18-661 Introduction to Machine Learning

Nearest Neighbors

Fall 2020

ECE – Carnegie Mellon University

Midterm Information

Midterm will be on Tuesday, 10/20 in-class.

- Conducted as an online exam on Gradescope, with multiple-choice and short-answer questions
- Closed-book except for one double-sided letter-size handwritten page of notes that you can prepare as you wish.
- We will provide formulas for relevant probability distributions.
- You will not need a calculator. Only pen/pencil and scratch paper are allowed.

Will cover all topics up to and including Nearest Neighbors (10/15)

- (1) point estimation/MLE/MAP, (2) linear regression, (3) naive Bayes, (4) logistic regression, (5) SVMs, (6) Graphical Models, (7) Nearest Neighbors.
- Practice Midterm exam has been posted on Gradescope

Outline

1. Nearest Neighbor Classifier

2. Practical Aspects of NN

Parametric vs. Nonparametric

- So far, we've discussed parametric machine learning models:

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    - Nearest neighbors
    - Decision trees

Parametric vs. Nonparametric

Key difference:

- Parametric models assume that the data can be characterized via some *fixed* set of parameters θ. Given this set of parameters, our future predictions are independent of the data $\mathcal{D}$, i.e., $P(x|\theta, \mathcal{D}) = P(x|\theta)$.

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  - More complex and expensive, but can learn more flexible patterns
- Both parametric and non-parametric methods can be used for either regression or classification.

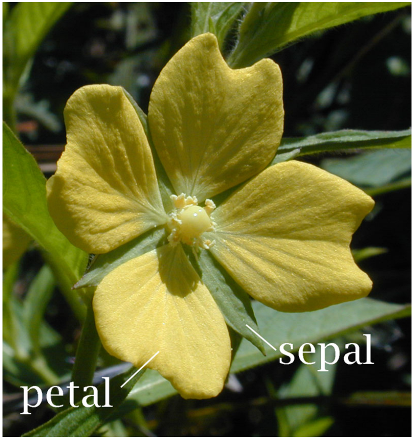
Nearest Neighbor Classifier

Recognizing flowers

Types of Iris: setosa, versicolor, and virginica

Measuring the properties of the flowers

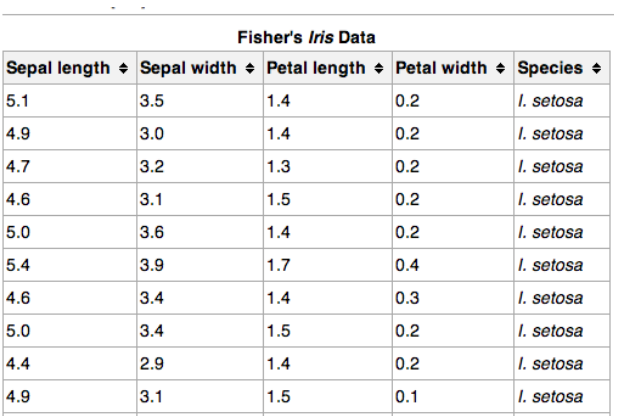
Features: the widths and lengths of sepal and petal



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*
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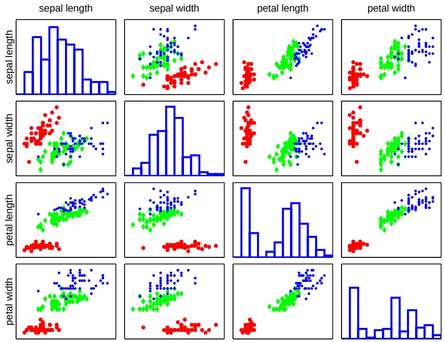
5.0	3.4	1.5	0.2	*I. setosa*
4.4	2.9	1.4	0.2	*I. setosa*
4.9	3.1	1.5	0.1	*I. setosa*

Pairwise scatter plots of 131 flower specimens

Visualization of data helps to identify the right learning model

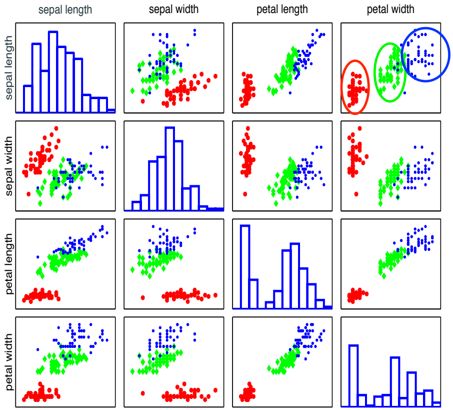
Which combination of features separates the three classes?

Figure 1: Each colored point is a flower specimen: setosa, versicolor, virginica

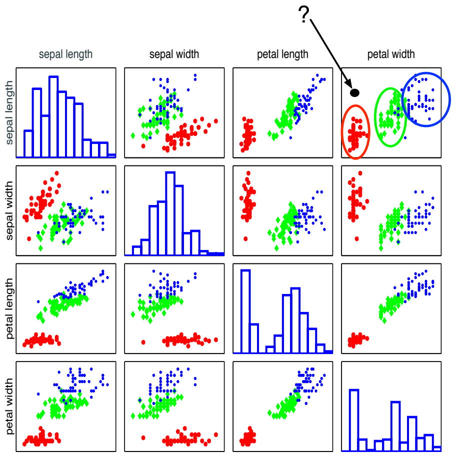


Different types seem well-clustered and separable

Using two features: petal width and sepal length



Labeling an unknown flower type



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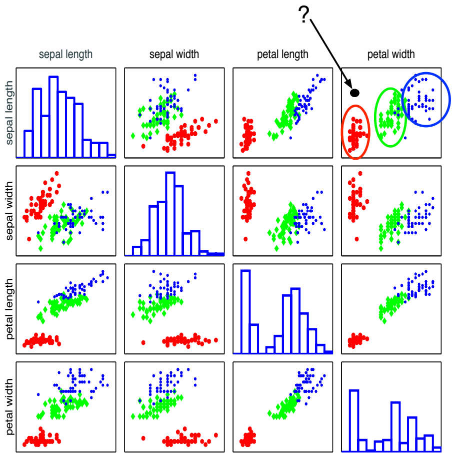

Closer to red cluster: so labeling it as setosa

Multi-class classification

Classify data into one of the multiple categories

- Input (feature vectors): $\boldsymbol{x} \in \mathbb{R}^{\mathsf{D}}$
- Output (label): $y \in [\mathsf{C}] = \{1, 2, \cdots, \mathsf{C}\}$
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Recall special case: binary classification

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

More terminology

Training data (set)

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

More terminology

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Test (evaluation) data

- M samples/instances: $\mathcal{D}^{\text{TEST}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_{\mathrm{M}}, y_{\mathrm{M}})\}$
- 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 of a (training or test) data point

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

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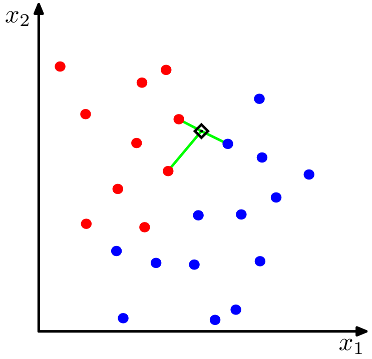
Example: if $\mathrm{nn}(\boldsymbol{x}) = 2$, then

$$y_{\mathrm{nn}(\boldsymbol{x})} = y_2,$$

which is the label of the 2nd data point.

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
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Calculating distance from (x_1, x_2) to (x_{n1}, x_{n2}): $(x_1 - x_{n1})^2 + (x_2 - x_{n2})^2$

ID	distance
1	4.25
2	0.52
3	0.58

Thus, the predicted category is 2 (*versicolor*)

How to measure "nearness" with other distances?

Previously, we used Euclidean distance

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

We can also use alternative distances

- E.g., the ℓ_1 distance (i.e., city block distance, or Manhattan distance):

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

- Or, the ℓ_∞ (supremum) distance:

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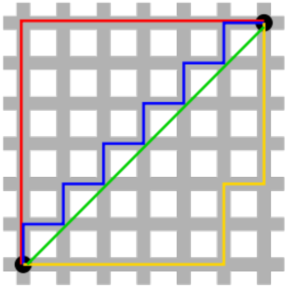

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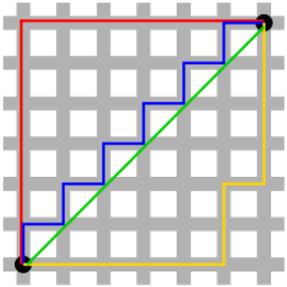
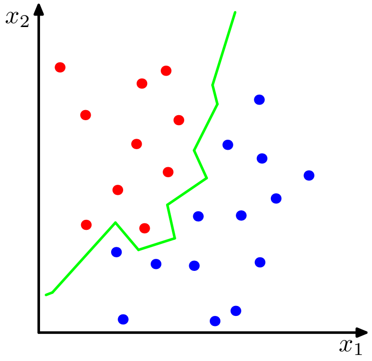


Figure 2: Green line is Euclidean distance. Red, Blue, and Yellow lines are L_1 distance

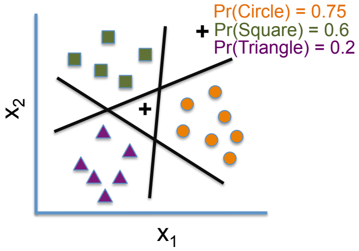
Decision boundary

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)

Recall: Multi-class classification



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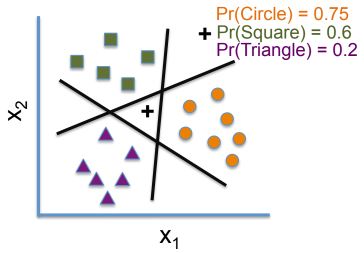
Recall: Multi-class classification



Previously, we learned a multi-class classifier by combining binary, linear decision boundaries to partition the feature space. Nearest neighbors can *naturally* learn multiple decision boundaries depending on which points are closest to which class's training data.

Nearest neighbors for regression

Recall the nearest neighbor of a (training or test) data point:

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Regression rule

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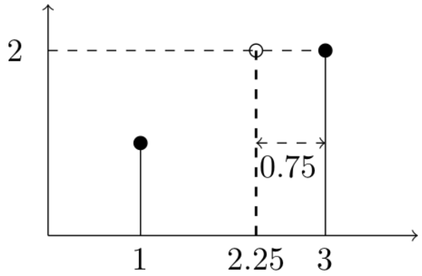
Label **x** with the label of its nearest neighbor!



Parametric vs. Nonparametric, revisited

Nonparametric models instead assume that the model features depend on the data $\mathcal{D}$. The number of features tends to grow with the size of the dataset.

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- But, we need to compare the test data point to *every sample in the training dataset*.

K-nearest neighbor (KNN) classification

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The set of K-nearest neighbors

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

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

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

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- Aggregate everyone's vote

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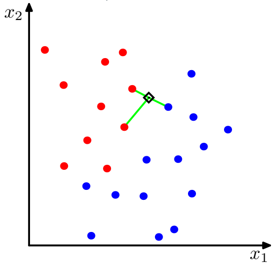
- Label with the majority, breaking ties arbitrarily

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

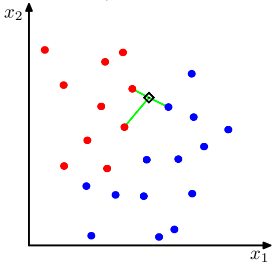
Example

K=1, Label: ??



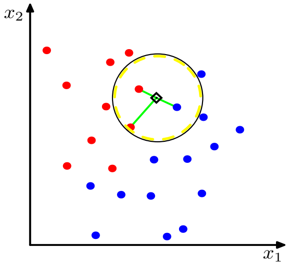
(a)

K=3, Label: ??



(a)

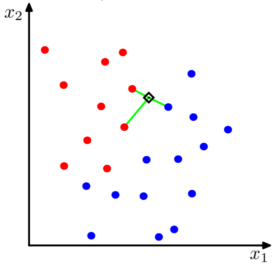
K=5, Label: ??



(a)

Example

K=1, Label: red



(a)

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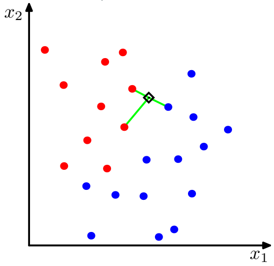
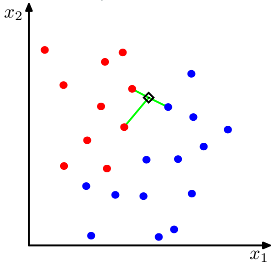


(a)

K=3, Label: red



(a)

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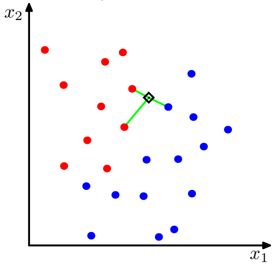
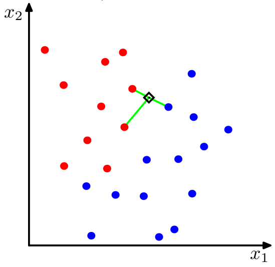
K=1, Label: red



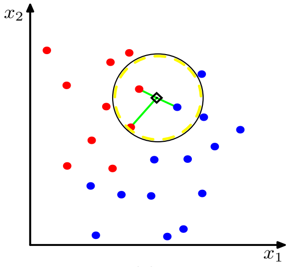
(a)

K=3, Label: red



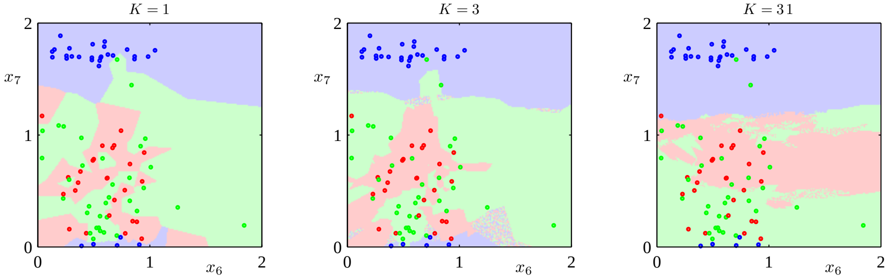
(a)

K=5, Label: blue



(a)

How to choose an optimal K?



When K increases, the decision boundary becomes smooth.

How to do regression with K neighbors?

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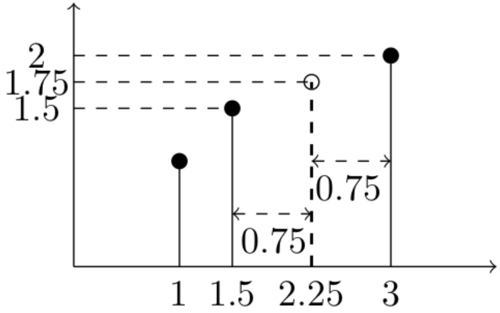

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Advantages of NNC

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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 difficult.

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    - More on this in the next lecture on decision trees.

Practical Aspects of NN

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Two crucial choices for NN

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

Hyperparameter tuning on a validation dataset

Training data

- N samples/instances: $\mathcal{D}^{\text{TRAIN}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_\mathsf{N}, y_\mathsf{N})\}$
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Validation data

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

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

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- For each possible value of the hyperparameter (say $K = 1, 3, \cdots, 100$)

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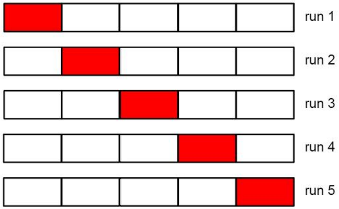
- Evaluate the model on $\mathcal{D}^{\text{TEST}}$

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 the model performs the best (based on average, variance, etc.)
- We re-train the model on the full training dataset with the best hyperparameter.

Figure 3: $S = 5$: 5-fold cross validation



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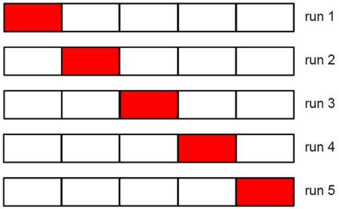

Special case: when $S = N$, this will be leave-one-out.

But how do we choose the distances?

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

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

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

Summary so far

- Described a simple *nonparametric* learning algorithm
- Discussed a few practical aspects, such as tuning hyperparameters, with cross-validation

Good luck on the midterm! Please come to office hours and/or the recitation with questions.