Applied Data Science

Machine Learning
Lecture 3

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Today's agenda — Classification

- The general problem
  - formulation
  - types of error

- (Gaussian) Model-based
  - linear discriminant analysis
  - quadratic discriminant analysis

- Regression methods
  - logistic regression
  - training and validation

- Other approaches
  - Nearest-neighbor methods

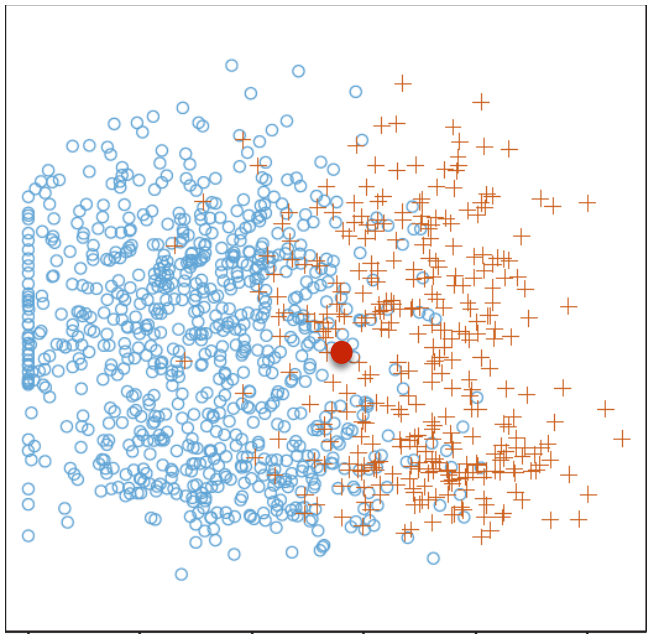
The general context — applications

$\mathbf{X}_1$	Y_1
$\vdots$	$\vdots$
$\vdots$	$\vdots$
$\mathbf{X}_n$	Y_n
$\mathbf{X}$	Y?

- Classify a data record into one of multiple categories, based on examples

$Y = 0, 1$ (binary)

$Y = 1, \ldots, m$ (m-ary)



$\mathbf{X}$: symptoms, test results — Y: cancer?

$\mathbf{X}$: an email message — Y: spam?

$\mathbf{X}$: image of a digit Y — Y: which digit is it? ($m = 10$)

$\mathbf{X}$: image of an animal Y — Y: cat, dog, cow,...

Example: prediction of loan default

Y	X_1	X_2	X_3
default	student	balance	income
No	No	729.5265	44361.63
No	Yes	817.1804	12106.13
No	No	1073.549	31767.14
No	No	529.2506	35704.49
No	No	785.6559	38463.5
No	Yes	919.5885	7491.559
No	No	825.5133	24905.23
No	Yes	808.6675	17600.45
No	No	1161.058	37468.53

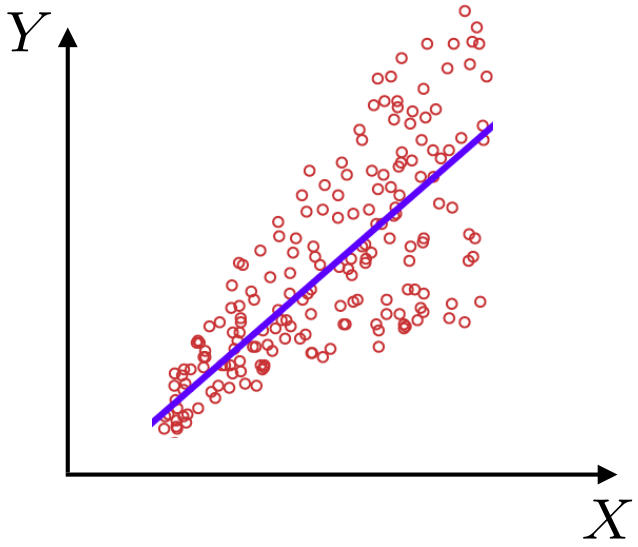
- 10,000 samples
  - 3.33% of the samples represent defaults
- encoding: "No" =0, "Yes" =1"

Predictors and classifiers

- In regression:

  predictor $\widehat{Y} = g(\mathbf{X})$

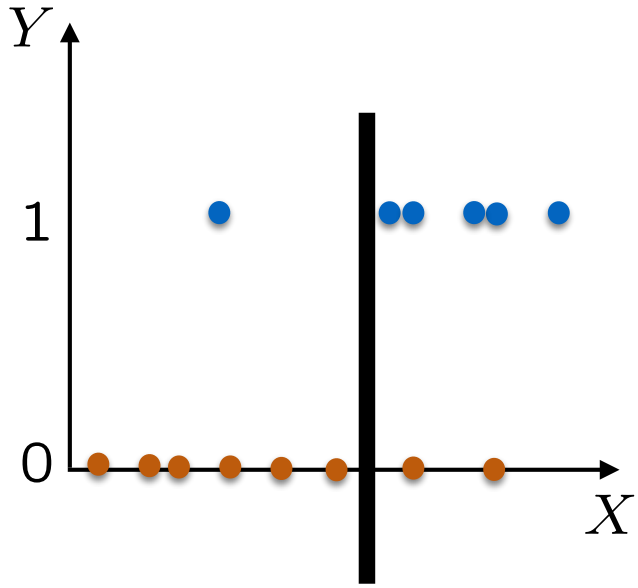
  metric $\mathbb{E}\left[(\widehat{Y} - Y)^2\right]$



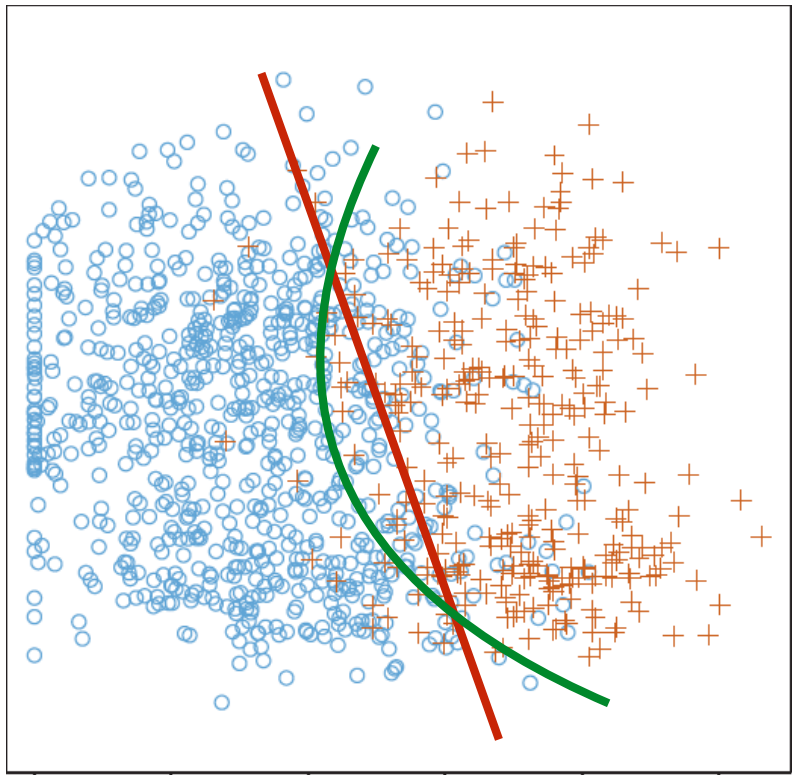
- In classification:

  classifier $\widehat{Y} = g(\mathbf{X}) \in \{1, \ldots, m\}$

  metric $\mathbb{P}(\text{mistake})$



Types of classifiers

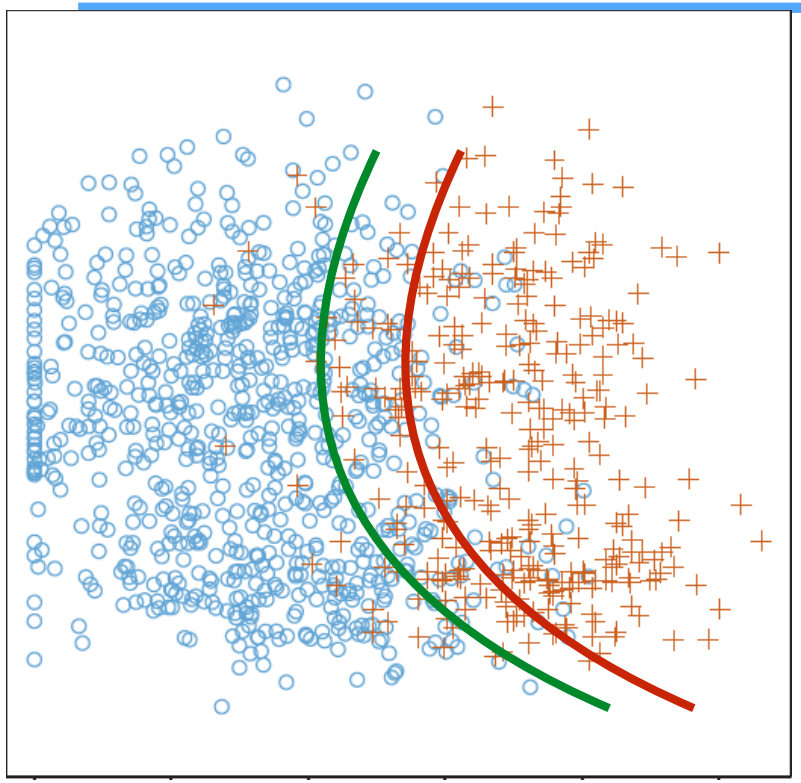


- Linear classifiers:
  compare $\boldsymbol{\theta}^T \mathbf{X}$ to a threshold
  - learn "good" vector $\boldsymbol{\theta}$ and threshold
- Nonlinear classifiers:
  compare $h(\mathbf{X})$ to a threshold
  - learn "good" function h and threshold

- Nonlinear classifier $\theta_1 X_1 + \theta_2 X_2 + \theta_{12} X_1 X_2$
  is actually linear if we redefine $\mathbf{X} = (X_1, X_2, X_1 X_2)$

- Feature-based linear classifier: compare $\boldsymbol{\theta}^T \phi(\mathbf{X})$ to a threshold

Error types and confusion matrix



- Binary classification, two error types:

  truth is "blue", decide $\widehat{Y}$ = "brown"

  truth is "brown", decide $\widehat{Y}$ = "blue"

Predicted labels \ True labels	blue	brown
blue	✓	✗
brown	✗	✓

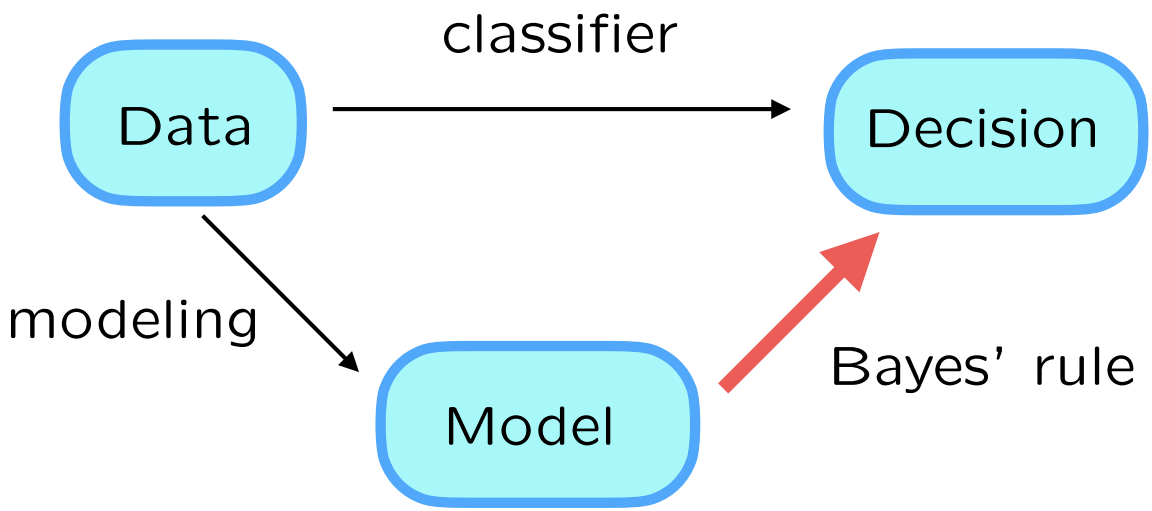
- Interested in having few errors on new data records
- Aim at few errors on training set
- Tradeoff between the two error types
- Similar confusion matrix, for m-ary classification

Predicted labels \ True labels	good	default
good	9644	252
default	23	81

Jargon: accuracy, precision, recall, sensitivity, specificity, false alarm,. . .

(GAUSSIAN) MODEL-BASED APPROACH

The model-based approach



1. Exemplify the Bayes' rule, for Gaussian models

2. Gaussian modeling

Gaussian model

- $\mathbb{P}(Y = k) = \pi_k \quad (k = 1, \ldots, m)$ "prior" probabilities

- $\mathbb{P}(\mathbf{X} \,|\, Y = k) \sim N(\boldsymbol{\mu}_k, C_k)$

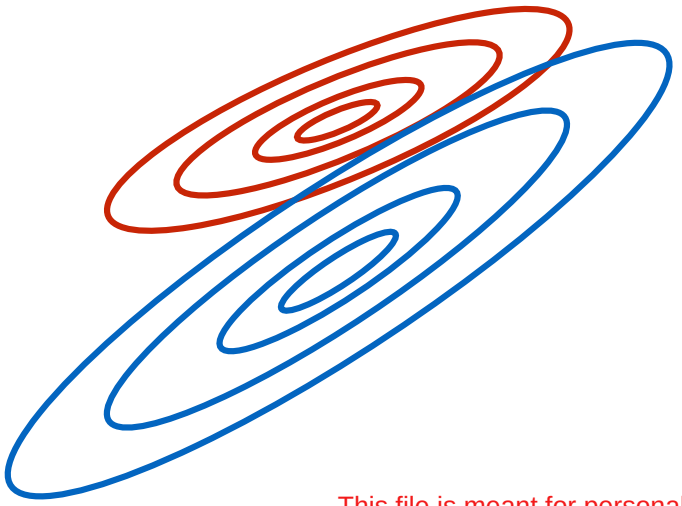
$$\gamma_k \cdot \exp\left\{ -\frac{(X - \mu_k)^2}{2\sigma_k^2} \right\}$$

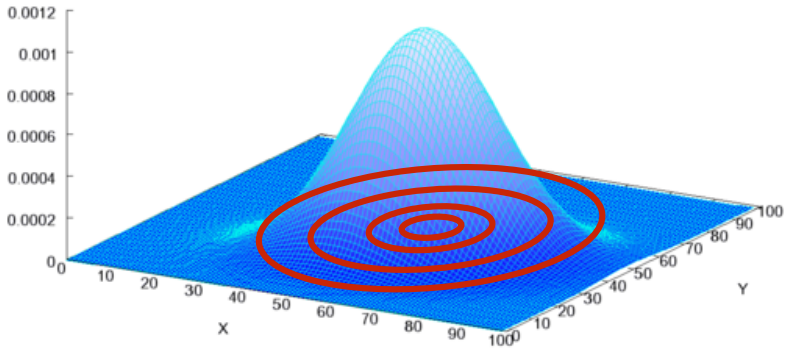
$$\gamma_k \cdot \exp\left\{ -\frac{1}{2}(\mathbf{X} - \boldsymbol{\mu}_k)^T C_k^{-1} (\mathbf{X} - \boldsymbol{\mu}_k) \right\}$$

$\boldsymbol{\mu}_k$: mean vector $\mathbb{E}[\mathbf{X} \,|\, Y = k]$

C_k: covariance matrix

$$\mathbb{E}\Big[(\mathbf{X} - \boldsymbol{\mu}_k)(\mathbf{X} - \boldsymbol{\mu}_k)^T \,|\, Y = k\Big]$$





https://en.wikipedia.org/wiki/Multivariate_normal_distribution

Bayes' rule

$$\mathbb{P}(Y = k \,|\, \mathbf{X}) = \frac{\pi_k \cdot \mathbb{P}(\mathbf{X} \,|\, Y = k)}{\mathbb{P}(\mathbf{X})} \qquad \text{(posterior)}$$

- Given value $\mathbf{X}$, choose k with largest posterior
  - minimizes $\mathbb{P}(\text{error})$ $\qquad \pi_k \cdot \gamma_k \cdot \exp\Big\{ -\frac{1}{2}(\mathbf{X} - \boldsymbol{\mu}_k)^T C_k^{-1} (\mathbf{X} - \boldsymbol{\mu}_k) \Big\}$

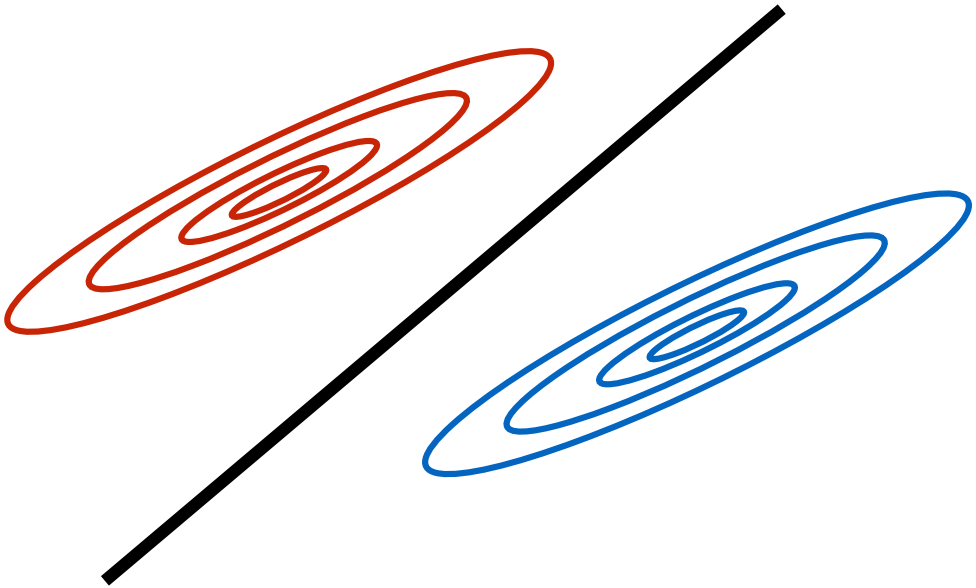
- Compare $\log(\pi_k \cdot \gamma_k) - \frac{1}{2}(\mathbf{X} - \boldsymbol{\mu}_k)^T C_k^{-1} (\mathbf{X} - \boldsymbol{\mu}_k)$, for different classes k
  - boundary: when same value for some k, $k' \longrightarrow$ quadratic in $\mathbf{X}$

  Quadratic discriminant analysis (QDA)

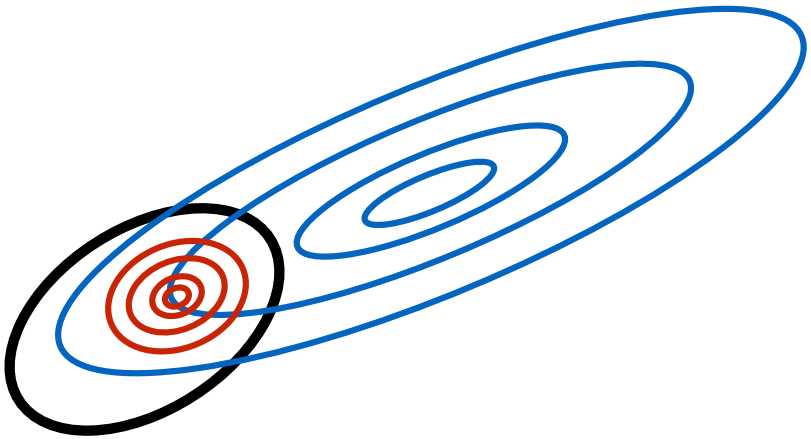
- When all $C_k = C$ (same), second-order terms in $\mathbf{X}$ are all the same
  - compare $\log(\pi_k \cdot \gamma_k) - (\boldsymbol{\mu}_k)^T C^{-1} \mathbf{X} - \frac{1}{2}(\boldsymbol{\mu}_k)^T C^{-1} \boldsymbol{\mu}_k$, for different k
  - boundary: when same value for some k, $k' \longrightarrow$ linear in $\mathbf{X}$

  Linear discriminant analysis (LDA)

LDA versus QDA



different means
same covariances



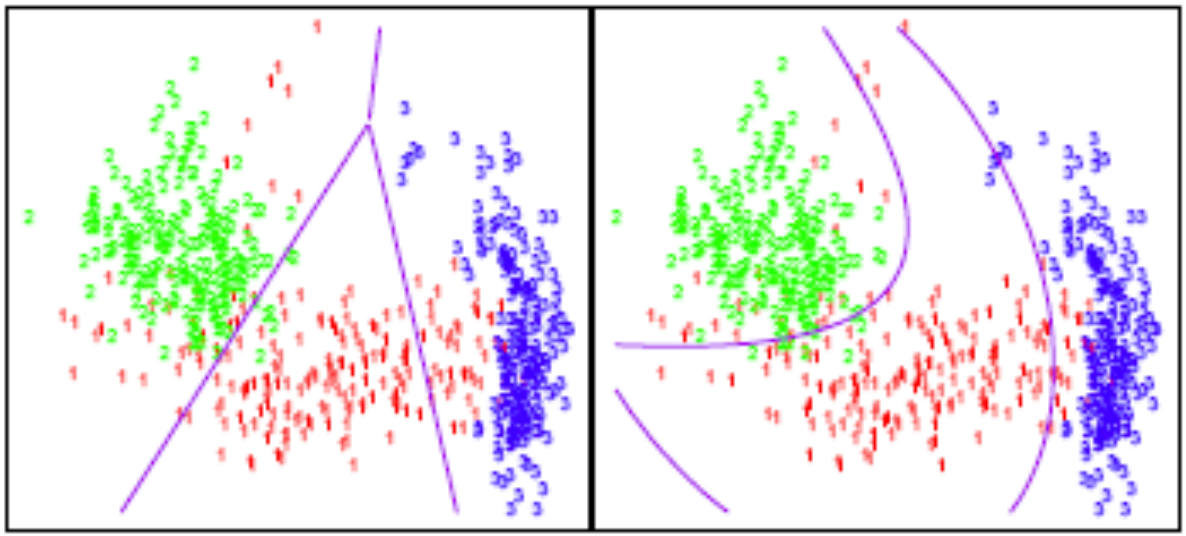
different means
different covariances

LDA versus QDA

Assume

same versus different

covariances



LDA QDA

The modeling part

- $\mathbb{P}(Y = k) = \pi_k$ $\qquad\qquad$ $\widehat{\pi}_k = \dfrac{\#\text{ samples of class } k}{\text{total } \#\text{ of samples}}$

- $\boldsymbol{\mu}_k = \mathbb{E}[\mathbf{X} \,|\, Y = k]$ $\qquad\qquad$ $\widehat{\boldsymbol{\mu}}_k =$ average value of $\mathbf{X}$ over all samples of class k

- $C_k = \mathbb{E}\Big[(\mathbf{X} - \boldsymbol{\mu}_k)(\mathbf{X} - \boldsymbol{\mu}_k)^T \,|\, Y = k\Big]$

$\widehat{C}_k =$ average value of $(\mathbf{X} - \widehat{\boldsymbol{\mu}}_k)(\mathbf{X} - \widehat{\boldsymbol{\mu}}_k)^T$, over all samples of class k

"plugin estimates"

(replace expectations with averages)

Prediction default example

- Performance on the training set

- Recall that only 3.33% of the records correspond to defaults
  - **Always decide "no default:"** Miss-classification rate 3.33%

- Make predictions using only one component of $\mathbf{X}$ ("balance")
  - LDA: 2.81%
  - QDA: 2.73%

- Make predictions using all of $\mathbf{X}$
  - LDA: 2.75%
  - QDA: 2.70%

Predicted labels \ True labels	good	default
good	9644	252
default	23	81

- Should validate performance on a holdout set or through cross-validation

Unbalanced costs

- some error types may be more costly

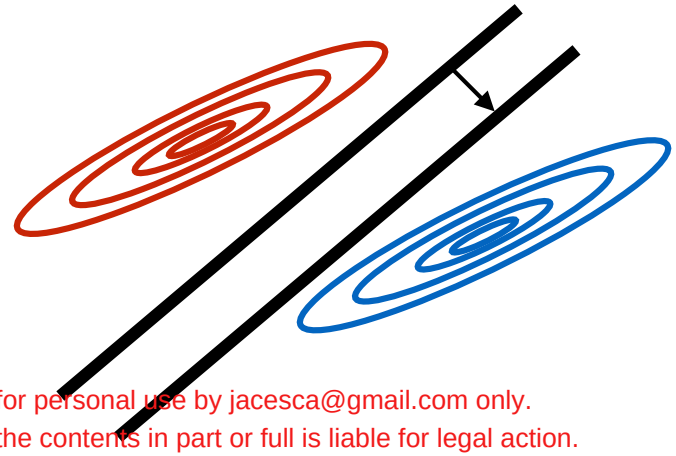
$$c_{\text{def}} \gg c_{\text{lost}}$$

Predicted labels \ True labels	good	default
good	9644	252 c_{def}
default	23 c_{lost}	81

- c_{def}: cost if $\widehat{Y} = \text{good}$ (give the loan) and $Y = \text{default}$
- c_{lost}: cost if $\widehat{Y} = \text{default}$ and $Y = \text{good}$ (lost customer)
- Minimize probability of error versus expected cost:

  compare $c_{\text{def}} \cdot \mathbb{P}(Y = \text{default} \mid \mathbf{X})$ to $c_{\text{lost}} \cdot \mathbb{P}(Y = \text{good} \mid \mathbf{X})$

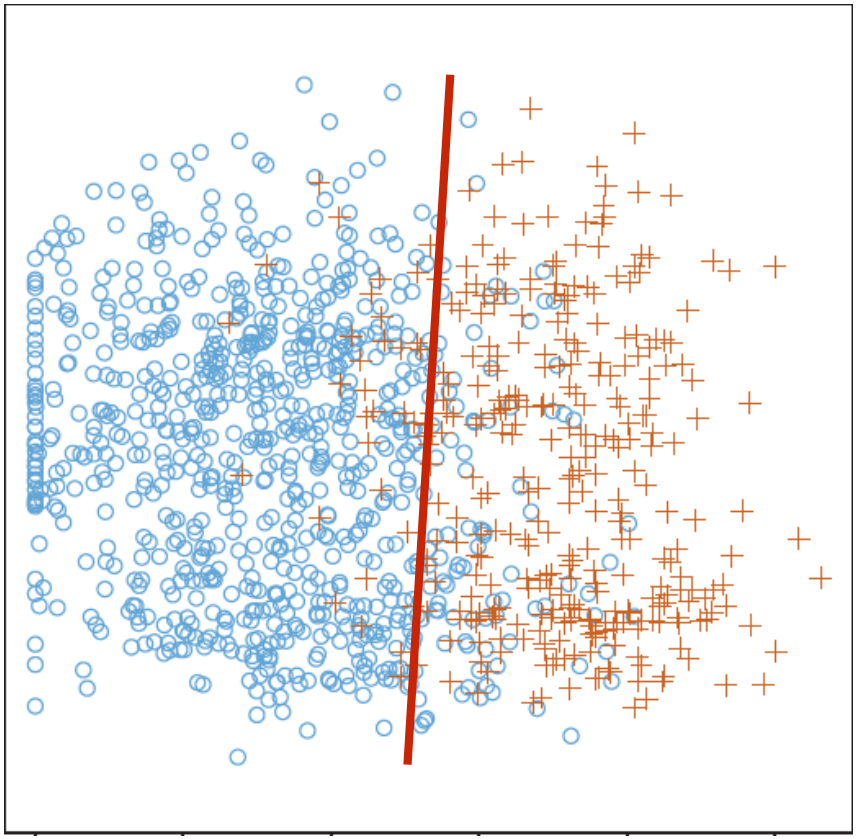
- Shifts the thresholds



LEARNING/REGRESSION METHODS FOR CLASSIFICATION

An approach that does not work

- Restrict to special family of classifiers (e.g., linear)
  - find classifier with fewest missclassified samples
  - computationally intractable

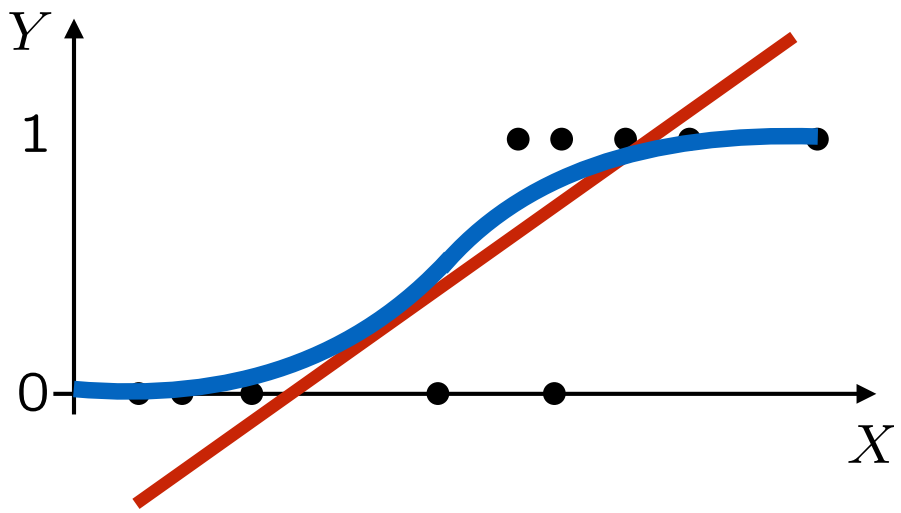


An attempt to use regression

- Regress Y on $\mathbf{X}$

$$\min_{\boldsymbol{\theta}} \sum_i (Y_i - \boldsymbol{\theta}^T \mathbf{X}_i)^2$$

– predict $\widehat{Y} = 1$ if $\widehat{\boldsymbol{\theta}}^T \mathbf{X} \geq 0.5$

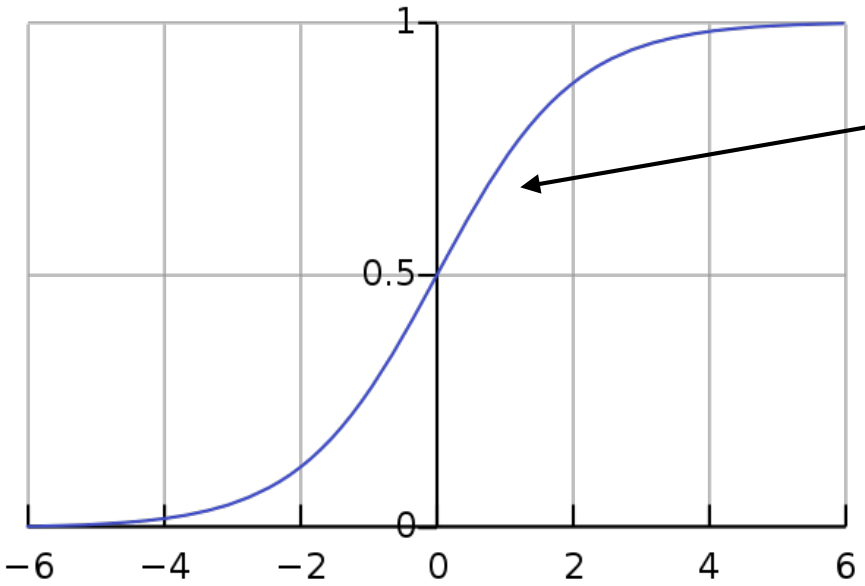


– error criterion is not meaningful

- **A better idea:** Fit a curve that ranges between 0 and 1 (must be nonlinear)

– interpret as (estimated) probability $\mathbb{P}(Y = 1 \,|\, \mathbf{X})$

The logistic model



$$\frac{e^x}{e^x + e^{-x}}$$

shift and scale

$$\frac{e^{\theta_1 x}}{e^{\theta_0 x} + e^{\theta_1 x}}$$

- Assume model of the form $\mathbb{P}(Y = k \,|\, \mathbf{X}) = \dfrac{\exp\{\boldsymbol{\theta}_k^T \mathbf{X}\}}{\sum_s \exp\{\boldsymbol{\theta}_s^T \mathbf{X}\}}$
- Use the data to find "best-fitting" vectors $\widehat{\boldsymbol{\theta}}_1, \ldots, \widehat{\boldsymbol{\theta}}_m$
- Decision rule: choose class k with biggest $\widehat{\boldsymbol{\theta}}_k^T \mathbf{X}$ linear!
- But we do not have training data for these probabilities

Training the logistic model: maximum likelihood

- Assume the $\mathbf{X}_i$ are somehow set (random or otherwise)
- Assume the model structure (+ independence) $\quad \mathbb{P}(Y = k \,|\, \mathbf{X}) = \dfrac{\exp\{\boldsymbol{\theta}_k^T \mathbf{X}\}}{\sum_s \exp\{\boldsymbol{\theta}_s^T \mathbf{X}\}}$
- Likelihood function of the observed data $\quad L(\text{data}; \boldsymbol{\theta}) = \prod_i \mathbb{P}(Y_i \,|\, \mathbf{X}_i)$

- Example data: $(\mathbf{X}_1, 1),\ (\mathbf{X}_2, 0),\ (\mathbf{X}_3, 1)$

  $L(\text{data}; \boldsymbol{\theta}) = \mathbb{P}(Y = 1 \mid \mathbf{X}_1) \cdot \mathbb{P}(Y = 0 \mid \mathbf{X}_2) \cdot \mathbb{P}(Y = 1 \mid \mathbf{X}_3)$

- $\log L(\text{data}; \boldsymbol{\theta}) = \sum_{i \text{ of class } 0} \log \mathbb{P}(Y = 0 \mid \mathbf{X}_i) + \sum_{i \text{ of class } 1} \log \mathbb{P}(Y = 1 \mid \mathbf{X}_i)$

- "Messy, but:
  - convex
  - gradients are easy to calculate
  - efficient algorithms

Comments, caveats

- Much from linear regression applies here too
- Good predictions do not imply causality
- Can use features $\exp\{\boldsymbol{\theta}_k^T \mathbf{X}\} \longrightarrow \exp\{\boldsymbol{\theta}_k^T \phi(\mathbf{X})\}$
- Can add regularization terms

  $$\log L(\text{data}; \boldsymbol{\theta}) - \gamma \cdot \|\boldsymbol{\theta}\|^2$$

  or sum of absolute values

  - tune hyperparameter γ "experimentally"

- Evaluating performance on the training set is not enough
  - use separate validation set
- Confidence intervals, various tests,...

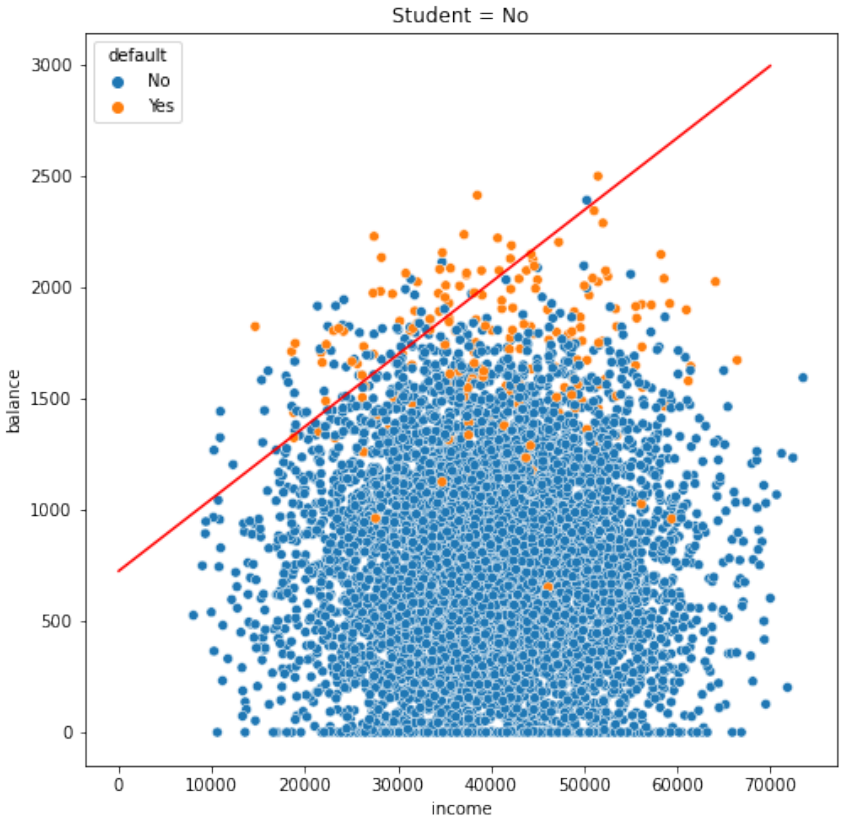
Results

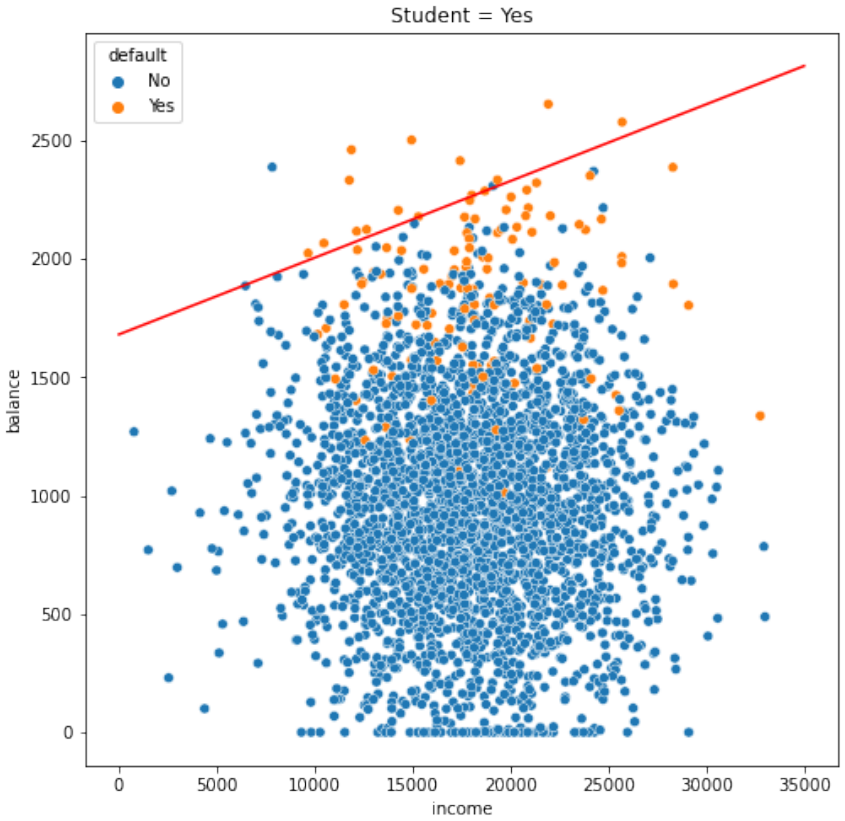
- Recall that only 3.33% of the records correspond to defaults
  - **Always decide "no default:"** Miss-classification rate 3.33%

- Make predictions using only one component of $\mathbf{X}$ ("balance")
  - LDA: 2.81%
  - QDA: 2.73%
  - Logistic: 2.73%

- Make predictions using all of $\mathbf{X}$
  - LDA: 2.75%
  - QDA: 2.70%
  - Logistic: 3.33%
  - Logistic with absolute value regularization: 2.66%

Results





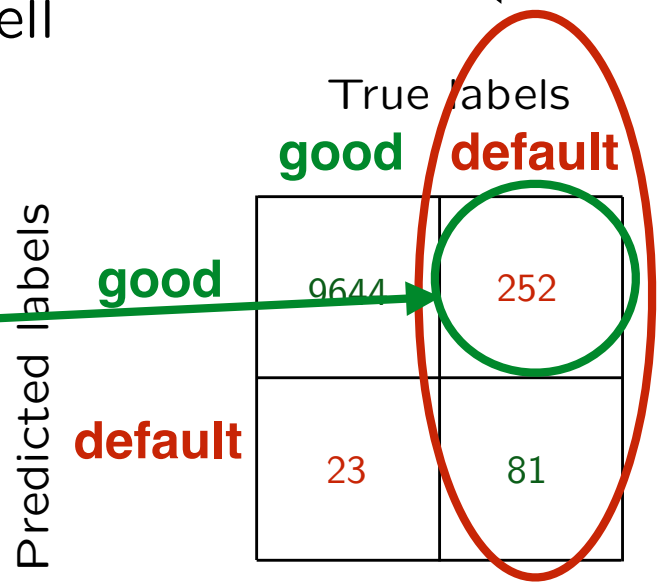
- Logistic: 3.33%

Unbalanced data sets and/or costs

- $\log L(\text{data};\theta) = \sum_{i \text{ of class } 0} \log \mathbb{P}(Y = 0 \mid \mathbf{X}_i) + \mathbf{w} \sum_{i \text{ of class } 1} \log \mathbb{P}(Y = 1 \mid \mathbf{X}_i)$

defaulting customers in the data set

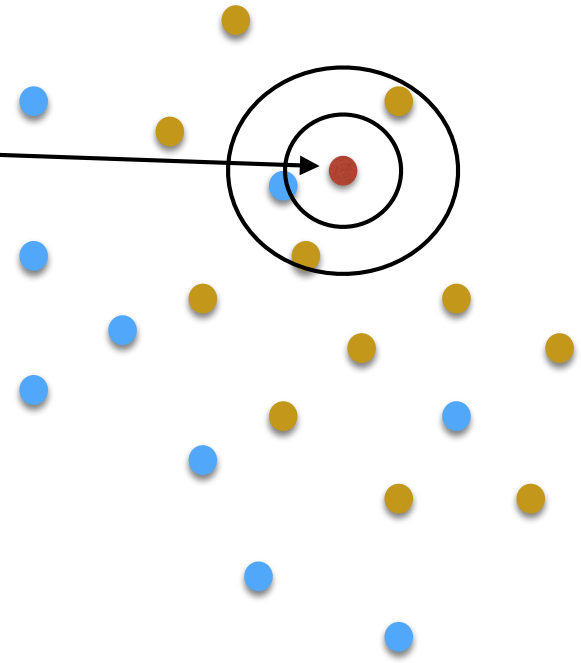
- Solution pays less attention to classes with few samples
  - always declaring "class 0" does pretty well
- Problem is exacerbated if errors on defaulting customers are much more costly
- Solution: increase weight of "red" sum
  - equivalent to adding to the data set replicas of the "class 1" samples



NEAREST-NEIGHBOR CLASSIFIERS

The k-NN classifier

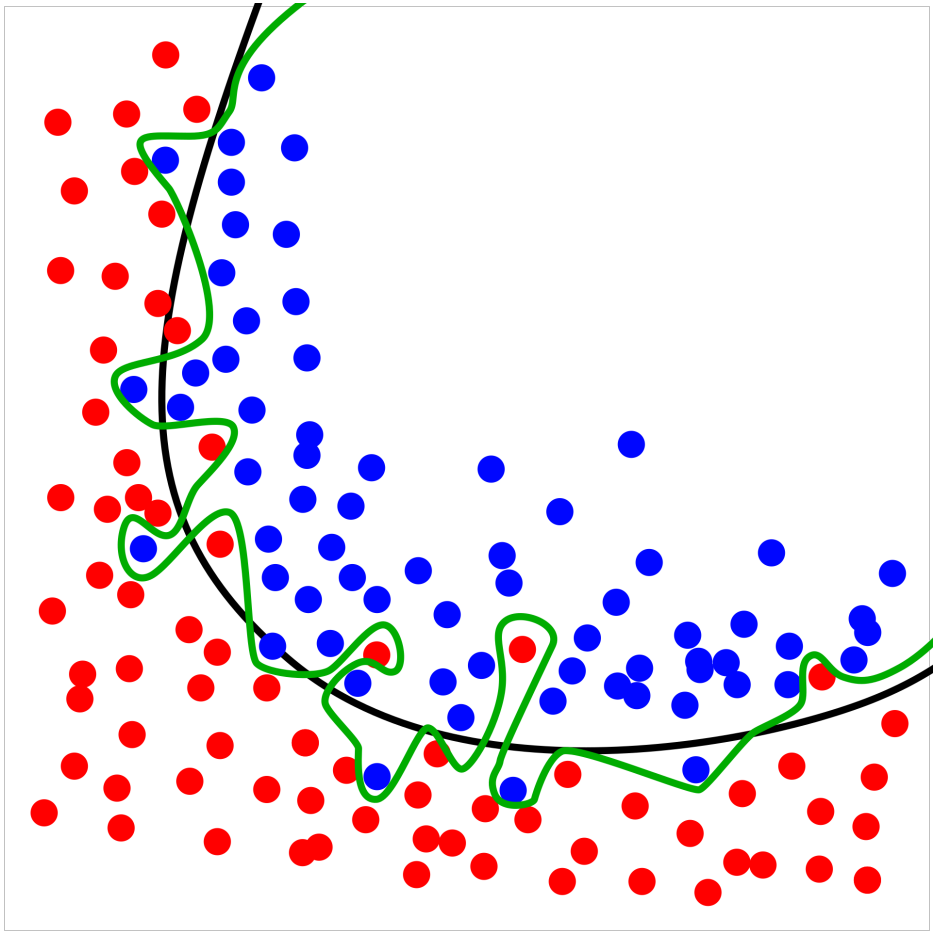
- The nearest-neighbor classifier:
  - given new $\mathbf{X}$
  - find closest $\mathbf{X}_i$ in the data set (with smallest $\|\mathbf{X} - \mathbf{X}_i\|$)
  - prediction: the label Y_i of $\mathbf{X}_i$



- The k-NN classifier:
  - given new $\mathbf{X}$
  - find k closest $\mathbf{X}_i$ in the data set
  - prediction: majority vote of the k labels

- Simple, no training required

Illustration

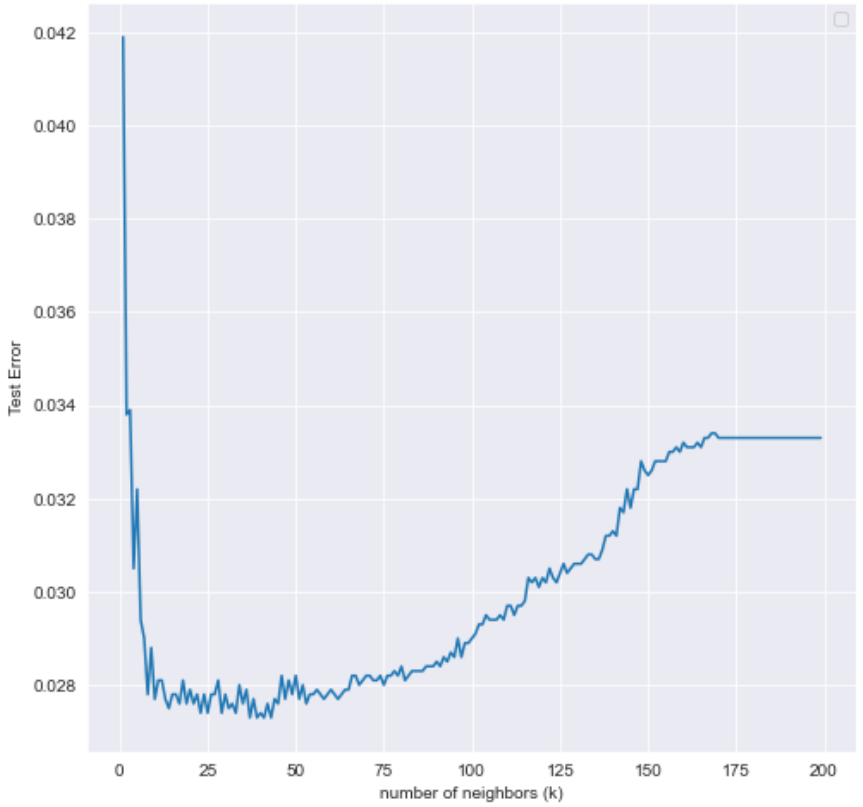


https://commons.wikimedia.org/wiki/File:Overfitting.svg#/media/File:Overfitting.svg

Selecting k

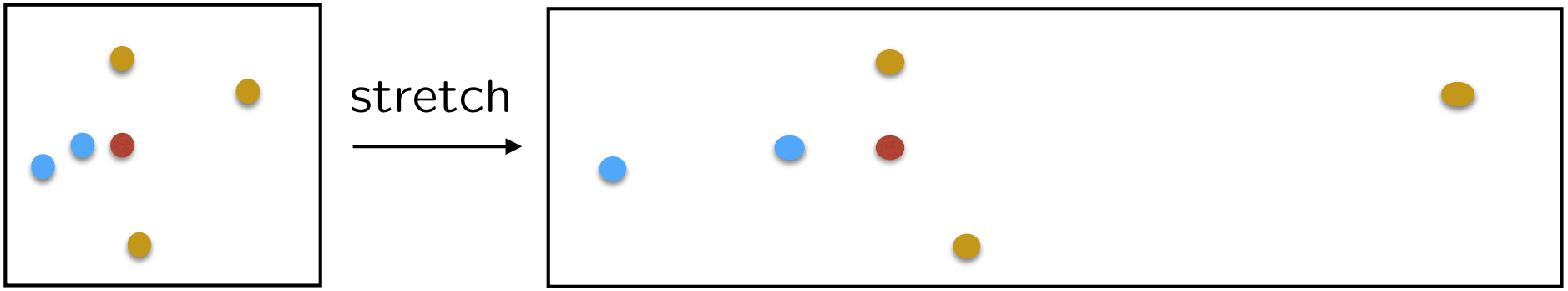
- Default data
  - LOOCV: classify a record, based on the remaining ones

Value of K	Error
5-NN	3.22
6-NN	2.94
7-NN	2.9
8-NN	2.78
9-NN	2.88
10-NN	2.77
11-NN	2.81
12-NN	2.81
13-NN	2.77
14-NN	2.75
15-NN	2.78



- This is an example of hyperparameter search to choose between models/algorithms

Scaling matters



$k = 3$

decide "blue"

$k = 3$

decide "brown"

- Scale so that the components of $\mathbf{X}$ have comparable ranges

- equivalently: use a weighted distance metric,

e.g. $\|x\| = \sqrt{x_1^2 + w \cdot x_2^2}$

Some other classification algorithms

- **Weighted NN**
  - k-NN: majority vote between k neighbors
  - Consider weighting the votes, as a function of the distance
  - every point could vote, far away points would have little weight

    - Similar idea applies to standard regression problems
      - estimate $\mathbb{E}[Y|\mathbf{X}]$ by weighing the Y_i's of nearby $\mathbf{X}_i$

        (kernel regression)

- **Support vector machines**

- **Decision trees**

- **Neural networks**

Interpretability of models; explainability of predictions

- A generic issue in machine learning
- In regression, coefficients $\boldsymbol{\theta}$ allow us to interpret the "logic" behind particular predictions

$$\widehat{\text{Sales}} = 2.94 + 0.046 \cdot (\text{TV}) + 0.19 \cdot (\text{Radio}) - 0.001 \cdot (\text{NewsP})$$

- Similarly in logistic regression $\mathbb{P}(Y = k \,|\, \mathbf{X}) = \dfrac{\exp\{\boldsymbol{\theta}_k^T \mathbf{X}\}}{\sum_s \exp\{\boldsymbol{\theta}_s^T \mathbf{X}\}}$
- Nearest neighbor methods do not yield an interpretable model
  - but allow us to explain the predictions

"Beth's profile is similar to that of Barbara, Beatrice, and Bo..."

- A challenge for more complex machine learning models

Wrapping up

- Saw a number of methods
  - for prediction and "model-building"

- Encountered the main general methodologies
  - empirical risk minimization
  - maximum likelihood
  - plugin estimates
  - Bayesian

- "Classical" methods (regression, LDA, QDA, NN, etc.) form the starting point for more complex methods

- General toolbox for performance assessment (validation, bootstrap)

- Need care to avoid misinterpretations