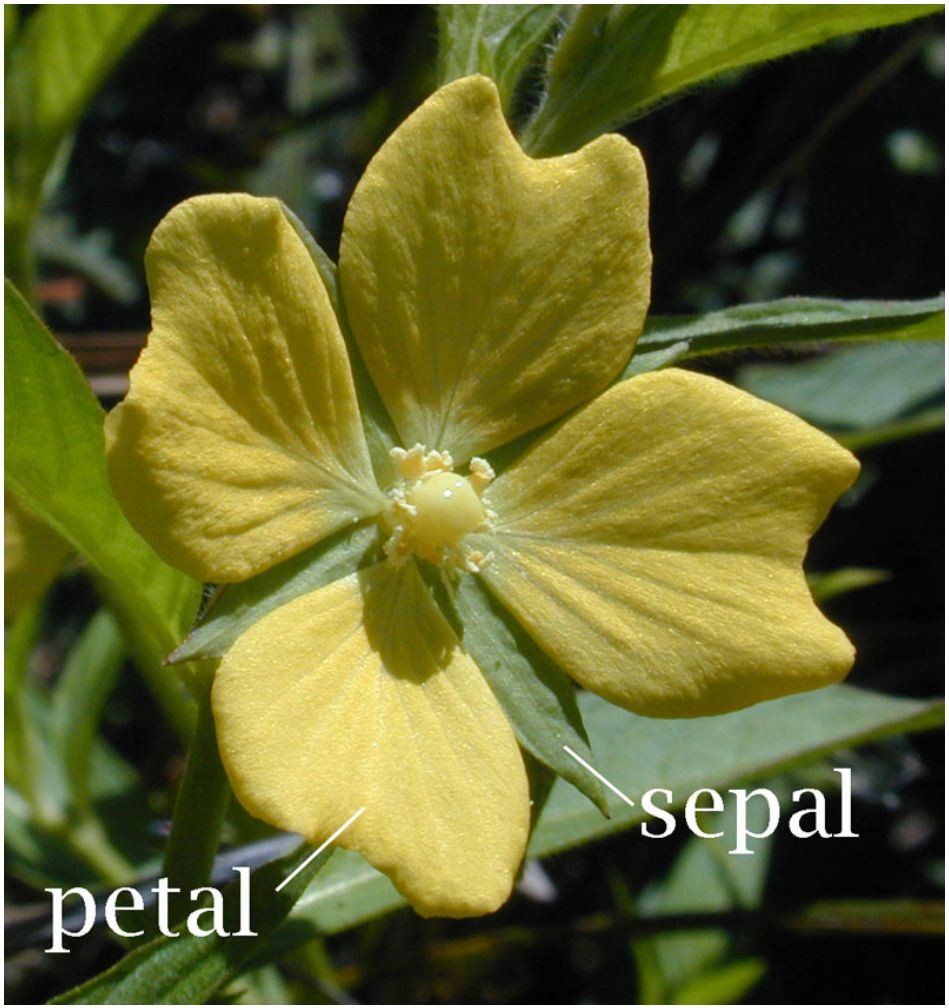
Recognizing flowers

Types of Iris: setosa, versicolor, and virginica



Measuring the properties of the flowers

Features: the widths and lengths of sepal and petal



Often, data is conveniently organized as a table

Ex: Iris data (click here for all data)

- 4 features
- 3 classes

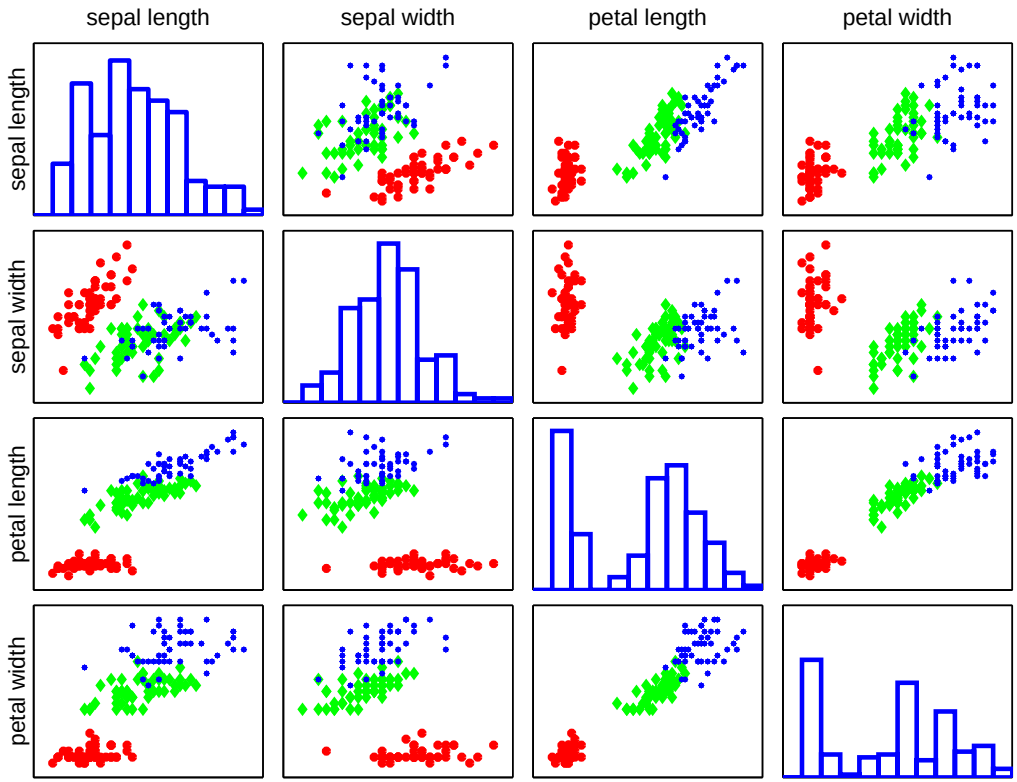
Fisher's *Iris* Data

Sepal length	Sepal width	Petal length	Petal width	Species
5.1	3.5	1.4	0.2	*I. setosa*
4.9	3.0	1.4	0.2	*I. setosa*
4.7	3.2	1.3	0.2	*I. setosa*
4.6	3.1	1.5	0.2	*I. setosa*
5.0	3.6	1.4	0.2	*I. setosa*
5.4	3.9	1.7	0.4	*I. setosa*
4.6	3.4	1.4	0.3	*I. setosa*
5.0	3.4	1.5	0.2	*I. setosa*
4.4	2.9	1.4	0.2	*I. setosa*
4.9	3.1	1.5	0.1	*I. setosa*

Pairwise scatter plots of 131 flower specimens

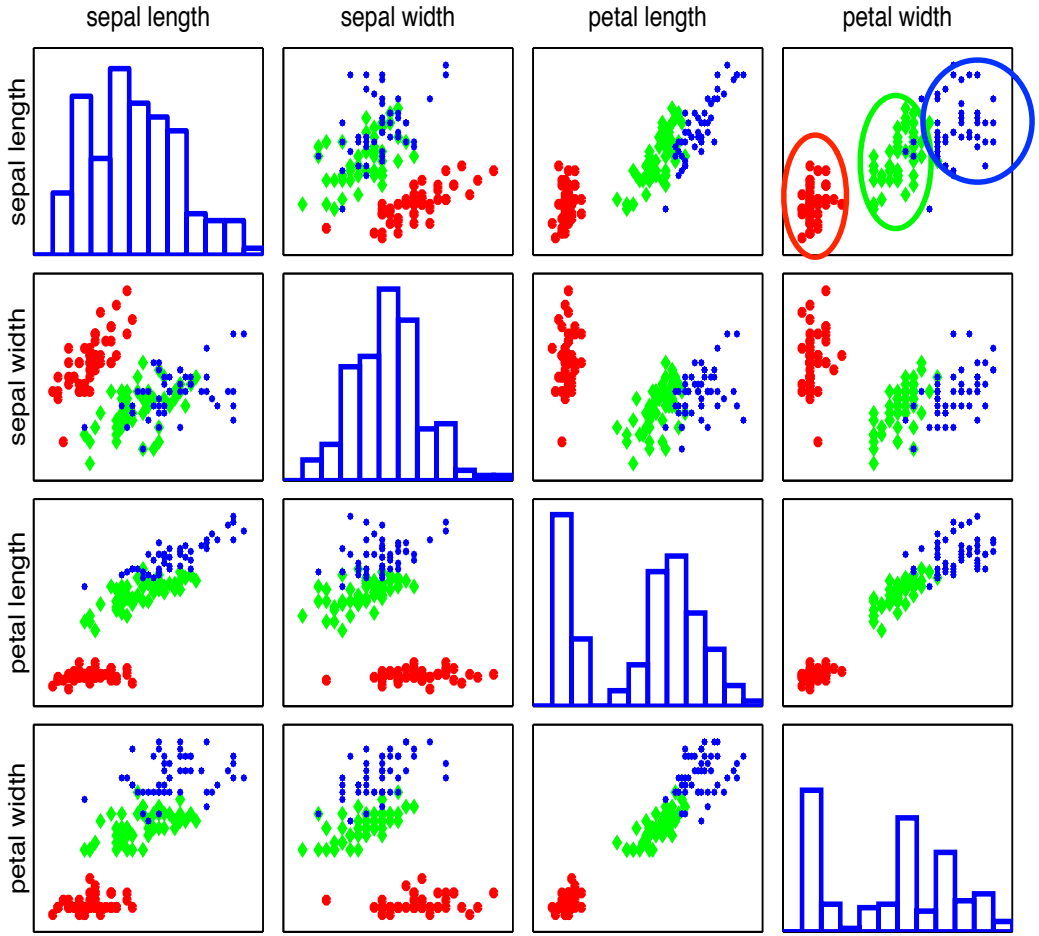
Visualization of data helps to identify the right learning model to use

Each colored point is a flower specimen: setosa, versicolor, virginica

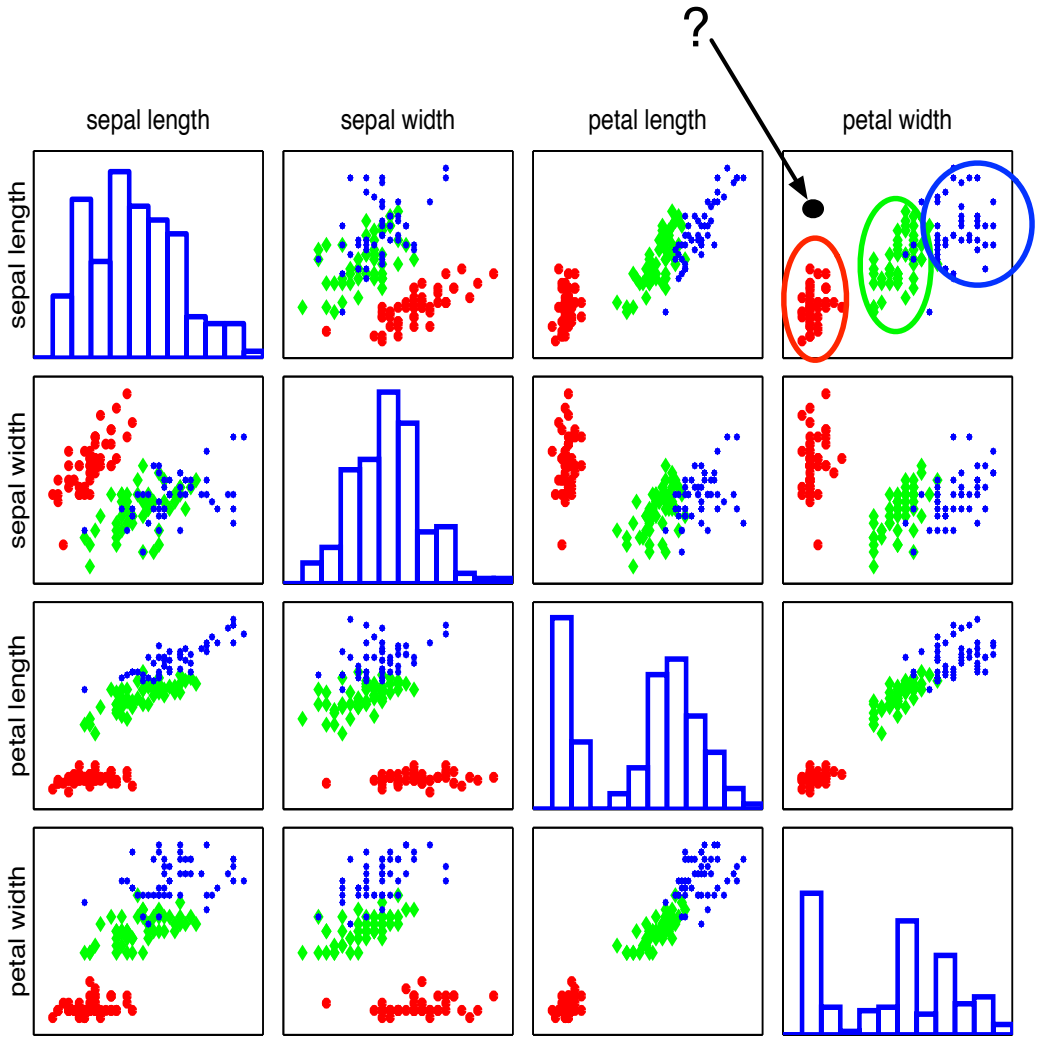


Different types seem well-clustered and separable

Using two features: petal width and sepal length



Labeling an unknown flower type



Closer to red cluster: so labeling it as setosa

Multi-class classification

Classify data into one of the multiple categories

- Input (feature vectors): $\boldsymbol{x} \in \mathbb{R}^{\mathsf{D}}$
- Output (label): $y \in [\mathsf{C}] = \{1, 2, \cdots, \mathsf{C}\}$
- Learning goal: $y = f(\boldsymbol{x})$

Special case: binary classification

- Number of classes: $\mathsf{C} = 2$
- Labels: $\{0, 1\}$ or $\{-1, +1\}$

More terminology

Training data (set)

- N samples/instances: $\mathcal{D}^{\text{TRAIN}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_{\text{N}}, y_{\text{N}})\}$
- They are used for learning $f(\cdot)$

Test (evaluation) data

- M samples/instances: $\mathcal{D}^{\text{TEST}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_{\text{M}}, y_{\text{M}})\}$
- They are used for assessing how well $f(\cdot)$ will do in predicting an unseen $\boldsymbol{x} \notin \mathcal{D}^{\text{TRAIN}}$

Training data and test data should *not* overlap: $\mathcal{D}^{\text{TRAIN}} \cap \mathcal{D}^{\text{TEST}} = \emptyset$

Nearest neighbor classification (NNC)

Nearest neighbor

$$\boldsymbol{x}(1) = \boldsymbol{x}_{\mathsf{nn}(\boldsymbol{x})}$$

where $\mathsf{nn}(\boldsymbol{x}) \in [\mathsf{N}] = \{1, 2, \cdots, \mathsf{N}\}$, i.e., the index to one of the training instances

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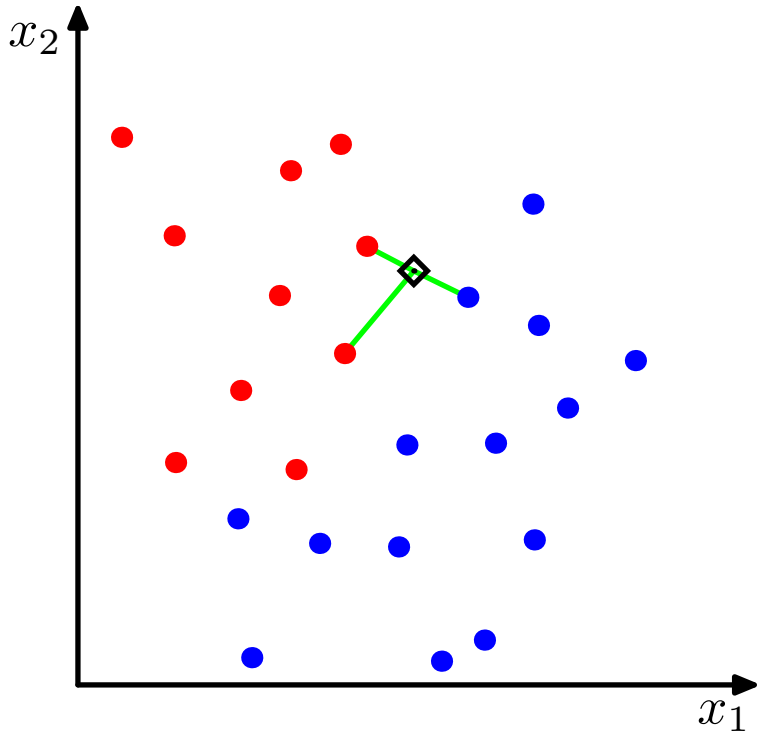
Classification rule

$$y = f(\boldsymbol{x}) = y_{\mathsf{nn}(\boldsymbol{x})}$$

Visual example

In this 2-dimensional example, the nearest point to $\boldsymbol{x}$ is a red training instance, thus, $\boldsymbol{x}$ will be labeled as red.



(a)

Example: classify Iris with two features

Training data

ID (n)	petal width (x_1)	sepal length (x_2)	category (y)
1	0.2	5.1	setosa
2	1.4	7.0	versicolor
3	2.5	6.7	virginica

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petal width $= 1.8$ and sepal width $= 6.4$

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Calculating distance $= \sqrt{x_1 - x_{n1})^2 + (x_2 - x_{n2})^2}$

ID	distance
1	1.75
2	0.72
3	0.76

Thus, the category is *versicolor* (the real category is *virginica*)

How to measure nearness with other distances?

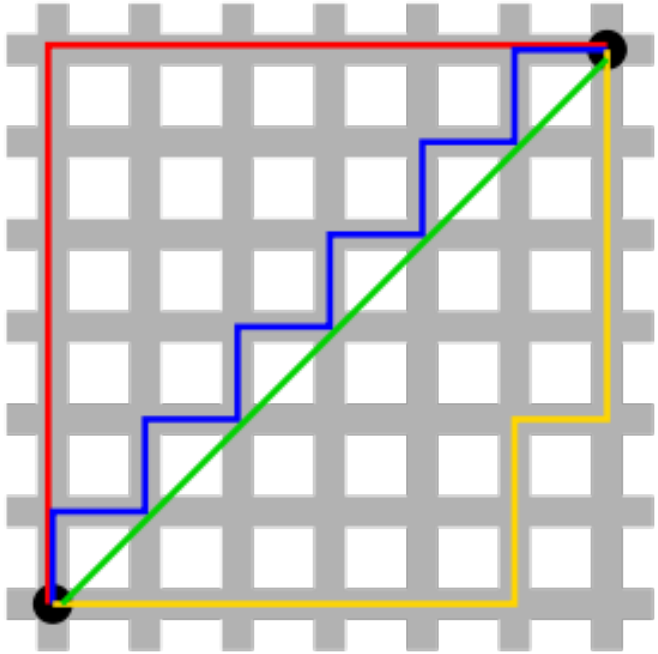
Previously, we use the Euclidean distance

$$\text{nn}(\boldsymbol{x}) = \arg\min_{n \in [\text{N}]} \|\boldsymbol{x} - \boldsymbol{x}_n\|_2^2$$

We can also use alternative distances

E.g., the following L_1 distance (i.e., city block distance, or Manhattan distance)

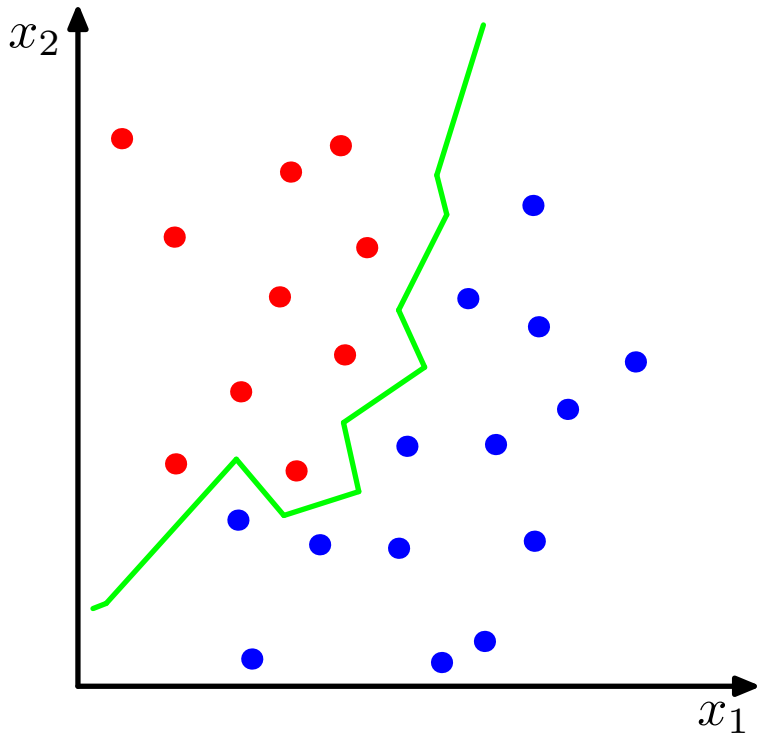
$$\begin{aligned}\text{nn}(\boldsymbol{x}) &= \arg\min_{n \in [\text{N}]} \|\boldsymbol{x} - \boldsymbol{x}_n\|_1 \\ &= \arg\min_{n \in [\text{N}]} \sum_{d=1}^{\text{D}} |x_d - x_{nd}|\end{aligned}$$



Green line is Euclidean distance. Red, Blue, and Yellow lines are L_1 distance

Decision boundary

For every point in the space, we can determine its label using the NNC rule. This gives rise to a *decision boundary* that partitions the space into different regions.



(b)

K-nearest neighbor (KNN) classification

Increase the number of nearest neighbors to use?

- 1-nearest neighbor: $\text{nn}_1(\boldsymbol{x}) = \arg\min_{n \in [\text{N}]} \|\boldsymbol{x} - \boldsymbol{x}_n\|_2^2$
- 2nd-nearest neighbor: $\text{nn}_2(\boldsymbol{x}) = \arg\min_{n \in [\text{N}] - \text{nn}_1(\boldsymbol{x})} \|\boldsymbol{x} - \boldsymbol{x}_n\|_2^2$
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The set of K-nearest neighbor

$$\mathsf{knn}(\boldsymbol{x}) = \{\mathsf{nn}_1(\boldsymbol{x}), \mathsf{nn}_2(\boldsymbol{x}), \cdots, \mathsf{nn}_K(\boldsymbol{x})\}$$

Let $\boldsymbol{x}(k) = \boldsymbol{x}_{\mathsf{nn}_k(\boldsymbol{x})}$, then

$$\|\boldsymbol{x} - \boldsymbol{x}(1)\|_2^2 \leq \|\boldsymbol{x} - \boldsymbol{x}(2)\|_2^2 \cdots \leq \|\boldsymbol{x} - \boldsymbol{x}(K)\|_2^2$$

How to classify with K neighbors?

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Classification rule

- Every neighbor votes: suppose y_n (the true label) for $\boldsymbol{x}_n$ is c, then
  - vote for c is 1
  - vote for $c' \neq c$ is 0

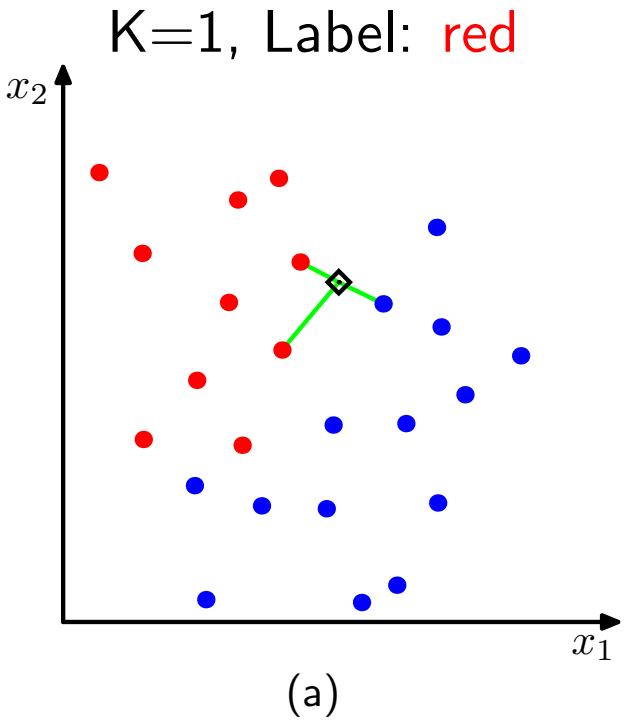
  We use the *indicator function* $\mathbb{I}(y_n == c)$ to represent.
- Aggregate everyone's vote

$$v_c = \sum_{n \in \text{knn}(\boldsymbol{x})} \mathbb{I}(y_n == c), \quad \forall \quad c \in [\text{C}]$$

- Label with the majority

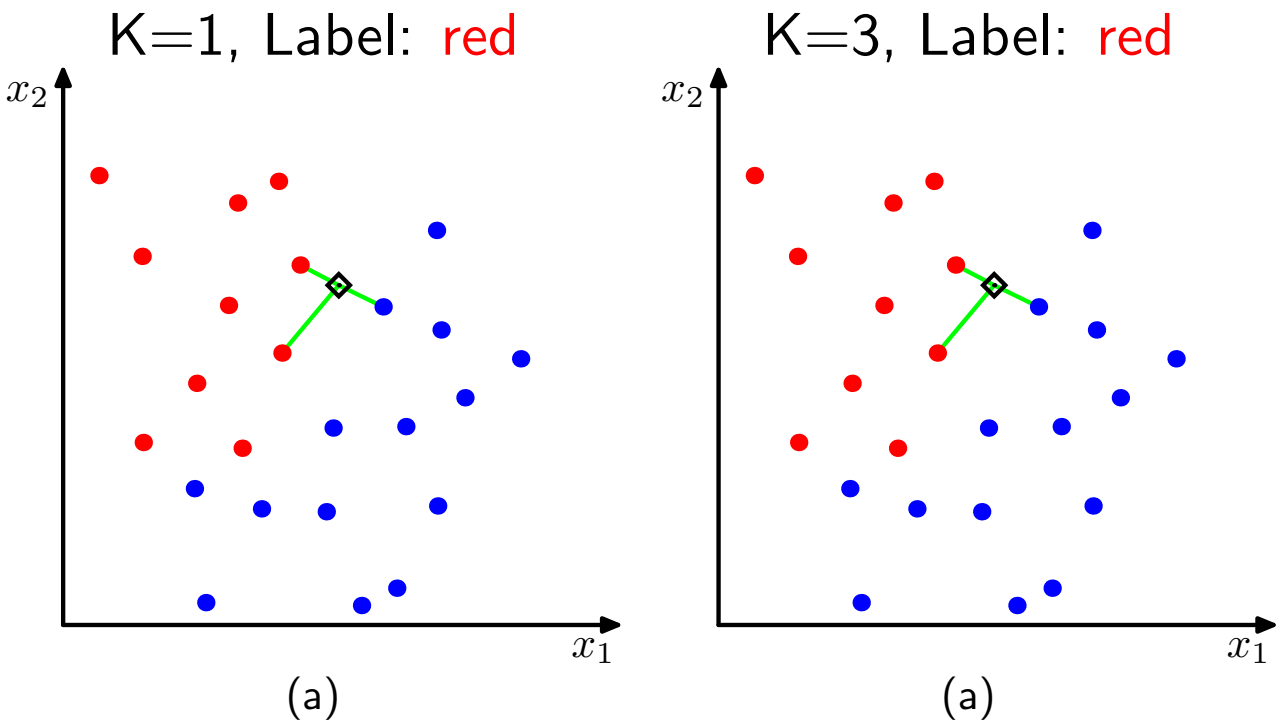
$$y = f(\boldsymbol{x}) = \arg\max_{c \in [\text{C}]} v_c$$

Example

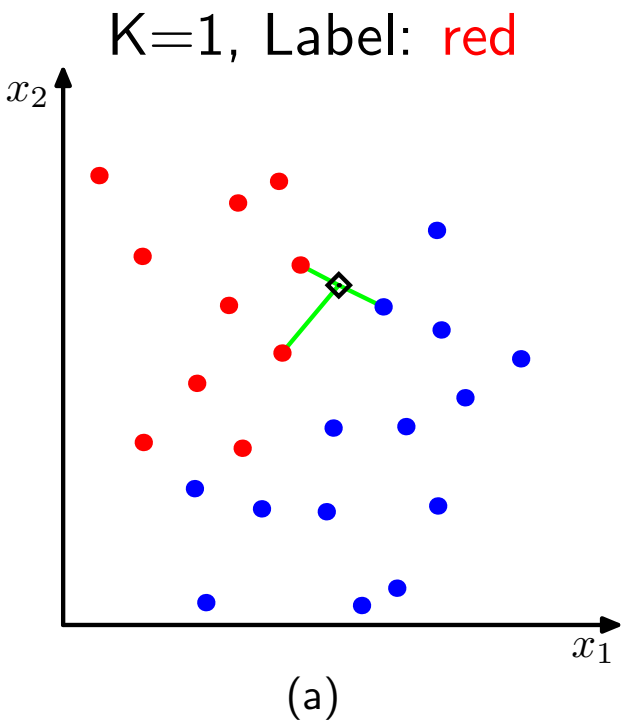


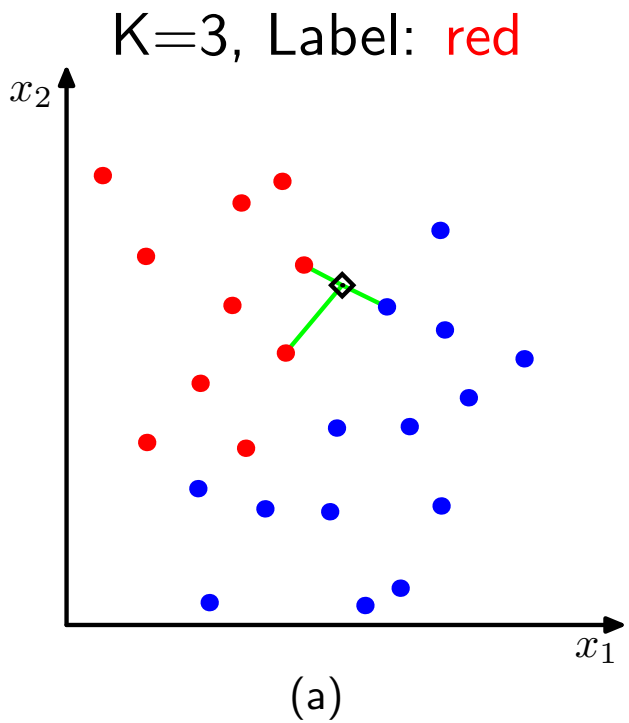
(a)

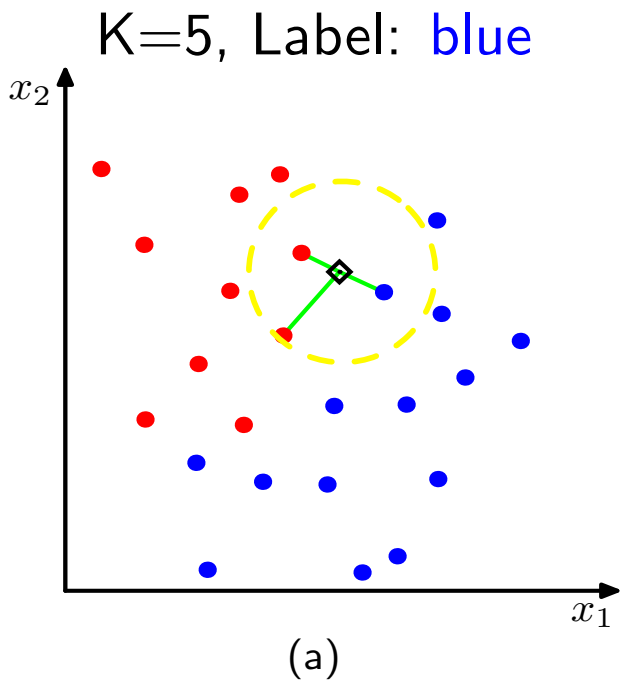
Example



Example







How to choose an optimal K?

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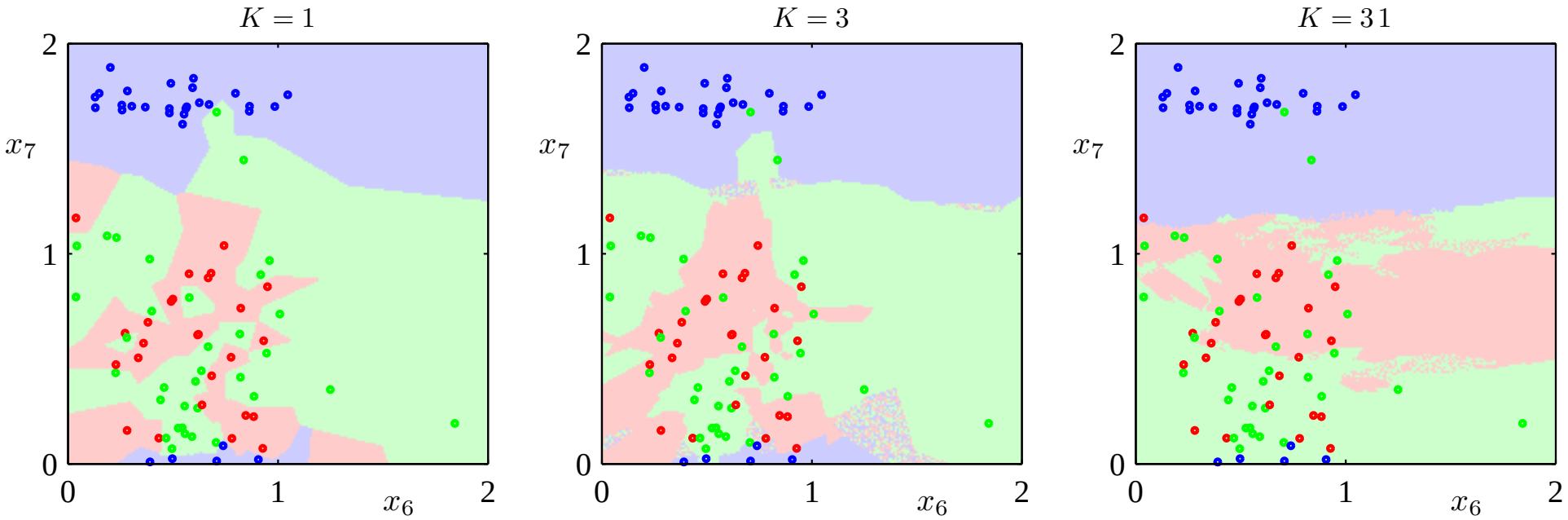


When K increases, the decision boundary becomes smooth.

Mini-summary

Advantages of NNC

- Computationally, simple and easy to implement – just computing the distance
- Theoretically, has strong guarantees "doing the right thing"

Disadvantages of NNC

- Computationally intensive for large-scale problems: $O(\mathrm{N}D)$ for labeling a data point
- We need to "carry" the training data around. Without it, we cannot do classification. This type of method is called *nonparametric*.
- Choosing the right distance measure and K can be involved.

Outline

Is NNC too simple to do the right thing?

To answer this question, we proceed in 3 steps

1. We define a performance metric for a classifier/algorithm.
2. We then propose an ideal classifier.
3. We then compare our simple NNC classifier to the ideal one and show that it performs nearly as well.

How to measure performance of a classifier?

Intuition

We should compute accuracy — the percentage of data points being correctly classified, or the error rate — the percentage of data points being incorrectly classified.

Two versions: which one to use?

- Defined on the training data set

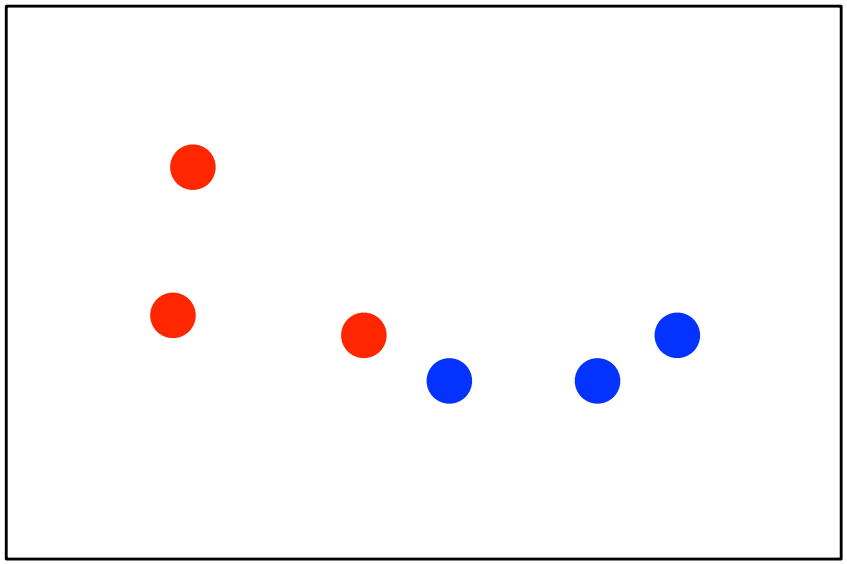
$$A^{\text{TRAIN}} = \frac{1}{\text{N}} \sum_{n} \mathbb{I}[f(\boldsymbol{x}_n) == y_n], \quad \varepsilon^{\text{TRAIN}} = \frac{1}{\text{N}} \sum_{n} \mathbb{I}[f(\boldsymbol{x}_n) \neq y_n]$$

- Defined on the test (evaluation) data set

$$A^{\text{TEST}} = \frac{1}{\text{M}} \sum_{m} \mathbb{I}[f(\boldsymbol{x}_m) == y_m], \quad \varepsilon^{\text{TEST}} = \frac{1}{\text{M}} \sum_{M} \mathbb{I}[f(\boldsymbol{x}_m) \neq y_m]$$

Example

Training data



What are A^{TRAIN} and $\varepsilon^{\text{TRAIN}}$?

Example

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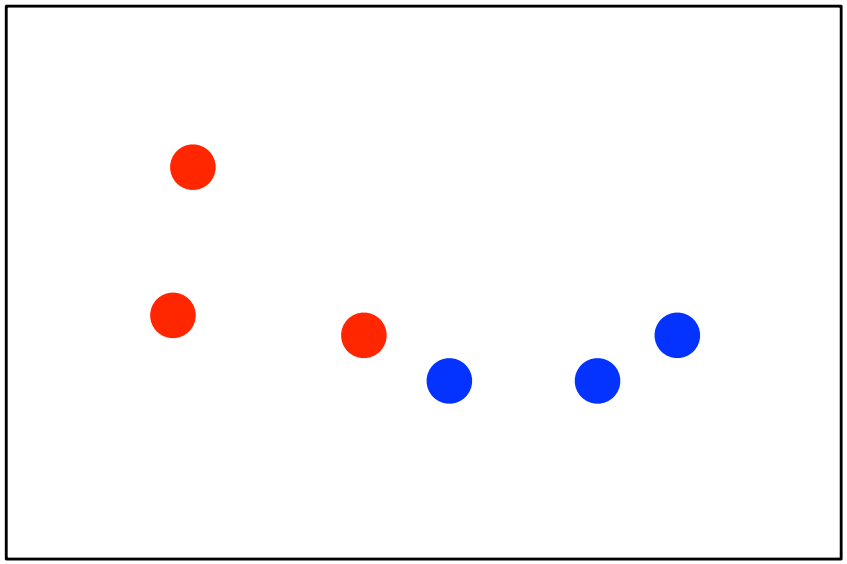

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$$A^{\text{TRAIN}} = 100\%, \quad \varepsilon^{\text{TRAIN}} = 0\%$$

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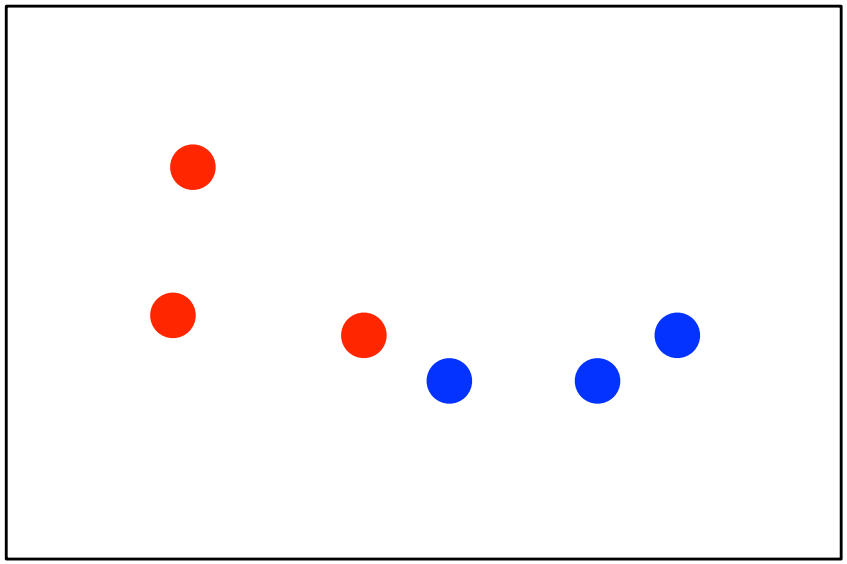
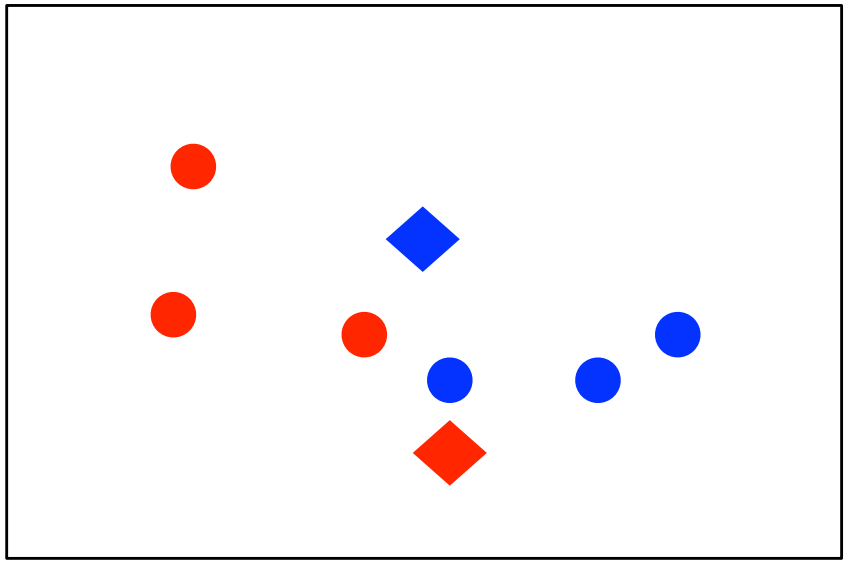


Test data



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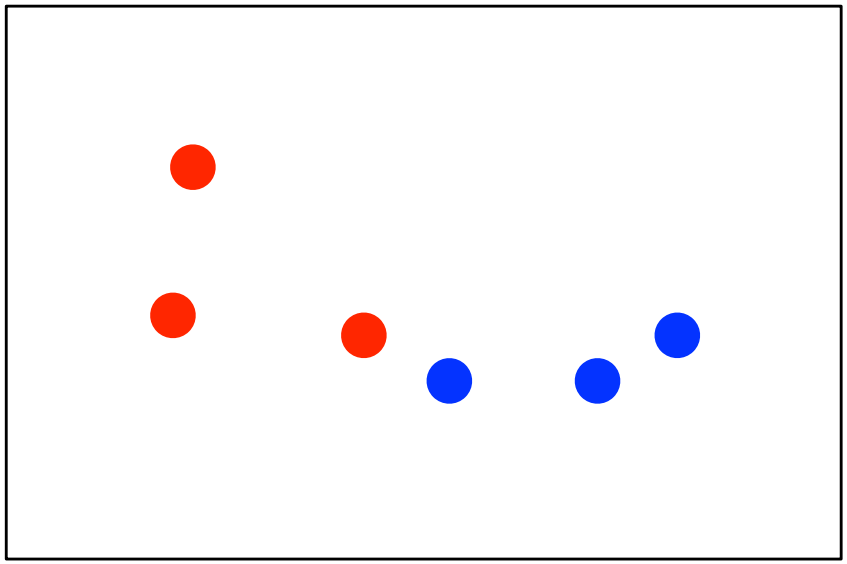

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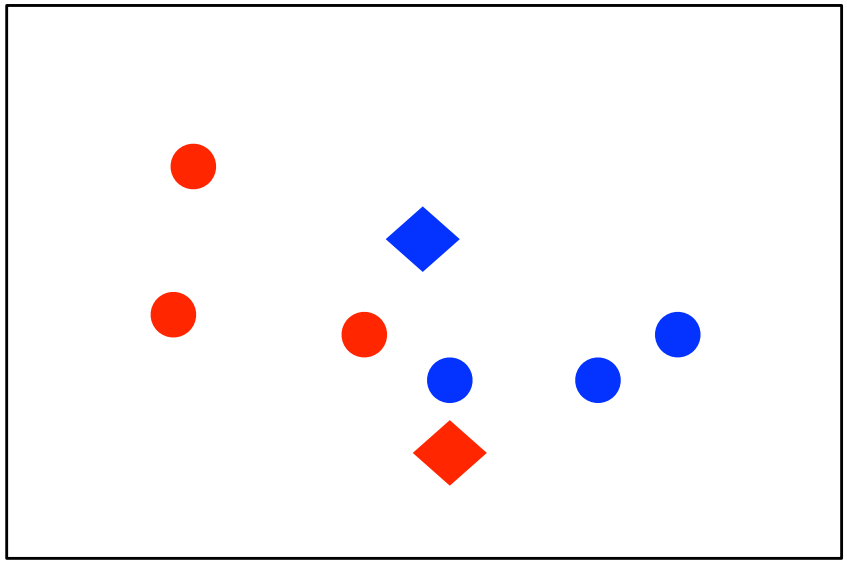

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Leave-one-out (LOO)

Idea

- For each training instance $\boldsymbol{x}_n$, take it out of the training set and then label it.
- For NNC, $\boldsymbol{x}_n$'s nearest neighbor will not be itself. So the error rate would not become 0 necessarily.

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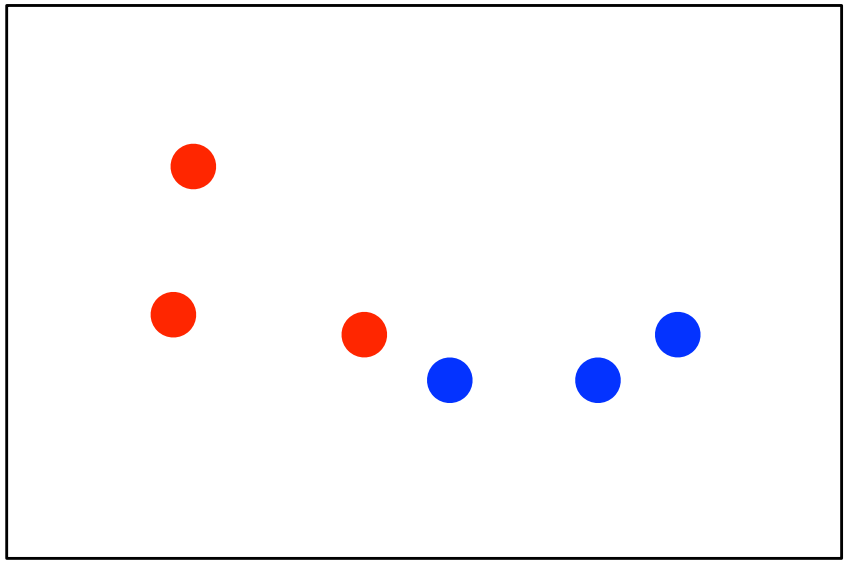

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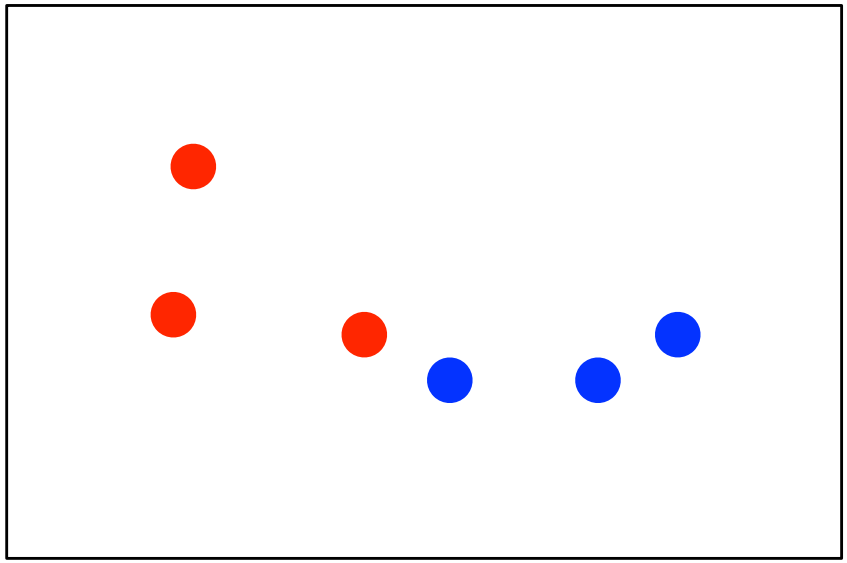

What are the LOO-version of A^{TRAIN} and $\varepsilon^{\text{TRAIN}}$?

$$A^{\text{TRAIN}} = 66.67\% (\text{i.e.}, 4/6)$$
$$\varepsilon^{\text{TRAIN}} = 33.33\% (\text{i.e.}, 2/6)$$

Drawback of the metrics

They are dataset-specific

- Given a different training (or test) dataset, A^{TRAIN} (or A^{TEST}) will change.
- Thus, if we get a dataset "randomly", these variables would be random quantities.

$$A^{\text{TEST}}_{\mathcal{D}_1}, A^{\text{TEST}}_{\mathcal{D}_2}, \cdots, A^{\text{TEST}}_{\mathcal{D}_q}, \cdots$$

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Can we understand the algorithm itself in a "more certain" nature, by removing the uncertainty caused by the datasets?

Expected mistakes

Setup

- Assume our data $(\boldsymbol{x}, y)$ is drawn from the joint and *unknown* distribution $p(\boldsymbol{x}, y)$
- Classification mistake on a single data point $\boldsymbol{x}$ with the ground-truth label y

$$L(f(\boldsymbol{x}), y) = \begin{cases} 0 & \text{if } f(x) = y \\ 1 & \text{if } f(x) \neq y \end{cases}$$

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(law of iterated expectations, tower property, smoothing)

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Terminology

- $L(f(\boldsymbol{x}), y)$ is called *0/1 loss function* — many other forms of loss functions exist for different learning problems.
- Expected conditional risk

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- Empirical risk

$$R_{\mathcal{D}}(f) = \frac{1}{\mathsf{N}} \sum_{n} L(f(\boldsymbol{x}_n), y_n)$$

(This is our empirical error from earlier.)

Ex: binary classification

Expected conditional risk of a single data point x

$$\begin{aligned} R(f, \boldsymbol{x}) &= \mathbb{E}_{y \sim p(y|\boldsymbol{x})} L(f(\boldsymbol{x}), y) \\ &= P(y = 1|\boldsymbol{x}) \mathbb{I}[f(\boldsymbol{x}) = 0] + P(y = 0|\boldsymbol{x}) \mathbb{I}[f(\boldsymbol{x}) = 1] \end{aligned}$$

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Let $\eta(\boldsymbol{x}) = P(y = 1|\boldsymbol{x})$, we have

$$\begin{aligned} R(f, \boldsymbol{x}) &= \eta(\boldsymbol{x}) \mathbb{I}[f(\boldsymbol{x}) = 0] + (1 - \eta(\boldsymbol{x})) \mathbb{I}[f(\boldsymbol{x}) = 1] \\ &= 1 - \underbrace{\{\eta(\boldsymbol{x}) \mathbb{I}[f(\boldsymbol{x}) = 1] + (1 - \eta(\boldsymbol{x})) \mathbb{I}[f(\boldsymbol{x}) = 0]\}}_{\text{expected conditional accuracy}} \end{aligned}$$

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Exercise: please verify the last equality.

Bayes optimal classifier

Consider the following classifier, using the posterior probability
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Theorem

For any labeling function $f(\cdot)$, $R(f^*, \boldsymbol{x}) \leq R(f, \boldsymbol{x})$. Similarly, $R(f^*) \leq R(f)$. Namely, $f^*(\cdot)$ is optimal.

Proof

From definition

$$R(f, \boldsymbol{x}) = 1 - \{\eta(\boldsymbol{x})\mathbb{I}[f(\boldsymbol{x}) = 1] + (1 - \eta(\boldsymbol{x}))\mathbb{I}[f(\boldsymbol{x}) = 0]\}$$
$$R(f^*, \boldsymbol{x}) = 1 - \{\eta(\boldsymbol{x})\mathbb{I}[f^*(\boldsymbol{x}) = 1] + (1 - \eta(\boldsymbol{x}))\mathbb{I}[f^*(\boldsymbol{x}) = 0]\}$$

Thus,

$$\begin{aligned} R(f, \boldsymbol{x}) - R(f^*, \boldsymbol{x}) = \eta(\boldsymbol{x}) &\{\mathbb{I}[f^*(\boldsymbol{x}) = 1] - \mathbb{I}[f(\boldsymbol{x}) = 1]\} \\ &+ (1 - \eta(\boldsymbol{x})) \{\mathbb{I}[f^*(\boldsymbol{x}) = 0] - \mathbb{I}[f(\boldsymbol{x}) = 0]\} \end{aligned}$$

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&= (2\eta(\boldsymbol{x}) - 1) \{\mathbb{I}[f^*(\boldsymbol{x}) = 1] - \mathbb{I}[f(\boldsymbol{x}) = 1]\}
\end{aligned}$$

Proof

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&= \eta(\boldsymbol{x}) \{\mathbb{I}[f^*(\boldsymbol{x}) = 1] - \mathbb{I}[f(\boldsymbol{x}) = 1]\} \\
&\quad + (1 - \eta(\boldsymbol{x})) \left\{ \left(1 - \mathbb{I}[f^*(\boldsymbol{x}) = 1]\right) - \left(1 - \mathbb{I}[f(\boldsymbol{x}) = 1]\right) \right\} \\
&= (2\eta(\boldsymbol{x}) - 1) \{\mathbb{I}[f^*(\boldsymbol{x}) = 1] - \mathbb{I}[f(\boldsymbol{x}) = 1]\} \\
&\geq 0
\end{aligned}$$

Bayes optimal classifier in general form

For multi-class classification problem

$$f^*(\boldsymbol{x}) = \arg\max_{c \in [\mathsf{C}]} p(y = c|\boldsymbol{x})$$

when $\mathsf{C} = 2$, this reduces to detecting whether or not $\eta(\boldsymbol{x}) = p(y = 1|\boldsymbol{x})$ is greater than $1/2$.

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Remarks

- The Bayes optimal classifier is generally not computable as it assumes the knowledge of $p(\boldsymbol{x}, y)$ or $p(y|\boldsymbol{x})$.
- However, it is useful as a conceptual tool to formalize how well a classifier can do *without* knowing the joint distribution.

Comparing NNC to Bayes optimal classifier

How well does our NNC do?

Theorem (Cover-Hart Inequality)

For the NNC rule f^{NNC} for binary classification, we have,

$$R(f^*) \leq R(f^{\mathrm{NNC}}) \leq 2R(f^*)(1 - R(f^*)) \leq 2R(f^*)$$

Namely, the expected risk by the classifier is at worst twice that of the Bayes optimal classifier.

In short, NNC seems doing a reasonable thing

Mini-summary

Advantages of NNC

- Computationally, simple and easy to implement – just computing the distance
- ✓ Theoretically, has strong guarantees "doing the right thing"

Disadvantages of NNC

- Computationally intensive for large-scale problems: $O(\mathrm{N}D)$ for labeling a data point
- We need to "carry" the training data around. Without it, we cannot do classification. This type of method is called *nonparametric*.
- Choosing the right distance measure and K can be involved.

Outline

Hypeparameters in NNC

Two practical issues about NNC

- Choosing K, i.e., the number of nearest neighbors (default is 1)
- Choosing the right distance measure (default is Euclidean distance), for example, from the following generalized distance measure

$$\|\boldsymbol{x} - \boldsymbol{x}_n\|_p = \left(\sum_d |x_d - x_{nd}|^p \right)^{1/p}$$

for $p \geq 1$.

Those are not specified by the algorithm itself — resolving them requires empirical studies and are task/dataset-specific.

Tuning by using a validation dataset

Training data (set)

- N samples/instances: $\mathcal{D}^{\text{TRAIN}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_{\text{N}}, y_{\text{N}})\}$
- They are used for learning $f(\cdot)$

Test (evaluation) data

- M samples/instances: $\mathcal{D}^{\text{TEST}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_{\text{M}}, y_{\text{M}})\}$
- They are used for assessing how well $f(\cdot)$ will do in predicting an unseen $\boldsymbol{x} \notin \mathcal{D}^{\text{TRAIN}}$

Development (or validation) data

- L samples/instances: $\mathcal{D}^{\text{DEV}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_{\text{L}}, y_{\text{L}})\}$
- They are used to optimize hyperparameter(s).

Training data, validation and test data should *not* overlap!

Recipe

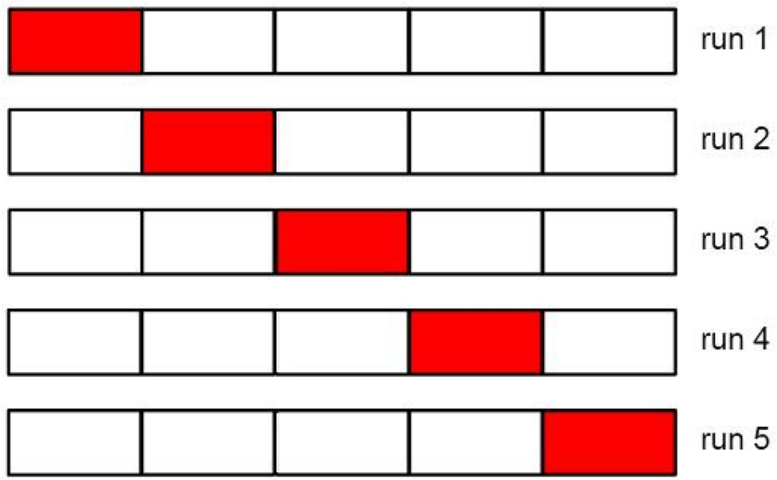
- for each possible value of the hyperparameter (say $K = 1, 3, \cdots, 100$)
  - Train a model using $\mathcal{D}^{\text{TRAIN}}$
  - Evaluate the performance of the model on $\mathcal{D}^{\text{DEV}}$
- Choose the model with the best performance on $\mathcal{D}^{\text{DEV}}$
- Evaluate the model on $\mathcal{D}^{\text{TEST}}$

Cross-validation

What if we do not have validation data?

- We split the training data into S equal parts.
- We use each part *in turn* as a validation dataset and use the others as a training dataset.
- We choose the hyperparameter such that *on average*, the model performing the best

$S = 5$: 5-fold cross validation



Special case: when S = N, this will be leave-one-out.

Recipe

- Split the training data into S equal parts. Denote each part as $\mathcal{D}_s^{\text{TRAIN}}$
- for each possible value of the hyperparameter (say $K = 1, 3, \cdots, 100$)
  - for every $s \in [1, \text{S}]$
    - ★ Train a model using $\mathcal{D}_{\setminus s}^{\text{TRAIN}} = \mathcal{D}^{\text{TRAIN}} - \mathcal{D}_s^{\text{TRAIN}}$
    - ★ Evaluate the performance of the model on $\mathcal{D}_s^{\text{TRAIN}}$
  - Average the S performance metrics
- Choose the hyperparameter corresponding to the best averaged performance
- Use the best hyerparamter to train on a model using all $\mathcal{D}^{\text{TRAIN}}$
- Evaluate the model on $\mathcal{D}^{\text{TEST}}$

Yet, another practical issue with NNC

Distances depend on units of the features!

Preprocess data

Normalize data to have zero mean and unit standard deviation in each dimension

- Compute the means and standard deviations in each feature

$$\bar{x}_d = \frac{1}{\mathrm{N}} \sum_n x_{nd}, \qquad s_d^2 = \frac{1}{N-1} \sum_n (x_{nd} - \bar{x}_d)^2$$

- Scale the feature accordingly

$$x_{nd} \leftarrow \frac{x_{nd} - \bar{x}_d}{s_d}$$

Many other ways of normalizing data — you would need/want to try different ones and pick them using (cross)validation

Outline

Summary so far

- Described a simple learning algorithm
  - Used intensively in practical applications — you will get a taste of it in your homework
  - Discussed a few practical aspects, such as tuning hyperparameters, with (cross)validation
- Briefly studied its theoretical properties
  - Concepts: loss function, risks, Bayes optimal
  - Theoretical guarantees: explaining why NNC would work

Administration Summary

- I've included a second optional textbook (*Elements of Statistical Learning*) that is free online
  - Course website will include readings from both books
- I'd like to bump up enrollment; I don't know if this will happen
  - No updates to waitlist and no PTEs until this is resolved
  - If enrollment does not go up, then priority will go to CS students who do well on the first problem set
- I will upload HW1 right after class to the course website
  - Due next Tuesday (10/6) at the beginning of class
  - Submission details are included in the assignment
  - Join Piazza if you haven't already