# Supervised Learning - I

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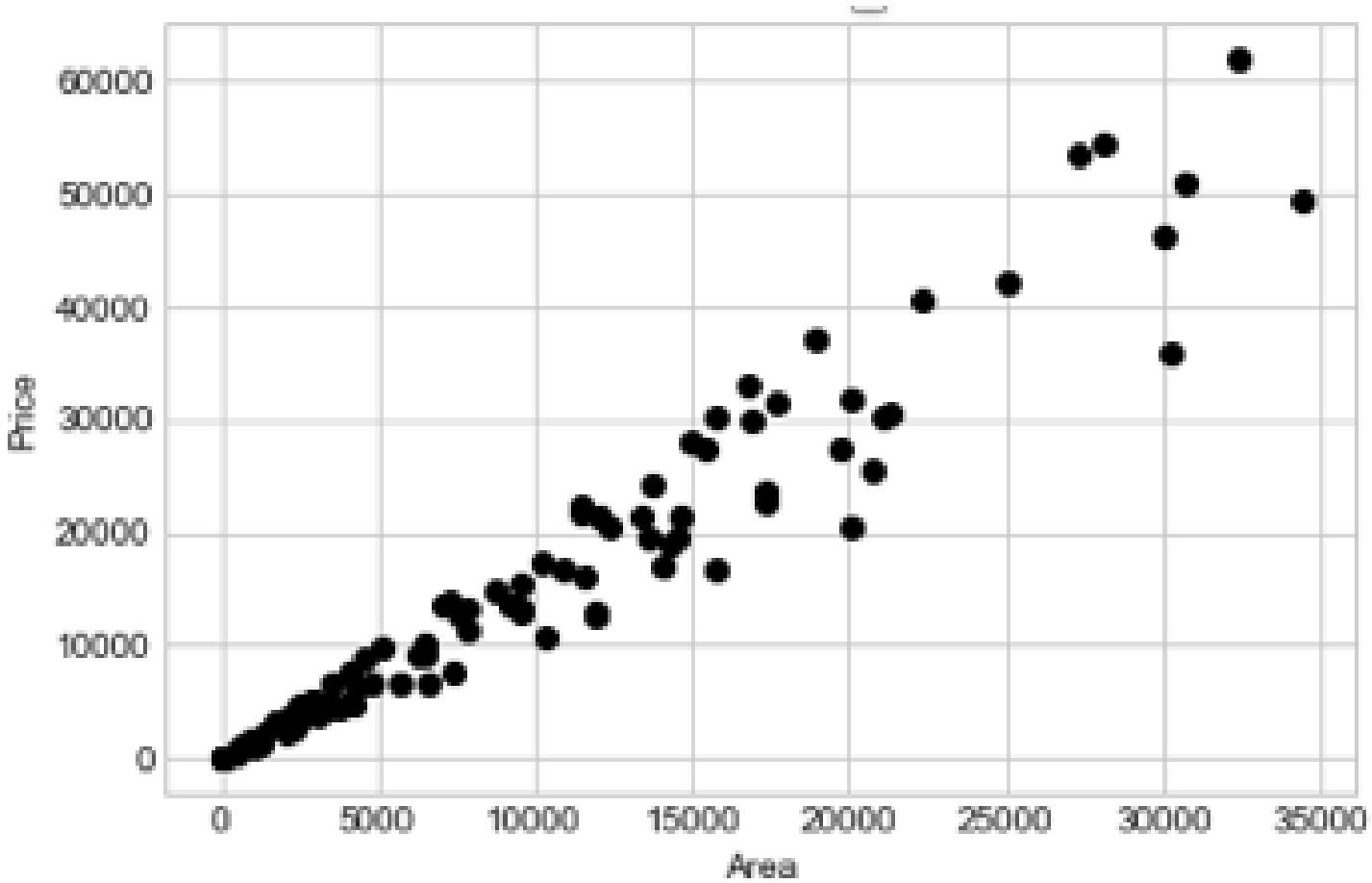
September, 2021

# Outline

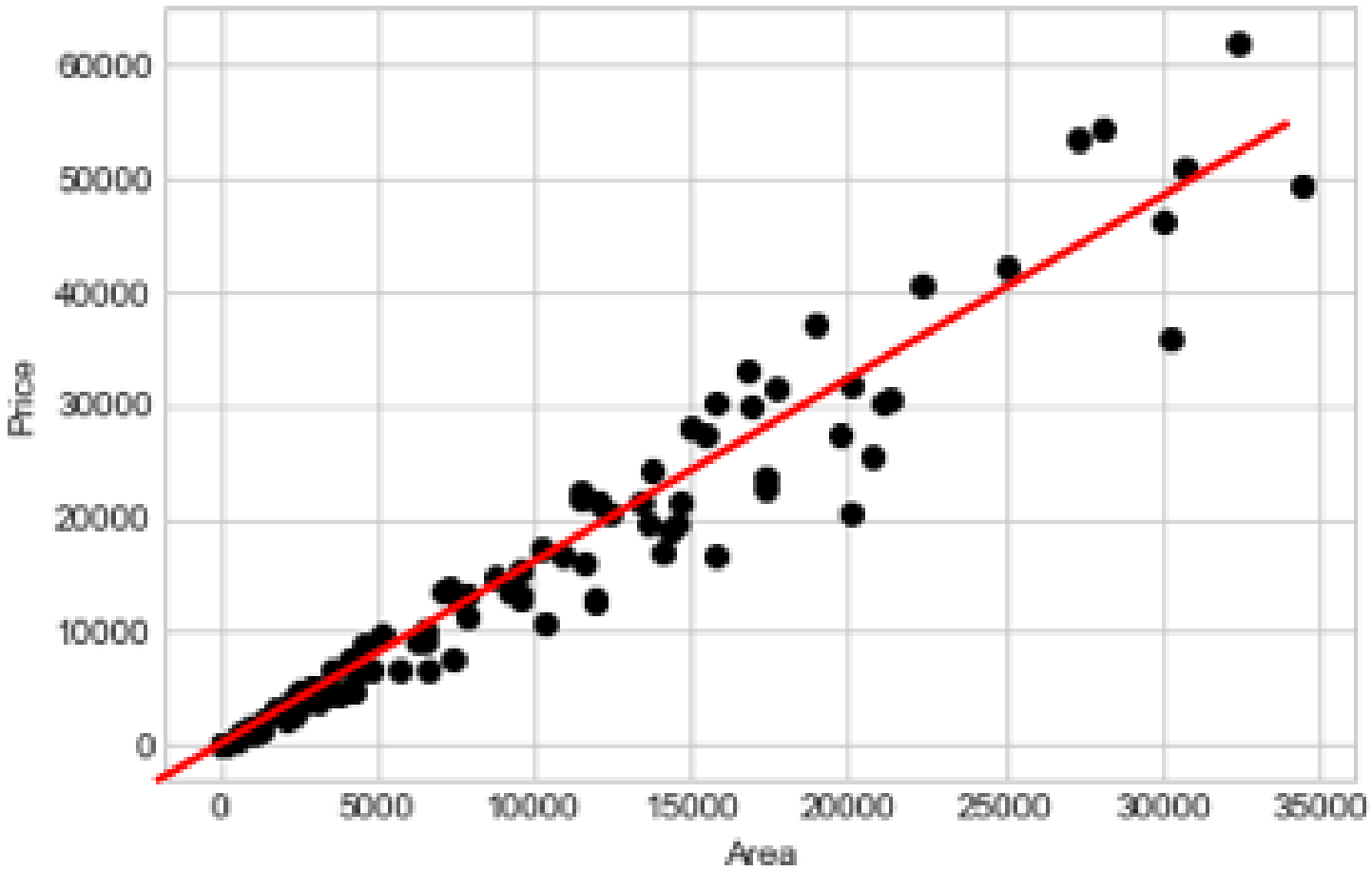
- Introduction to supervised learning
- K-nn
- Naïve Bayes
- Logistic Regression

# Supervised Learning




Can we predict the price of a parcel based on its size (surface in $m\hat{2}$) ?

# Supervised Learning




Can we predict the price of a parcel based on its size (surface in $m\hat{2}$) ?

# Supervised learning

- $X = X_1, X_2, ..., X_p$: input variables (features)
- $Y$: "output" or target variable that we try to predict
- A pair $(x_i, y_i)$ is called a training example, where:

$$x_i \in X = X_1 \times ... \times X_p \text{ and } y_i \in Y$$

- The training set is a list of training examples:

$$\{(x_i, y_i) \; ; \; i = 1...m\}$$

- The supervised learning problem is formulated as:
  - Given a training set,
  - Learn a function $h : X \to Y$ such that $h(x)$ is "good" predictor for the corresponding value of $y$.

For historical reasons, the function $h$ is called a *hypothesis*.

# Supervised Learning – Performance evaluation

Goal: find a hypothesis $h : X \to Y$ minimizing

$$Error(h) = E_{X,Y} L(Y, h(X))$$

Classification (Y label values, i.e. Y=yes,no ) - Error: 0-1 loss:

$$L(Y, h(X)) = 1(Y! = h(X))$$

Regression Y: number, i.e. Y = stock_price - Error: square loss:

$$L(Y, h(X)) = (Y - h(X))^2$$

# Generative vs. Discriminative classifiers

- Generative algorithm
  - Data generated by a distribution of feature
  - Assume $x$ features of an animal and $y$ the animal genre (i.e cat, dog).
  - For unknown classification data $x$ find the class maximizing the posterior $p(y|x)$ based on Bayes rules

$$p(y|x) = \frac{p(x|y)p(y)}{p(x)}$$

  - Therefore

$$p(y|x) = argmax_y(p(x|y)p(y))$$

# Generative vs. Discriminative classifiers

- Discriminative algorithm
  - Learn directly $p(y|x)$or learn mappings directly from the space of inputs $X$ to the labels $0, 1$
  - Do not care about how the data was generated - simply categorizes a given vector
  - Generally discriminative classifiers are more effective - better accuracy.

# Some Classes of classifiers

- Class-conditional probabilistic based on $p(x \mid c_k)$
  - Naïve Bayes: simple, often effective in high dimensions
  - Parametric generative models, e.g., Gaussian (can be effective in low-dimensional problems: leads to quadratic boundaries in general)
- Regression-based $p(c_k \mid x)$ directly
  - Logistic regression: simple
  - Neural networks: non-linear extension of logistic regression

# Some Classes of classifiers

- Discriminative models, focus on locating optimal decision boundaries
  - Linear discriminants: perceptron - simple, sometimes effective.
  - Support vector machines: Generalization of linear discriminants, can be quite effective, computational complexity is an issue
  - Nearest neighbor: Simple, can scale poorly in high dimensions
  - Decision trees: Often effective in high dimensions

# Classification: Results & Evaluation

- Confusion matrix

| Predicted class | Actual class | |
|---|---|---|
| | 1 | 0 |
| 1 | True Positive | False positive |
| 0 | False negative | True negative |

- Precision $\frac{\text{TP}}{\text{TP}+\text{FP}}$
- Recall $\frac{\text{TP}}{\text{TP}+\text{FN}}$
- Accuracy $\frac{\text{TP}+\text{TN}}{\text{TP}+\text{TN}+\text{FP}+\text{FN}}$
- $F1 = \frac{2*\text{precision}*\text{recall}}{\text{precision}+\text{recall}}$

# Classification: Results & Evaluation

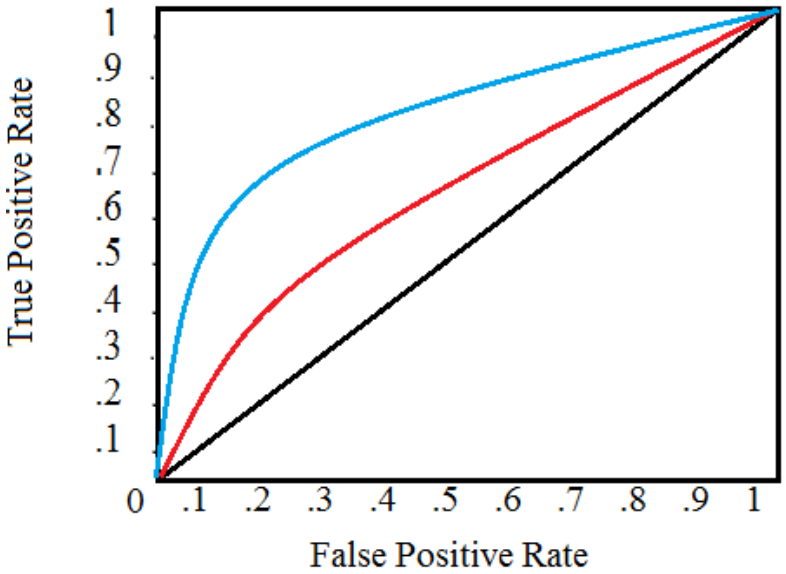
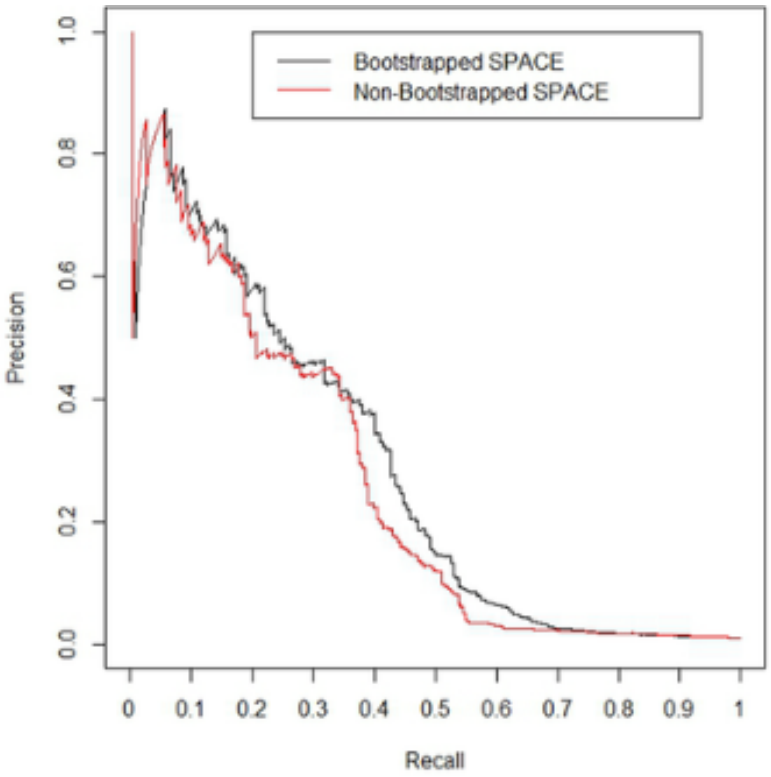



Figure: ROC curve




Precision recall curve

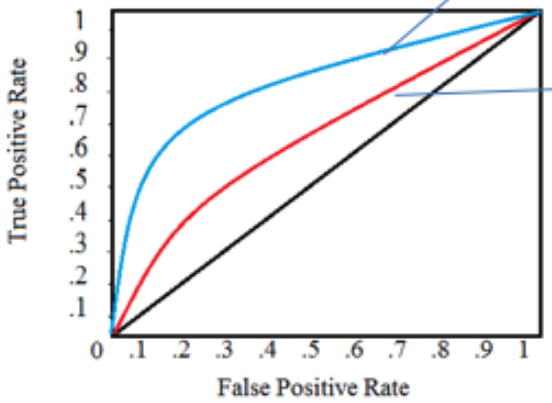
# ROC/AUC curve

- True positive rate:

$$TPR = \frac{TP}{TP + FN}$$

- False negative rate:

$$FPR = \frac{FP}{FP + TN}$$



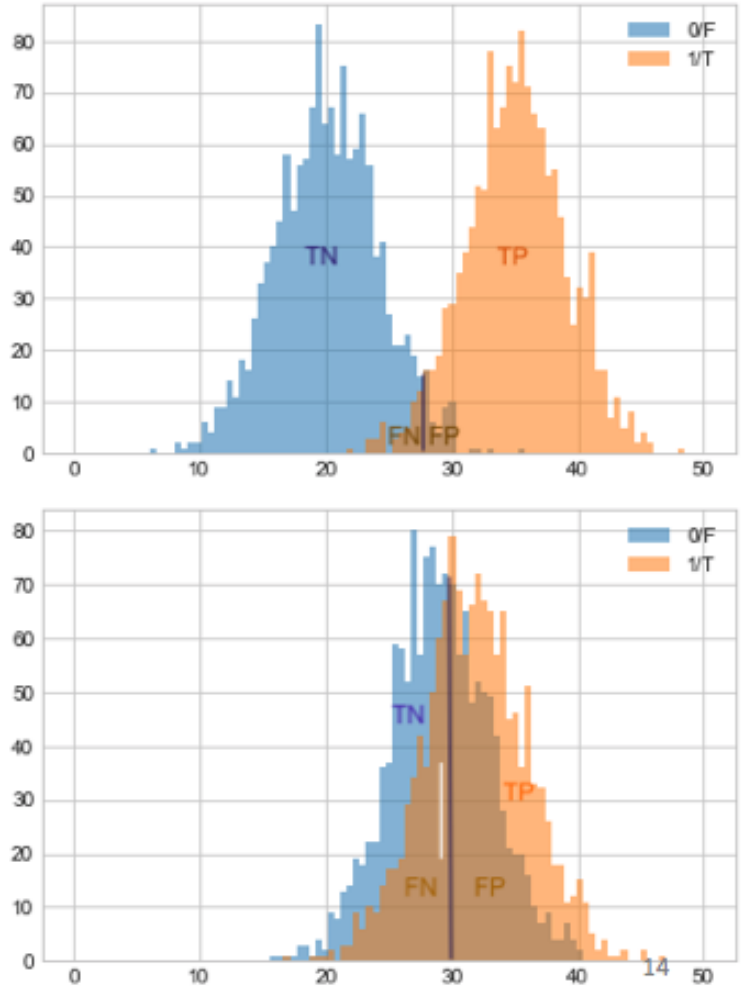




Figure:

# Classification: Results & Evaluation

- Log-loss: more refined evaluation of the classification
- Capitalizing on the classifier probability

$$\text{log -loss} = -\frac{1}{N}\sum_{i=1}^{N} y_i \log p_i + (1 - y_i) \log p_i(1 - p_i)$$

- Log loss  cross entropy $H(p, q) = -\sum_x p(x) \log q(x)$ between the distribution of true labels and predictions
- Closely related to Kullback-Leibler divergence

$$KL(p|q) = \sum_x p(x) \log \frac{p(x)}{q(x)}$$

- Minimizing cross entropy, maximize accuracy of the classifier.

# Outline

- Introduction to supervised learning
- **K-nn**
- Naïve Bayes
- Logistic Regression

# $k$-NN Algorithm

- $K$-NN is an non parametric lazy learning algorithm.
  - No assumptions for the data (i.e. distribution, linearly separable)
  - No training lack of generalization
- K-nn classification: by majority voting
- K-nn regression: average value of k nearest neighbors

# K-NN classification example

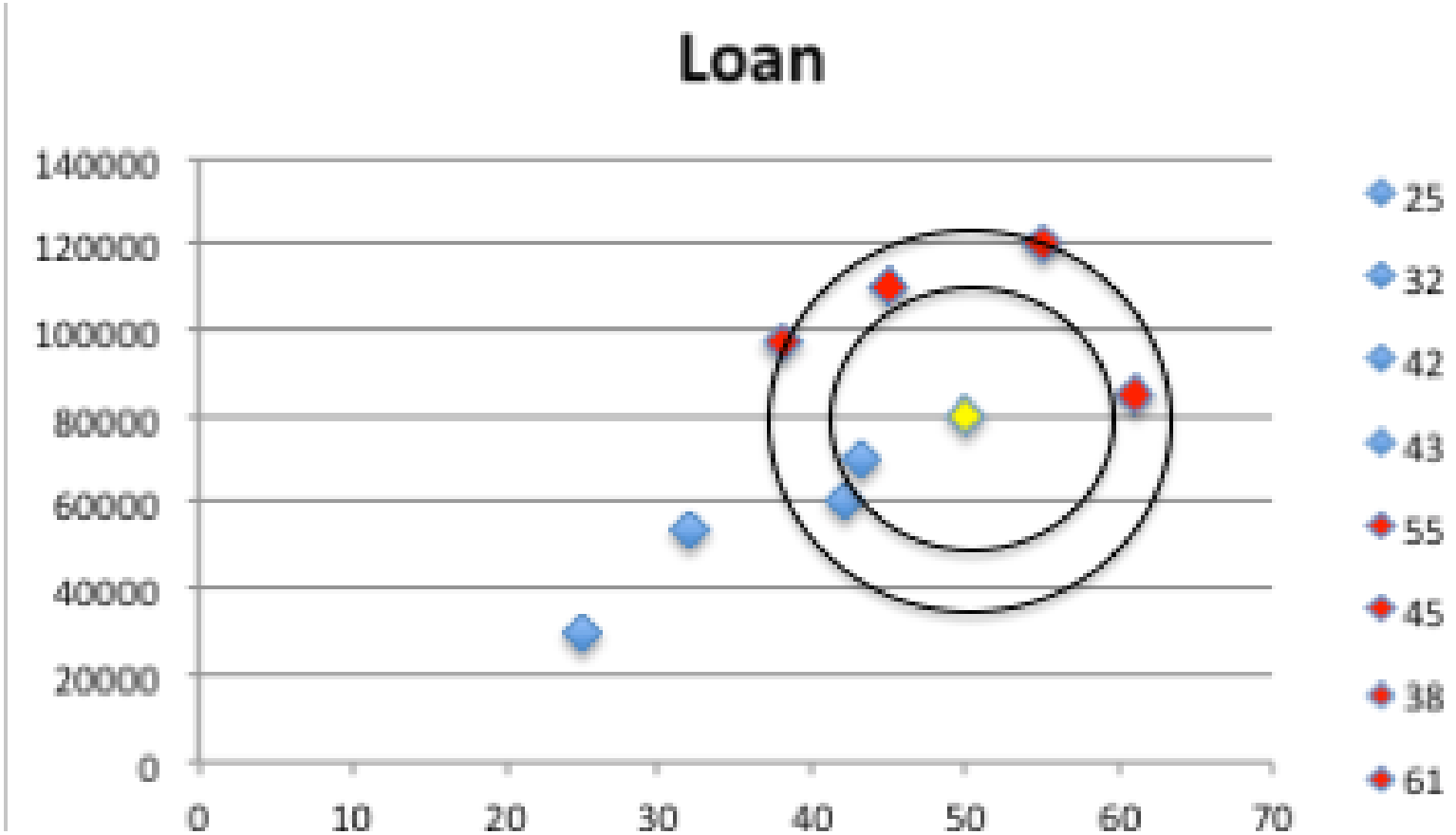



Figure: Loan amount vs. age: decide class by majority of nns

# K-NN classification example

| Age | Loan | Default | Distance |
|---|---|---|---|
| 25 | 30000 | N | 50000,0062 |
| 32 | 54000 | N | 26000,0062 |
| 42 | 60000 | N | 20000,0016 |
| 43 | 70000 | N | 10000,0024 |
| 55 | 120000 | Y | 40000,0003 |
| 45 | 110000 | Y | 30000,0004 |
| 38 | 97000 | Y | 17000,0042 |
| 61 | 85000 | Y | 5000,0121 |
| 50 | 80000 | ? | |

Figure: Loan amount vs. age: decide class by majority of nns

$$D(x, y) = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$$

# K-NN classification example

| Age | Loan | Default | Distance |
|---|---|---|---|
| 0 | 0 | N | 0,88932 |
| 0,1944 | 0,2667 | N | 0,57746 |
| 0,4722 | 0,3333 | N | 0,31427 |
| 0,5 | 0,4444 | N | 0,22395 |
| 0,8333 | 1 | Y | 0,46564 |
| 0,5556 | 0,8889 | Y | 0,36111 |
| 0,3611 | 0,7444 | Y | 0,38313 |
| 1 | 0,6111 | Y | 0,31056 |
| 0,6944 | 0,5556 | ? | |

Figure: Loan amount vs. age: decide class by majority of nns

$$\frac{X_i - min(X)}{max(X) - min(X)}$$

# K-NN regression

- k-NN algorithm to estimate continuous variables.
- weighted average of the k nearest neighbors, weighted by the inverse of their distance:
  - Compute distance of query example to the labeled examples.
  - Order labeled examples by increasing distance.
  - Find a heuristically optimal number k of nearest neighbors, based on RMSE – with cross validation.
  - Calculate inverse distance weighted average with k-nearest multivariate neighbors.

# K-NN issues

- K: larger values reduce noise effect but make classes boundaries blur
- Dimensionality affects the performance
- Feature selection/scaling (mutual information)
- Binary classification: k odd number
- popular way for empirically optimal k via bootstrap method
- Assume large number of points and c classes:

$$E_{k-nn} \leq E_{Bayes}(2 - \frac{c}{c-1} E_{Bayes})$$

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# Bayesian Classification: Why?

- Probabilistic learning
  - Calculate explicit probabilities for hypothesis,
  - practical approaches to certain types of learning problems
- Incremental
  - Each training example can incrementally increase/decrease the probability that a hypothesis is correct.
  - Prior knowledge combined with observed data.
- Probabilistic prediction
  - Predict multiple hypotheses, weighted by their probabilities

# Bayesian Classification

- Problem formalized using a-posteriori probabilities:
- $p(C|X)$ = prob. vector $X =< x_1, \ldots, x_k >$ is class $C$.
  - e.g. $p(class = N|outlook = sunny, windy = true, \ldots)$
- Assign to sample $X$ class label $C$: $p(C|X)$ is maximal
- Bayes theorem:

$$p(C|X) = \frac{p(X|C)p(C)}{p(X)}$$

- $p(X)$: prior probability of vector X
- $p(C)$ = prior probability of class C in training data
- $p(X|C)$ = probability of X given C
- $p(C|X)$ = probability of X given C

# Learn probabilistic models with dependence

- Problem: computing $P(X|C)$ not unfeasible! – Why?
- $p(C)$: assume p classes
- $p(X =< x_1, \ldots, x_k >)$: k binary features
- $p^{(2k-1)}$ parameters
- Likelihood: $p(X|C)$
  - Need a value for each possible $p(X =< x_1, \ldots, x_k > |C))$

# Naive Bayesian Classification

- Naïve assumption: attribute independence

$$p(X|C) = \prod_i p(x_i|C)$$

- $p(x_i|C)$: relative frequency of $x_i$ as i-th attribute in class $C$
- Computationally feasible
- Generative probabilistic model with conditional independence assumption
- Prediction:

$$p(C|X) = argmax_C(p(X|C)p(C)) = argmax_C(\prod_i^k p(x_i|C)p(C))$$

# Naive Bayesian Classification

- Simple to train
- estimate conditional probabilities for each feature-class pair
- Often very good baseline
- Feature selection can be helpful, e.g., information gain
- However.... on most problems can usually be outperformed by a more complex model

# Playtennis example: estimating $P(xi|C)$

| Outlook | Temperature | Humidity | Windy | Class |
|---|---|---|---|---|
| sunny | hot | high | false | N |
| sunny | hot | high | true | N |
| overcast | hot | high | false | P |
| rain | mild | high | false | P |
| rain | cool | normal | false | P |
| rain | cool | normal | true | N |
| overcast | cool | normal | true | P |
| sunny | mild | high | false | N |
| sunny | cool | normal | false | P |
| rain | mild | normal | false | P |
| sunny | mild | normal | true | P |
| overcast | mild | high | true | P |
| overcast | hot | normal | false | P |
| rain | mild | high | true | N |

| |
|---|
| **p(P) = 9/14** |
| **p(N) = 5/14** |

| **outlook** | |
|---|---|
| **p(sunny\|P) = 2/9** | **p(sunny\|N) = 3/5** |
| **p(overcast\|P) = 4/9** | **p(overcast\|N) = 0** |
| **p(rain\|P) = 3/9** | **p(rain\|N) = 2/5** |
| **temperature** | |
| **p(hot\|P) = 2/9** | **p(hot\|N) = 2/5** |
| **p(mild\|P) = 4/9** | **p(mild\|N) = 2/5** |
| **p(cool\|P) = 3/9** | **p(cool\|N) = 1/5** |
| **humidity** | |
| **p(high\|P) = 3/9** | **p(high\|N) = 4/5** |
| **p(normal\|P) = 6/9** | **p(normal\|N) = 2/5** |
| **windy** | |
| **p(true\|P) = 3/9** | **p(true\|N) = 3/5** |
| **p(false\|P) = 6/9** | **p(false\|N) = 2/5** |

# Naive Bayesian Classification

- unseen sample $X =< rain, hot, high, false >$
- $p(X|P)p(P) = p(rain|P)p(hot|P)p(high|P)p(false|P)p(P) = 3/9 * 2/9 * 3/9 * 6/9 * 9/14 = 0.010582$
- $p(X|N)p(N) = P(rain|N)P(hot|N)P(high|N)P(false|N)P(N) = 2/5 * 2/5 * 4/5 * 2/5 * 5/14 = \mathbf{0.018286}$
- Sample X is classified in class N (don't play)

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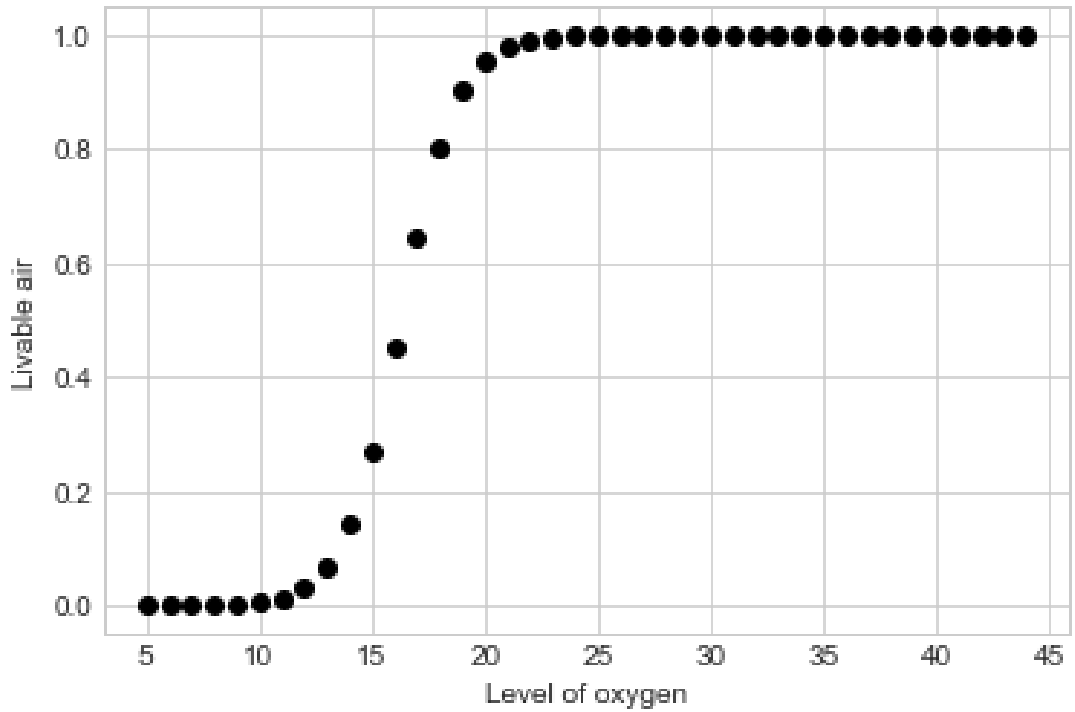
# Solving a supervised learning problem

Given data, a real-world classification problem, and constraints, you need to determine:

- classifier to use
- optimization method to employ
- loss function to minimize
- features to consider from the data
- evaluation metric to use

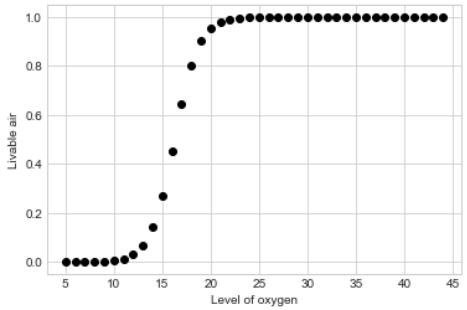
# Logistic Regression

- Fits binary classification problems
- Output in [0,1]
- Need a function that takes data vector $x$ and produces as output p(x) in [0,1]



# Why linear regression does not do..

- Linear regression: output y is continuous – need binary classification
- Need a $p(X)$ in [0,1] – linear regression does not guarantee it.
- homoscedasticity assumption: variance of Y constant across values of X.
- significance testing assumes prediction errors (y-f(x)) are normally distributed.
- But y takes values 0 and 1,



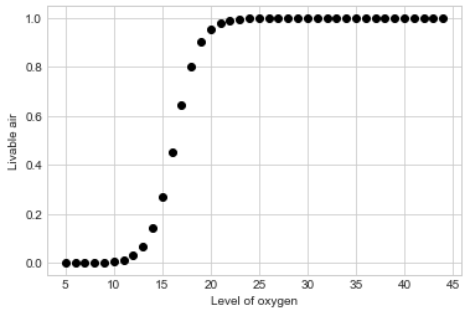
# Logistic function – design

- Classification: $\mathbf{x} \in R^p, y \in \{0, 1\}$
- Assumption (odds p(y=1)):

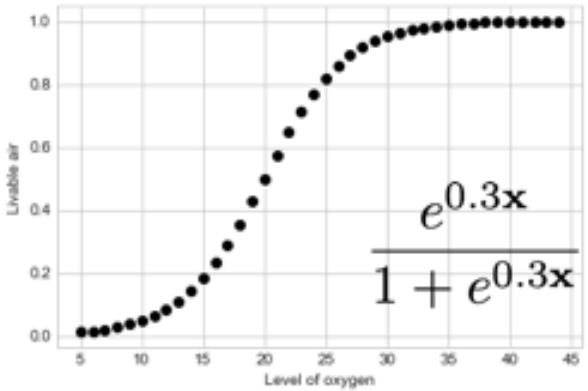
$$log(\frac{p(y=1|\mathbf{x})}{1-p(y=1|\mathbf{x})}) = \alpha\mathbf{x} + \beta$$

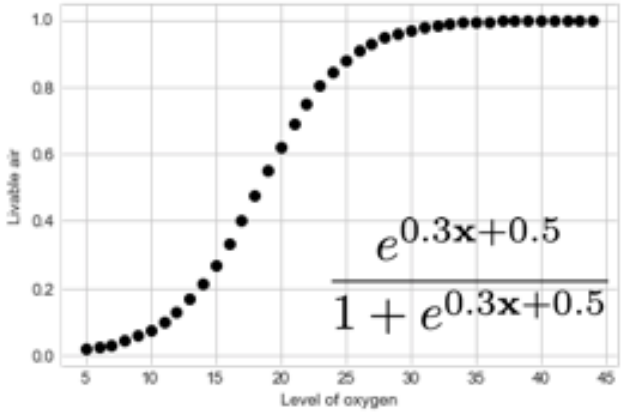
- therefore

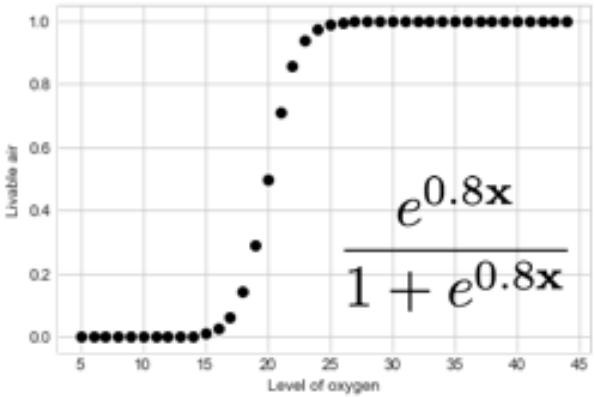
$$p(y=1|\mathbf{x}) = \frac{e^{\alpha\mathbf{x}+\beta}}{1+e^{\alpha\mathbf{x}+\beta}} = \frac{1}{1+e^{-(\alpha\mathbf{x}+\beta)}}$$

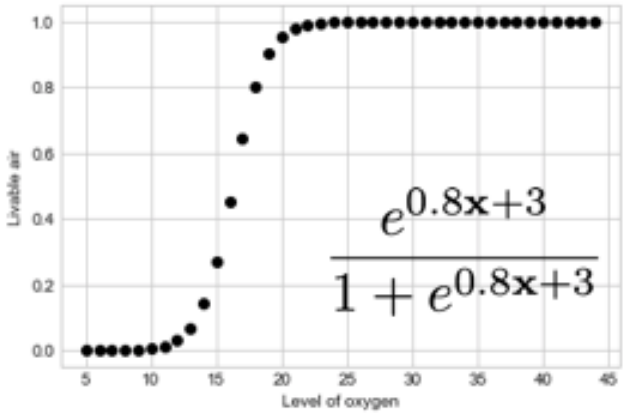


# Examples of logistic function - parameters



# Click prediction example

- Web site publishing ads
- Predict user $i$ click an ad.
- Assume class $c_i$ (1: clicked, 0: otherwise)
- $x_i$ data for user $i$ (history of URLs visited)
- logit( P(¡user i clicks on the ad¿) = linear function of the features $x_i$

# Click Prediction: Logistic regression model

- linear model for $c_i$,
- take the log of the odds ratio:

$$log(p(c_i = 1|x_i)/(1 - p(c_i = 1|x_i)) = \alpha + \beta^T x_i$$

- Or

$$p(c_i = 1|x_i) = \frac{e^{\alpha+\beta^T x_i}}{1 + e^{\alpha+\beta^T x_i}}$$

- $\alpha$: base rate, unconditional probability of $c_i = 1$ (click)
- $\beta$: dependence on the user data
  - slope of the logit function
  - Determines the relevance of features (i.e. pages visited) to the likelihood of the ad being clicked

# Click Prediction: $\alpha$,$\beta$ parameter estimation

- Parameters: $\theta = \{\alpha, \beta\}$,
- Likelihood: $L(\theta|X_1, ..., X_n) = p(X|\theta) = p(X_1|\theta)...p(X_n|\theta)$,
- $X_i$ users are independent:

$$\theta_{MLE} = argmax_\theta \prod_{k=1}^{N} p(X_i|\theta)$$

- Setting:

$$p_i = \frac{1}{1 + e^{-(\alpha+\beta^T x_i)}}$$

- Then:

$$\theta_{MLE} = argmax_\theta \prod_{k=1}^{N} p_i^c (1 - p_i)^c$$

  $c$: number of clicks

- MLE with either i. Newton-Raphson method or ii. Stochastic gradient descent