CSCI567 Machine Learning (Spring 2021)

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Outline

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Homeworks

- HW 0 is due on Friday. It will not be graded, only to get everyone familiar with the submission mechanism.
- HW 1 will be released on Friday (01/22/2021). Starting HW 1 assignments will be graded.

Outline

Last Class: Foundations of ML

- We discussed different flavors of learning problems
- Tools from probability, information theory, and optimization
- **Today:** We will start our journey of Supervised learning starting with classification.

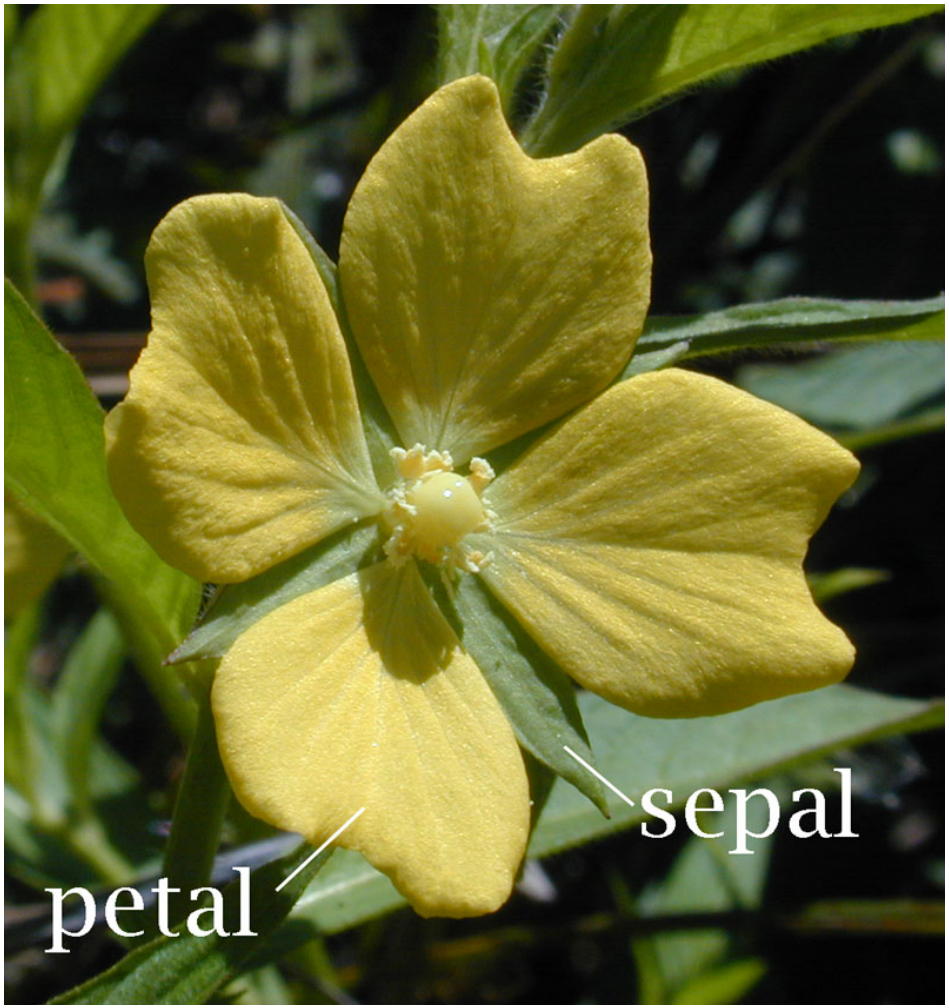
Outline

Recognizing flowers

Types of Iris: setosa, versicolor, and virginica

Measuring the properties of the flowers

Features and attributes: the widths and lengths of sepal and petal



Often, data is conveniently organized as a table

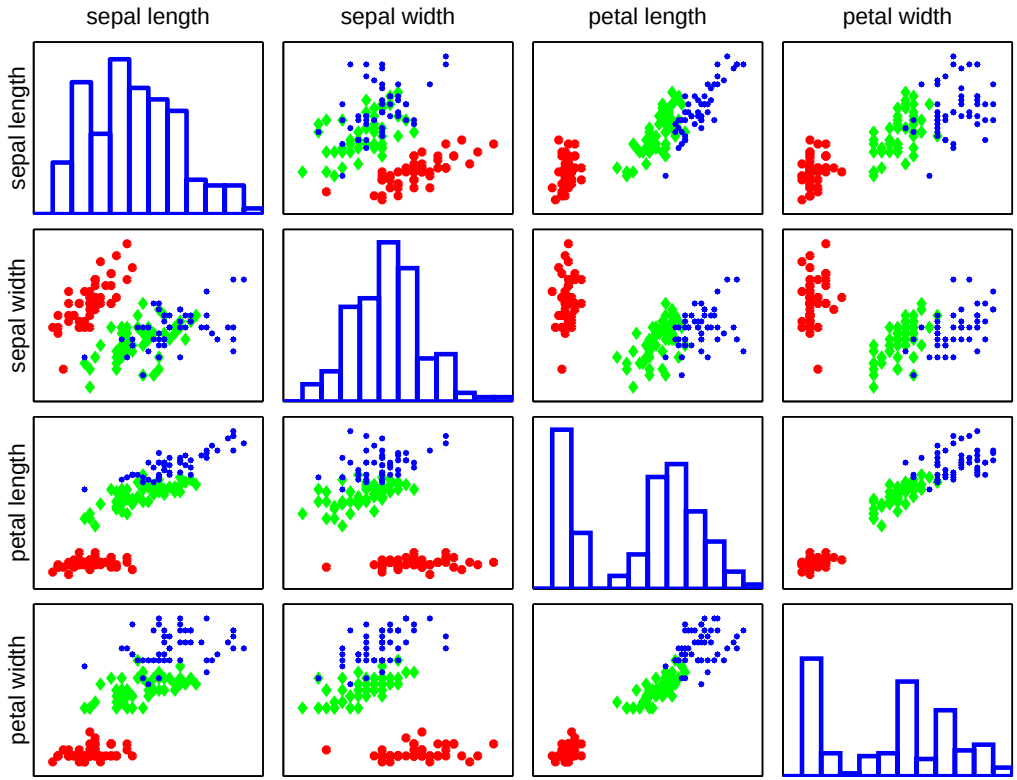
Fisher's *Iris* Data

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

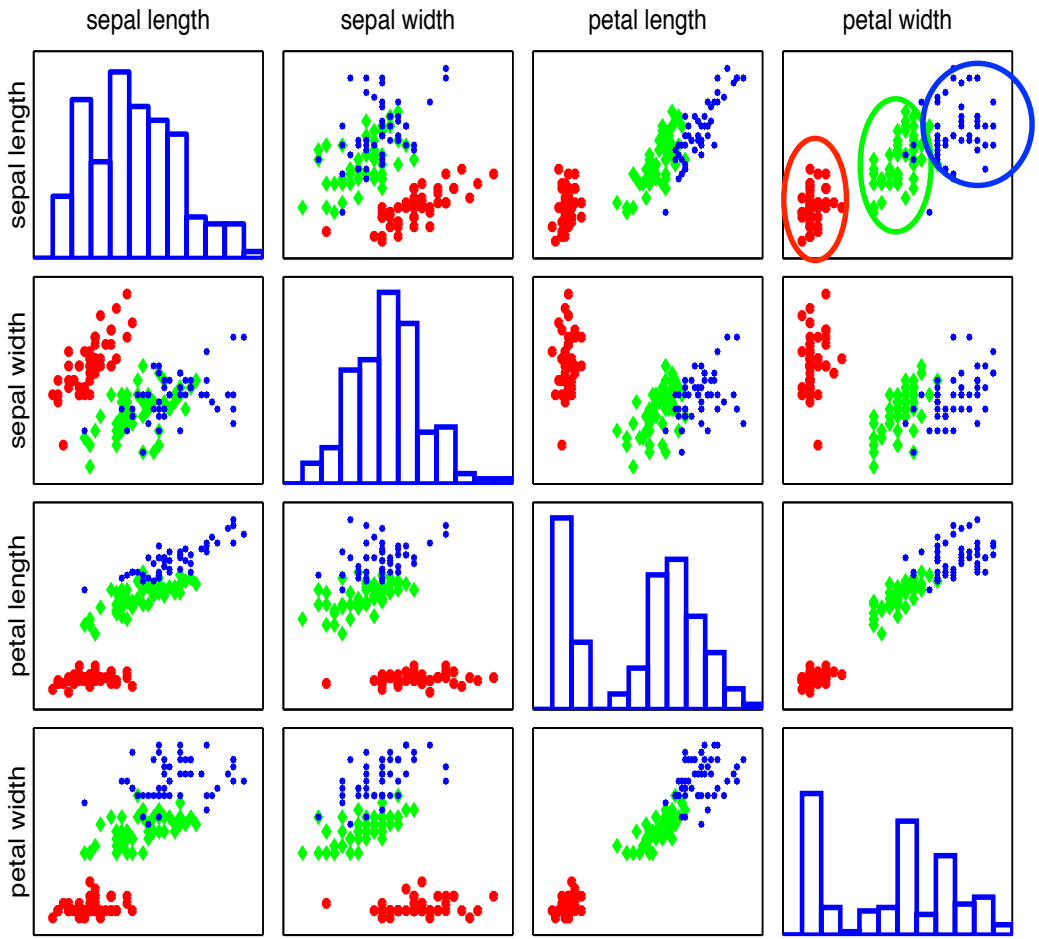
Visualization of data helps identify the right learning model to use

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



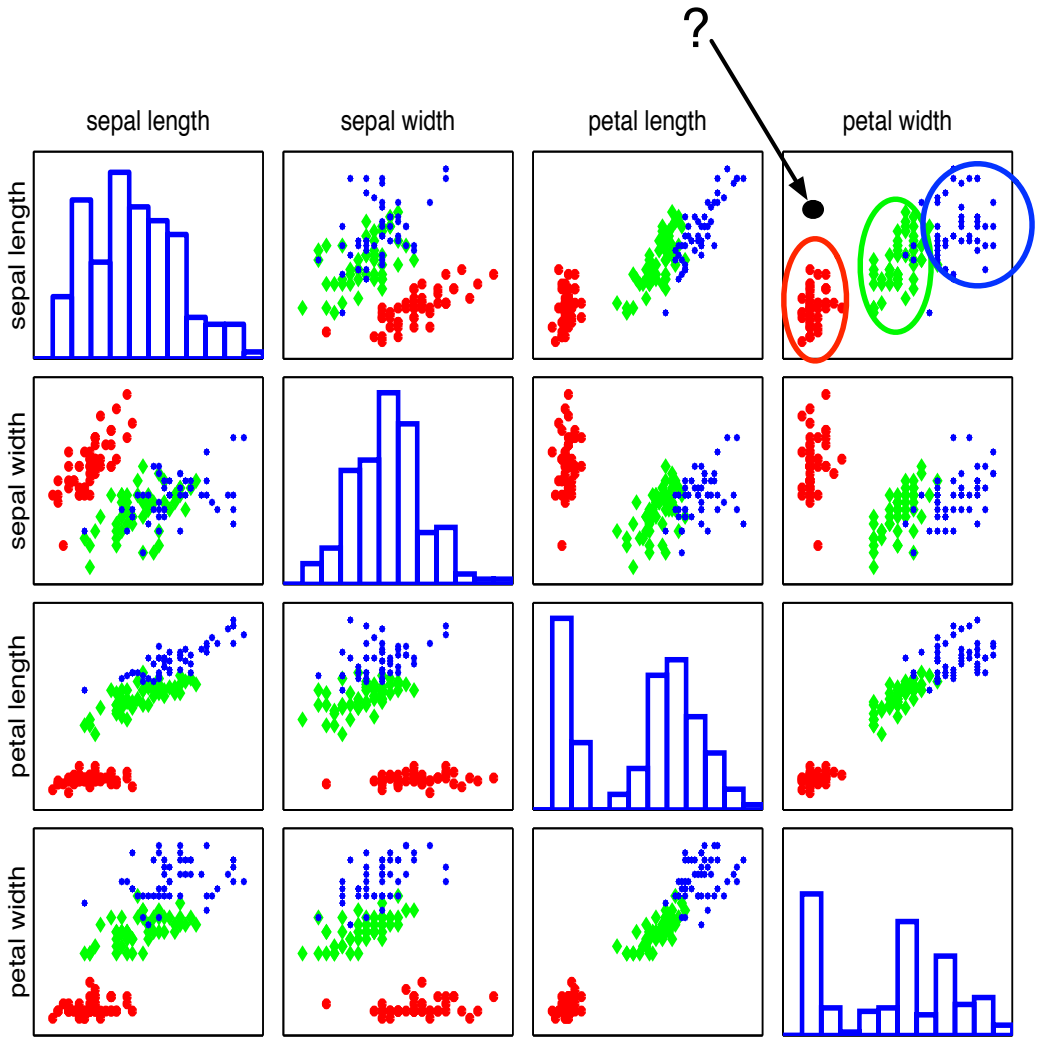
Different types seem well-clustered and separable

Using two features: petal width and sepal length



Labeling an unknown flower type

Closer to red cluster: so labeling it as setosa



General setup for multi-class classification

Training data (set)

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

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Special case: binary classification

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

Nearest neighbor classification (NNC)

The index of the **nearest neighbor** of a point $\boldsymbol{x}$ is

$$\mathsf{nn}(\boldsymbol{x}) = \operatorname*{argmin}_{n \in [\mathsf{N}]} \|\boldsymbol{x} - \boldsymbol{x}_n\|_2 = \operatorname*{argmin}_{n \in [\mathsf{N}]} \sqrt{\sum_{d=1}^{\mathsf{D}} (x_d - x_{nd})^2}$$

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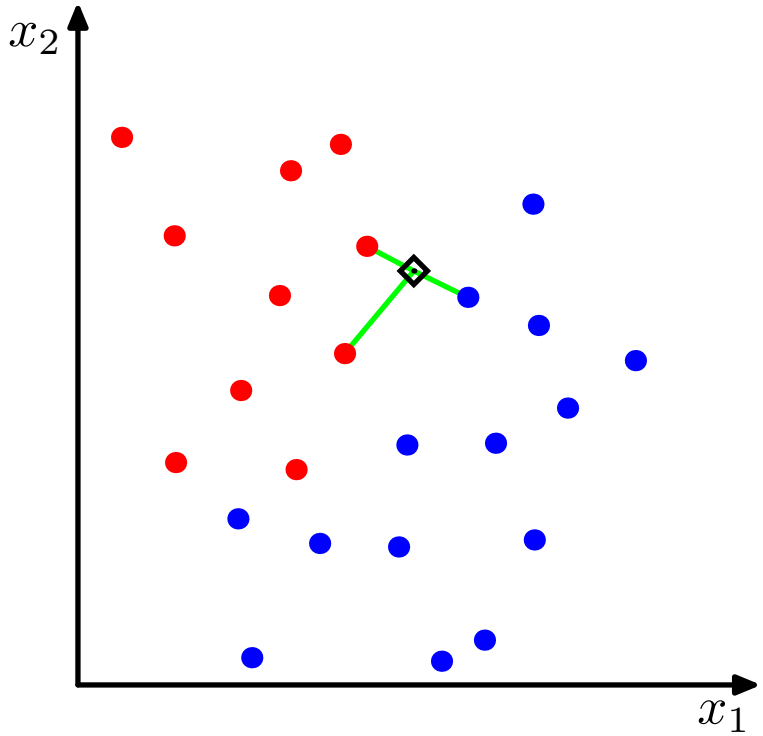
Classification rule

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

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	setoas
2	1.4	7.0	versicolor
3	2.5	6.7	virginica
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Flower with unknown category

petal width $= 1.8$ and sepal length $= 6.4$ (i.e. $\boldsymbol{x} = (1.8, 6.4)$)

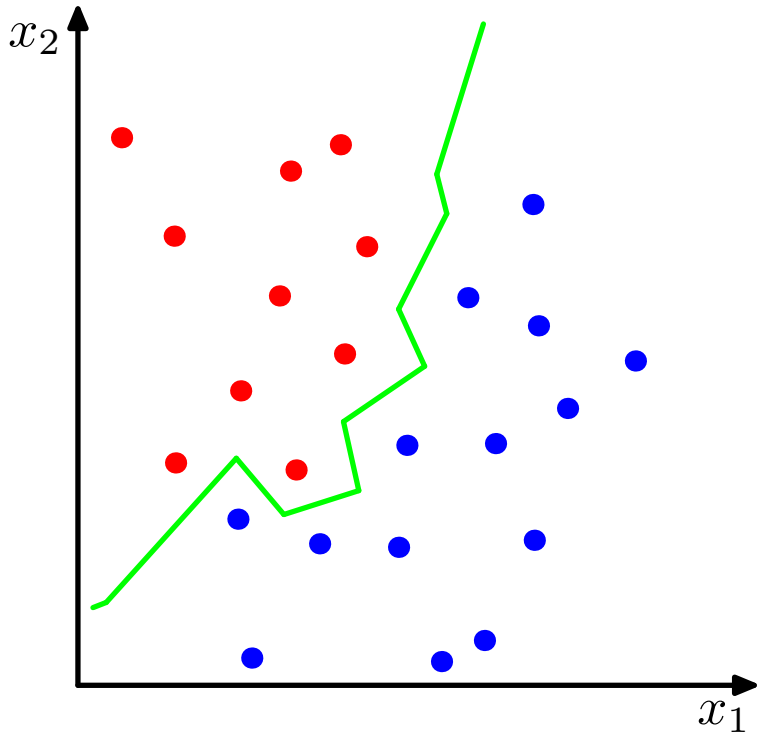
Calculating distance $\|\boldsymbol{x} - \boldsymbol{x}_n\|_2 = \sqrt{(x_1 - x_{n1})^2 + (x_2 - x_{n2})^2}$

ID	distance
1	1.75
2	0.72
3	0.76

Thus, the category is *versicolor*.

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)

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Intuition

We should compute accuracy (A) — the percentage of data points being correctly classified, or the error rate (ϵ)— the percentage of data points being incorrectly classified. (accuracy + error rate = 1)

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where $\mathbb{I}[\cdot]$ is the indicator function.

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Is this the right measure?

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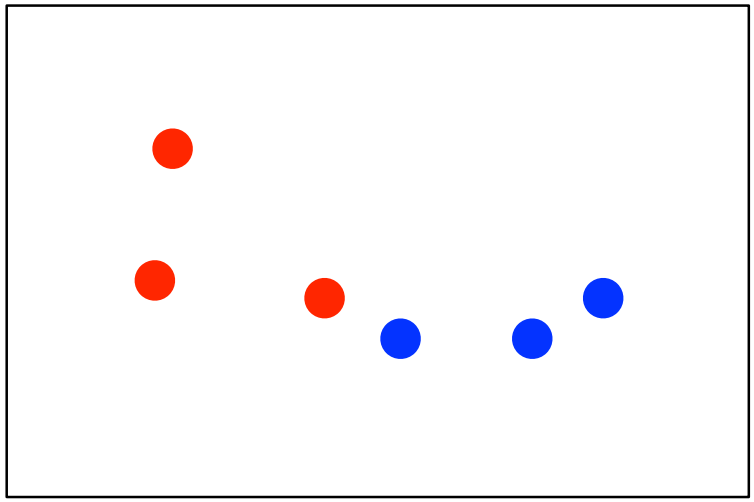

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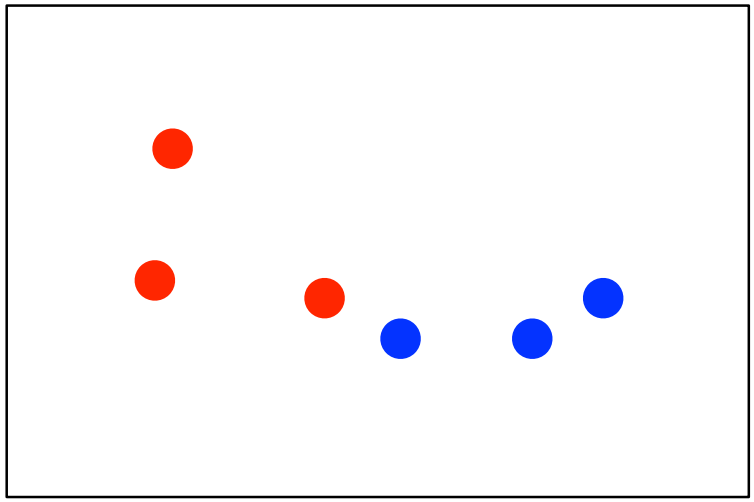

What are A^{TRAIN} and ϵ^{TRAIN}?

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

For every training data point, its nearest neighbor is itself.

Test Error

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- Good measurement of a classifier's performance

Variant 1: measure nearness with other distances

Previously, we use the Euclidean distance

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

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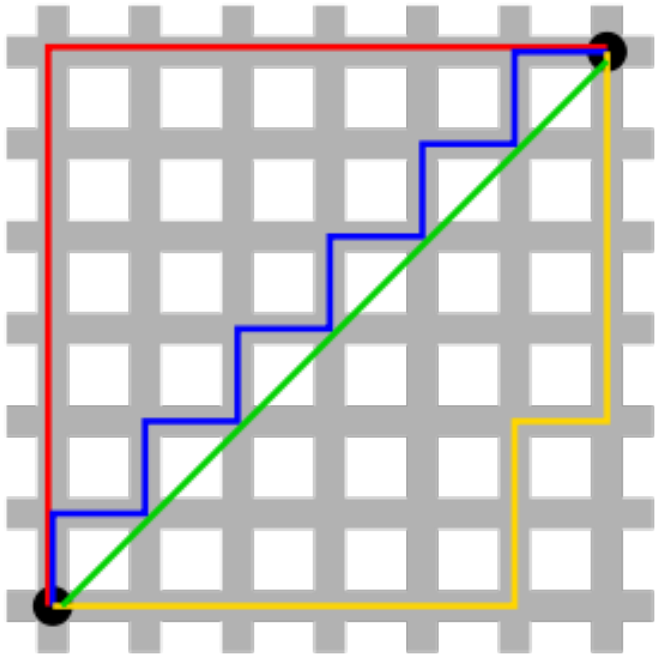

Green line is Euclidean distance. Red, Blue, and Yellow lines are L_1 distance

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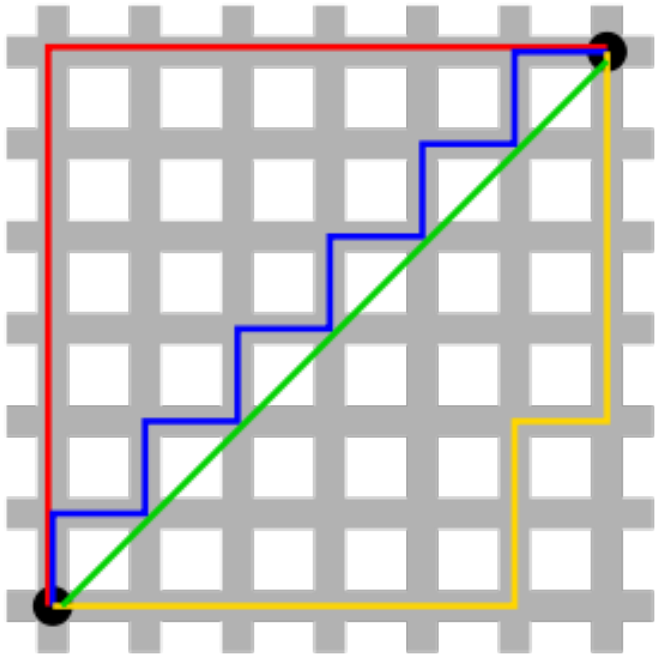
More generally, L_p distance (for $p \geq 1$):

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



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Note: we have

$$\|\boldsymbol{x} - \boldsymbol{x}_{\mathsf{nn}_1(\boldsymbol{x})}\|_2 \leq \|\boldsymbol{x} - \boldsymbol{x}_{\mathsf{nn}_2(\boldsymbol{x})}\|_2 \cdots \leq \|\boldsymbol{x} - \boldsymbol{x}_{\mathsf{nn}_K(\boldsymbol{x})}\|_2$$

How to classify with K neighbors?

Classification rule

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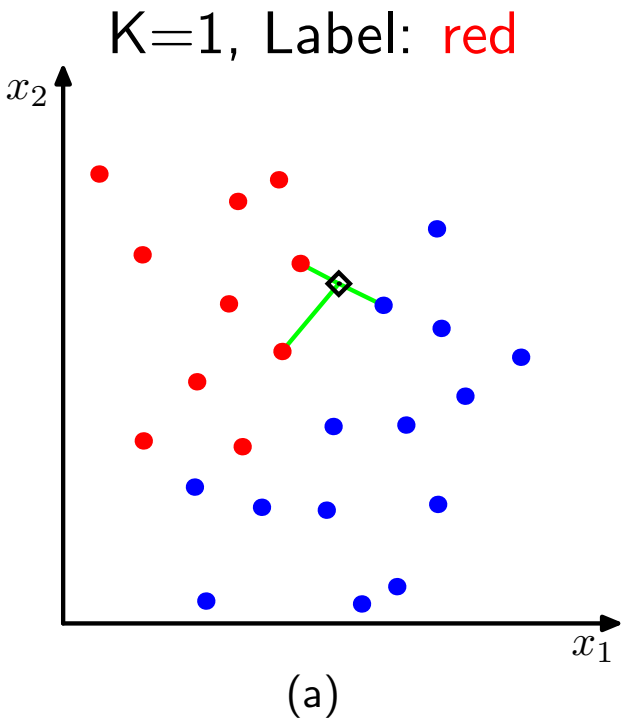
- Predict with the majority

$$f(\boldsymbol{x}) = \operatorname*{argmax}_{c \in [\mathsf{C}]} v_c$$

Example



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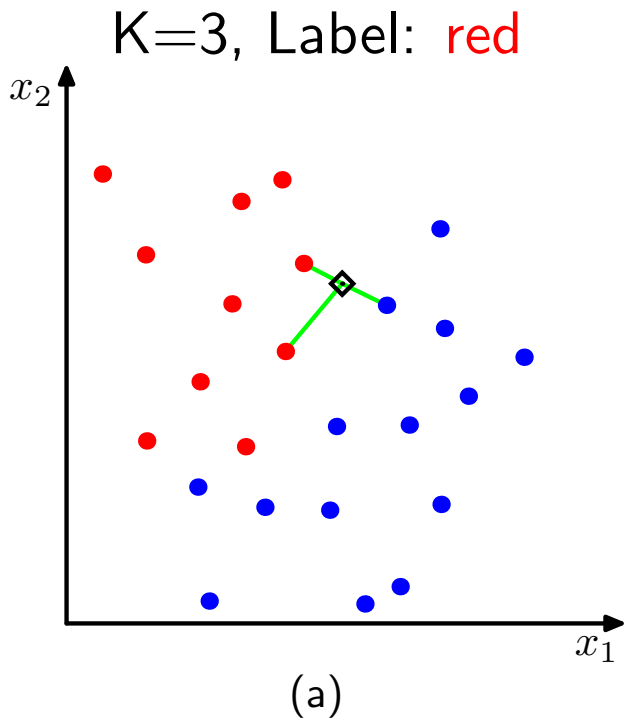

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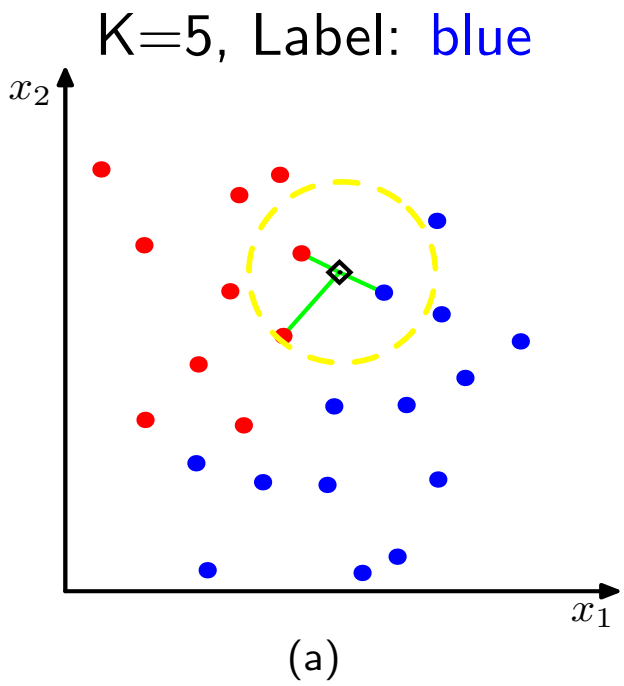
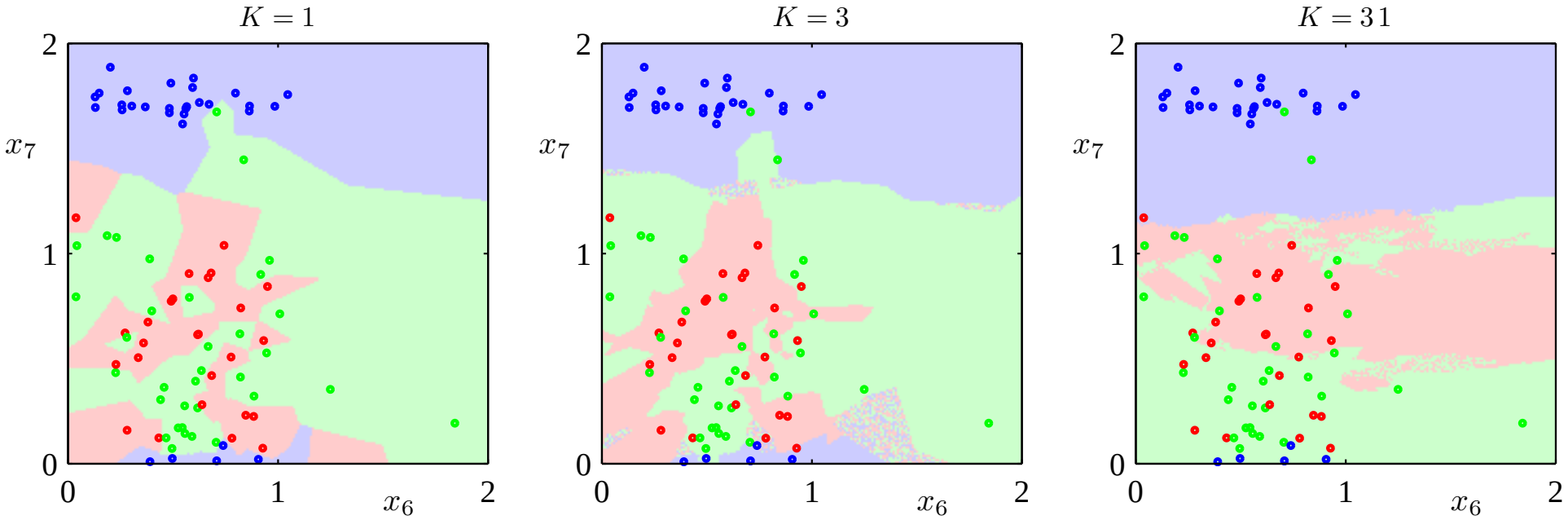


(a)

Decision boundary



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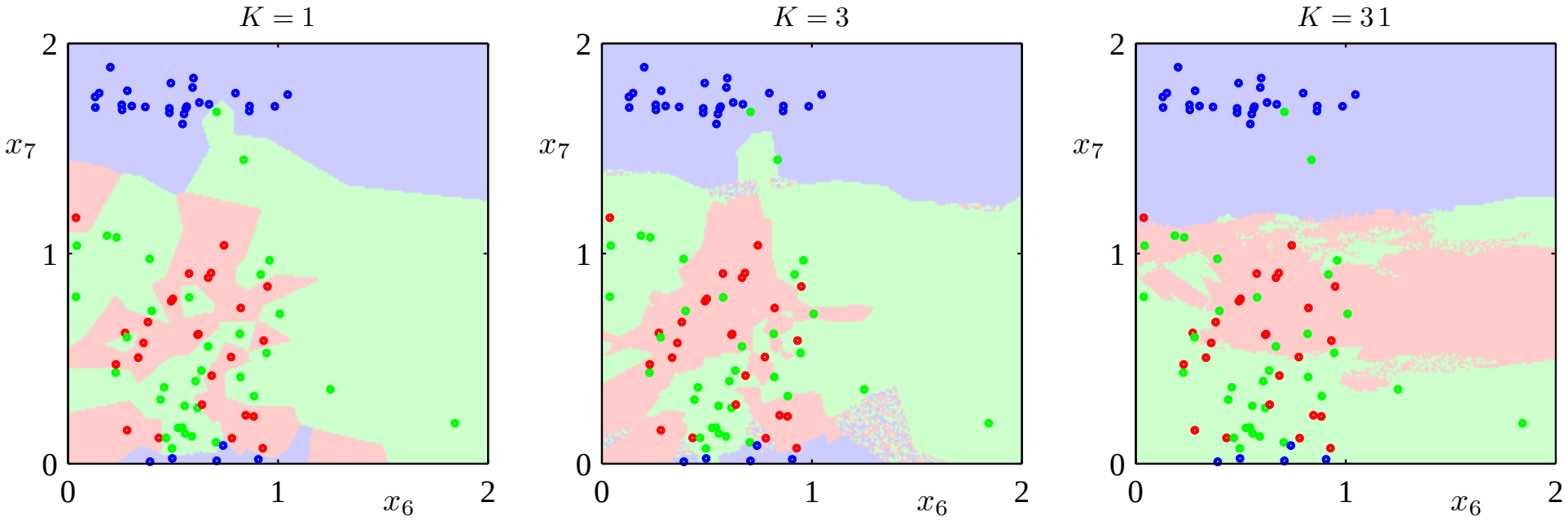

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What happens when $K = N$?

Variant 3: Preprocessing data

One issue of NNC: *distances depend on units of the features!*

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Example:

- 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

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Many other ways of normalizing data.

Which variants should we use?

Hyper-parameters in NNC

- The distance measure (e.g. the parameter p for L_p norm)
- K (i.e. how many nearest neighbor?)
- Different ways of preprocessing

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- Different ways of preprocessing

Most algorithms have hyper-parameters. Tuning them is a significant part of applying an algorithm.

Tuning via a development dataset

Training data

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

Test data

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

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These three sets should *not* overlap!

Recipe

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

S-fold Cross-validation

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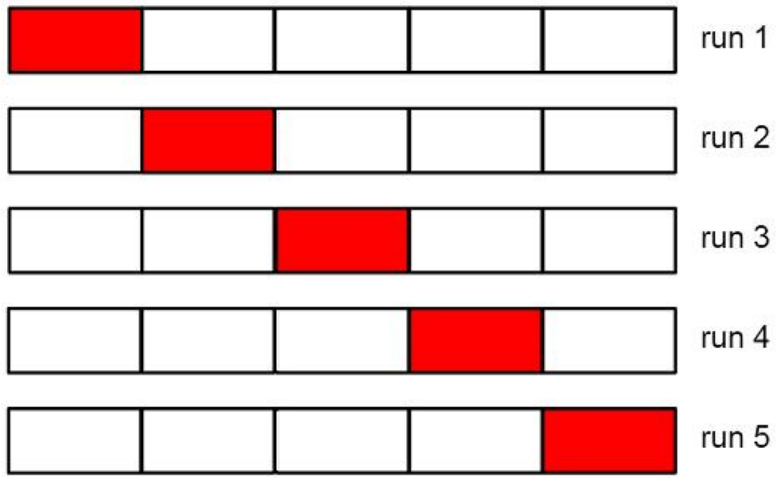

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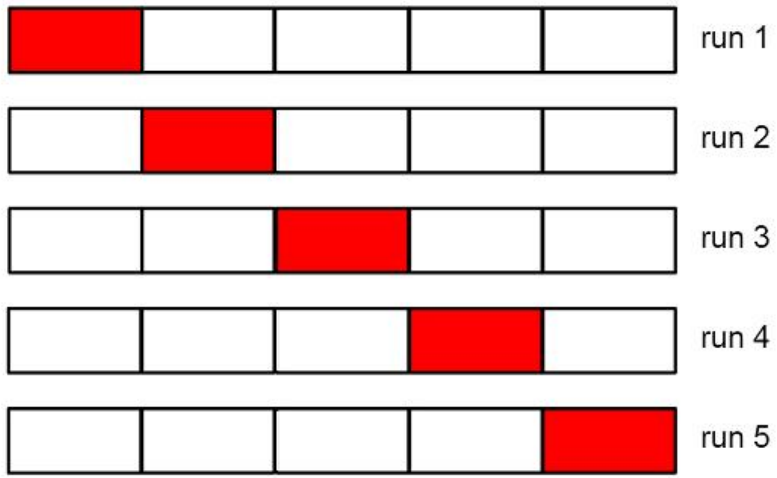

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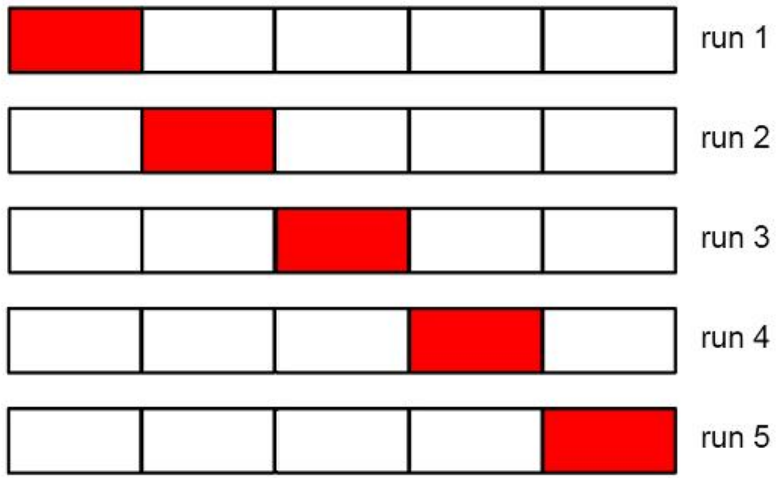

Special case: S = N, called leave-one-out.

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- Need to *"carry"* the training data around. This type of method is called *nonparametric*.
- Choosing the right hyper-parameters can be involved.

Summary

Typical steps of developing a machine learning system:

- Collect data, split into training, development, and test sets.
- Train a model with a machine learning algorithm. Most often we apply cross-validation to tune hyper-parameters.
- Evaluate using the test data and report performance.
- Use the model to predict future/make decisions.

Outline

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Most standard assumption: every data point $(\boldsymbol{x}, y)$ (from $\mathcal{D}^{\text{TRAIN}}$, $\mathcal{D}^{\text{DEV}}$, or $\mathcal{D}^{\text{TEST}}$) is an *independent and identically distributed (i.i.d.)* sample of an unknown joint distribution $\mathcal{P}$.

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Need a more "certain" measure of performance (so it's easy to compare different classifiers for example).

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What about the expectation of training error? Is training error a good proxy of expected error?

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More generally, for a loss function $L(y', y)$,

- e.g. $L(y', y) = \mathbb{I}[y' \neq y]$, called *0-1 loss*.
- many more other losses as we will see.

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For special case $C = 2$, let $\eta(\boldsymbol{x}) = \mathcal{P}(0|\boldsymbol{x})$, then

$$\begin{aligned} R(f^*) &= \mathbb{E}_{\boldsymbol{x}\sim\mathcal{P}_{\boldsymbol{x}}}[\mathbb{E}_{\boldsymbol{y}|\boldsymbol{x}}[\mathbb{I}_{f^*(\boldsymbol{x})\neq y}]] \\ &= \mathbb{E}_{\boldsymbol{x}\sim\mathcal{P}_{\boldsymbol{x}}}[\eta(\boldsymbol{x})\mathbb{I}_{f^*(\boldsymbol{x})=1} + (1-\eta(\boldsymbol{x}))\mathbb{I}_{f^*(\boldsymbol{x})=0}] \\ &= \mathbb{E}_{\boldsymbol{x}\sim\mathcal{P}_{\boldsymbol{x}}}[\min\{\eta(\boldsymbol{x}), 1-\eta(\boldsymbol{x})\}], \end{aligned}$$

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Theorem (Cover and Hart, 1967)

Let f_N be the 1-nearest neighbor binary classifier using N training data points, we have (under mild conditions)

$$R(f^*) \leq \lim_{N \to \infty} \mathbb{E}[R(f_N)] \leq 2R(f^*)$$

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A pretty strong guarantee.
In particular, $R(f^*) = 0$ implies $\mathbb{E}[R(f_N)] \to 0$.

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