Lecture 6: Supervised Learning

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WESTLAKE UNIVERSITY | SCHOOL OF ENGINEERING

This lecture:

- Basic concept of regression and classification
- Linear Regression
  - Definition
  - Gradient Descent (GD) optimization
  - Least Square
  - The probabilistic interpretation of Linear Regression
- Logistic Regression

Next lecture:

- Over-fitting and under-fitting
- Polynomial Regression and Ridge Regression
- Model selection
- Bias-Variance Decomposition

Reading materials

- Chapter 1, Stanford CS 229 Lecture Notes,
  `https://cs229.stanford.edu/notes2022fall/main_notes.pdf`
- Chapter 3.1, Bishop, Pattern Recognition and Machine Learning

Reference

- EPFL, CS-433 Machine Learning, `https://github.com/epfml/ML_course`

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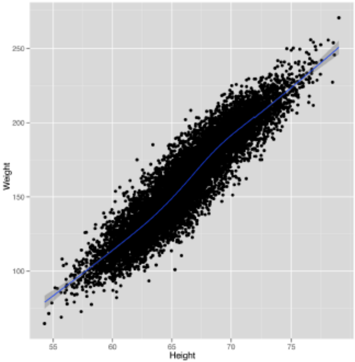
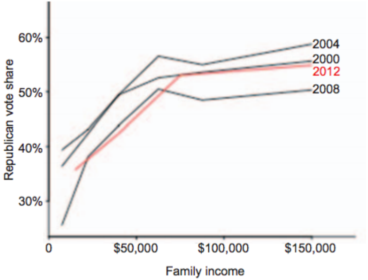
What is regression?



(a) Height is correlated with weight. Taken from “Machine Learning for Hackers"



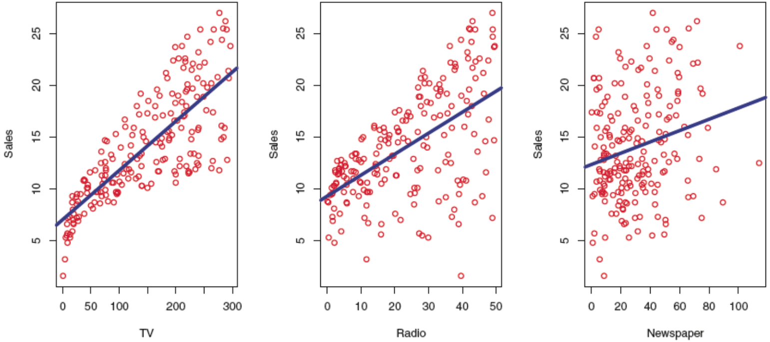
(b) Do rich people vote for republicans? Taken from Avi Feller et. al. 2013, Red state/blue state in 2012 elections.

Regression is to relate input variables to the output variable.

Dataset for regression

$$\mathcal{D} = \{\mathbf{x}_n, y_n\}_{n=1}^{N} \in \mathcal{X} \times \mathcal{Y} \quad (1)$$

- data consists of pairs $(\mathbf{x}_n, y_n)$, where y_n is the n'th output and $\mathbf{x}_n$ is a vector of D inputs.



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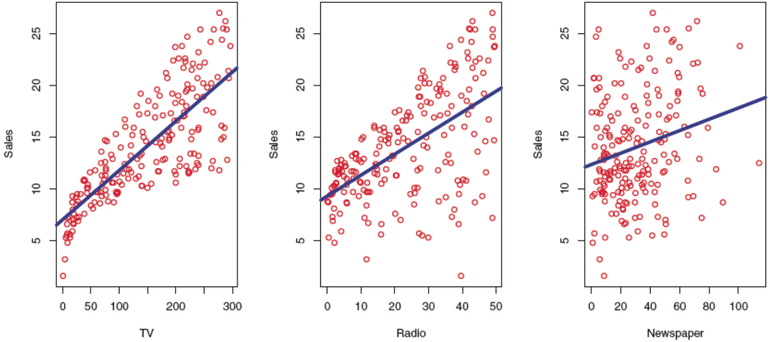
- The number of pairs N is the data-size and D is the dimensionality.



Two goals of regression

The regression function approximates the output y_n "well enough" given inputs $\mathbf{x}_n$.

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Regression finds a correlation not a causal relationship, so interpret your results with caution.

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Remark 2 (Shortcut learning in Deep Learning)

Models may only learn spurious correlation (and thus sensitive to distribution shifts).

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We observe some data

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Remark 3

no ordering between classes.

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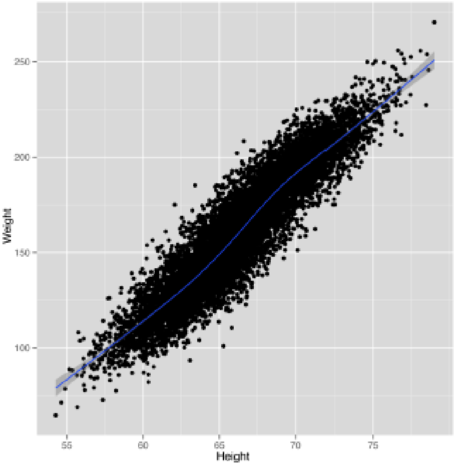

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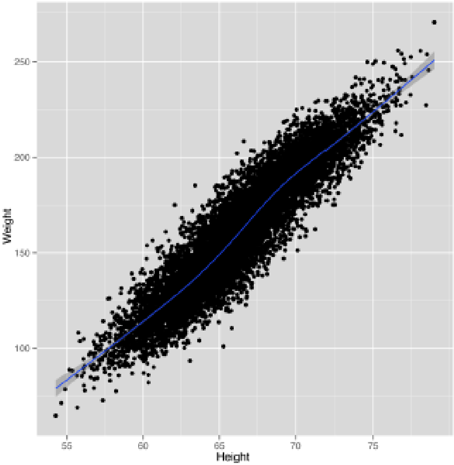

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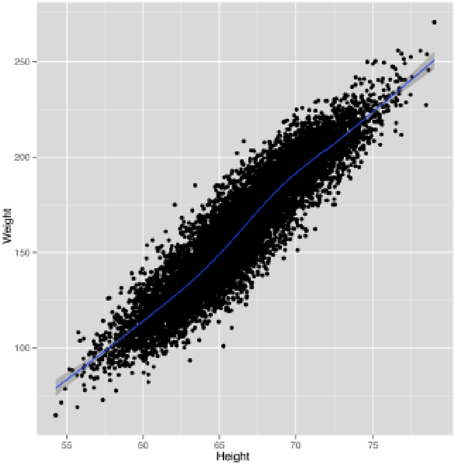
- $y_n \approx f(\mathbf{x}_n)$ for all n and $\mathcal{D} = \{\mathbf{x}_n, y_n\}_{n=1}^N \in \mathcal{X} \times \mathcal{Y}$
- a linear relationship is assumed for f



Detailed definition

Simple linear regression (w/ only one input dimension):

$$y_n \approx f(\mathbf{x}_n) := w_0 + w_1 x_{n1}$$

Here, $\mathbf{w} = (w_0, w_1)$ are the two parameters of the model. They describe f.

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We need an optimization algorithm!

Why learn about *linear* regression?

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- easily generalized to non-linear models
- we can learn almost all fundamental concepts of ML with regression alone

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Motivation

Consider the following models.

$$\text{1-parameter model: } y_n \approx w_0$$
$$\text{2-parameter model: } y_n \approx w_0 + w_1 x_{n1}$$

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- the cost penalizes "large" mistakes and "very-large" mistakes similarly

Mean Squared Error (MSE) and Outliers

$$\text{MSE}(\mathbf{w}) := \frac{1}{N} \sum_{n=1}^{N} \left[y_n - f_{\mathbf{w}}(\mathbf{x}_n) \right]^2 \tag{7}$$

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+ MAE is more robust to outliers.
– MAE is not differentiable at zero.

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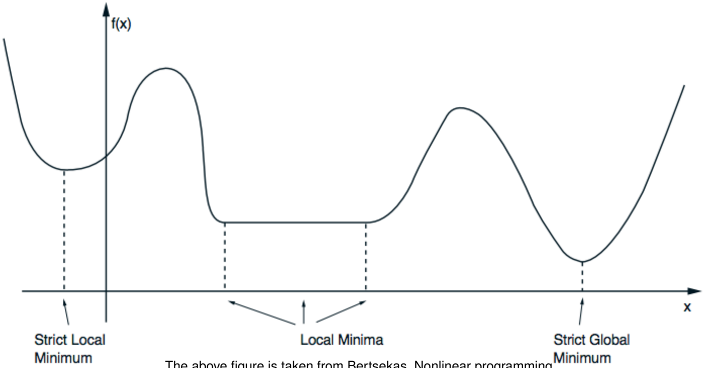
We will use an optimization algorithm to solve the problem (to find a good $\mathbf{w}$).

Optimization Landscapes



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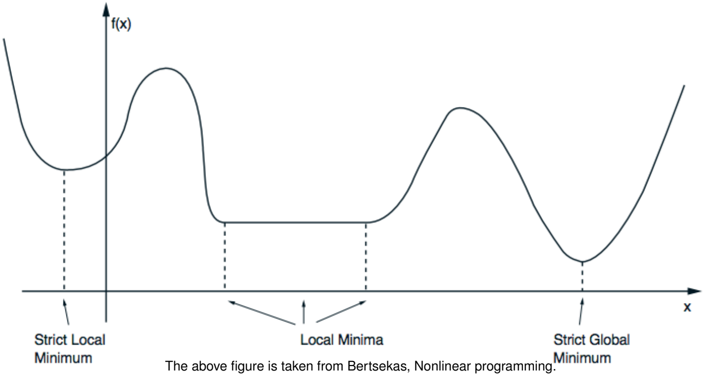

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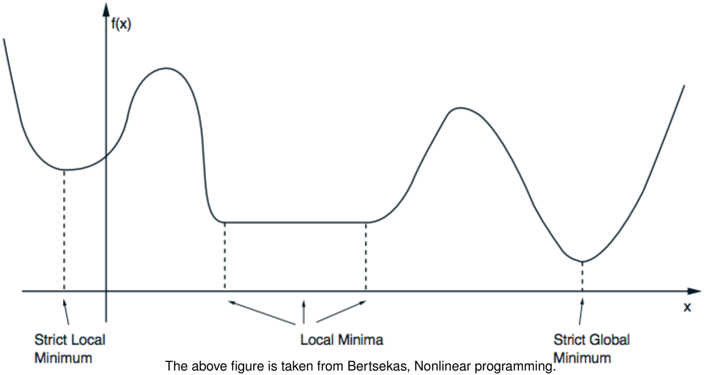

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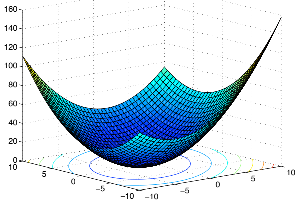
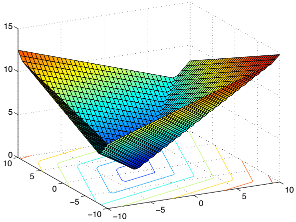
For a 2-parameter model, MSE$(\mathbf{w})$ and MAE$(\mathbf{w})$ are shown below.

(We used $\mathbf{y}_n \approx w_0 + w_1 x_{n1}$ with $\mathbf{y}^\top = [2, -1, 1.5]$ and $\mathbf{x}^\top = [-1, 1, -1]$).





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where $\gamma > 0$ is the step-size (or learning rate). Then repeat with the next t.

Gradient Descent for Linear Regression with MSE

Considering a dataset $\mathcal{D} = \{\mathbf{X}, \mathbf{y}\}$ and learnable weights $\mathbf{w} \in \mathbb{R}^D$ for $f_{\mathbf{w}}(\mathbf{X}) = \mathbf{X}\mathbf{w}$.

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \in \mathbb{R}^N, \qquad \mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1D} \\ x_{21} & x_{22} & \dots & x_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \dots & x_{ND} \end{bmatrix} \in \mathbb{R}^{N \times D} \tag{12}$$

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We define the error vector $\mathbf{e}$:

$$\mathbf{e} = \mathbf{y} - \mathbf{X}\mathbf{w} = \begin{pmatrix} e_1 \\ \vdots \\ e_N \end{pmatrix} \in \mathbb{R}^N, \tag{13}$$

where $e_i := y_n - \mathbf{x}_n^\top \mathbf{w}$.

Gradient Descent for Linear Regression with MSE

Considering a dataset $\mathcal{D} = \{\mathbf{X}, \mathbf{y}\}$ and learnable weights $\mathbf{w} \in \mathbb{R}^D$ for $f_{\mathbf{w}}(\mathbf{X}) = \mathbf{X}\mathbf{w}$.

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \in \mathbb{R}^N, \qquad \mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1D} \\ x_{21} & x_{22} & \dots & x_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \dots & x_{ND} \end{bmatrix} \in \mathbb{R}^{N \times D} \tag{12}$$

We define the error vector $\mathbf{e}$:

$$\mathbf{e} = \mathbf{y} - \mathbf{X}\mathbf{w} = \begin{pmatrix} e_1 \\ \vdots \\ e_N \end{pmatrix} \in \mathbb{R}^N, \tag{13}$$

where $e_i := y_n - \mathbf{x}_n^\top \mathbf{w}$. The MSE is defined as:

$$\mathcal{L}(\mathbf{w}) := \frac{1}{2N} \sum_{n=1}^{N} \left(y_n - \mathbf{x}_n^\top \mathbf{w}\right)^2 = \tfrac{1}{2N} \mathbf{e}^\top \mathbf{e}, \tag{14}$$

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and then the gradient is given by

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- Here its solution can be obtained explicitly, by solving a linear system of equations.

$\Rightarrow$ These equations are sometimes called the normal equations.

$\Rightarrow$ Solving the normal equations is called the least squares.

Recall that the cost function for linear regression with MSE is given by

$$\mathcal{L}(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N}\left(y_n - \mathbf{x}_n^\top \mathbf{w}\right)^2 = \frac{1}{2N}(\mathbf{y} - \mathbf{X}\mathbf{w})^\top(\mathbf{y} - \mathbf{X}\mathbf{w}), \tag{16}$$

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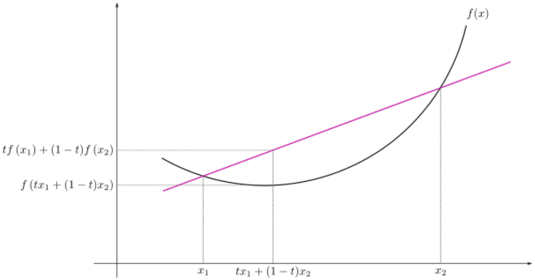
A function $h(\mathbf{u})$ with $\mathbf{u} \in \mathbb{R}^D$ is convex, if for any $\mathbf{u}, \mathbf{v} \in \mathbb{R}^D$ and for any $0 \leq \lambda \leq 1$, we have:

$$h(\lambda\mathbf{u} + (1-\lambda)\mathbf{v}) \leq \lambda h(\mathbf{u}) + (1-\lambda)h(\mathbf{v}) \quad (18)$$



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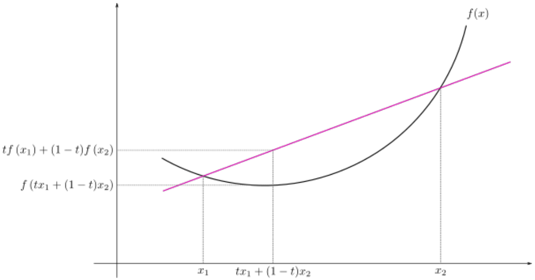

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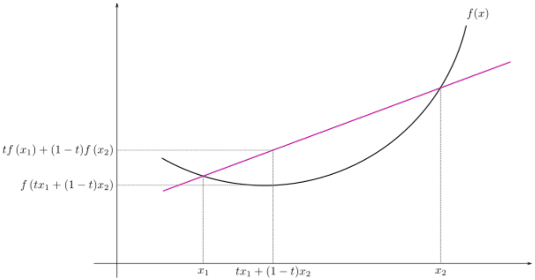

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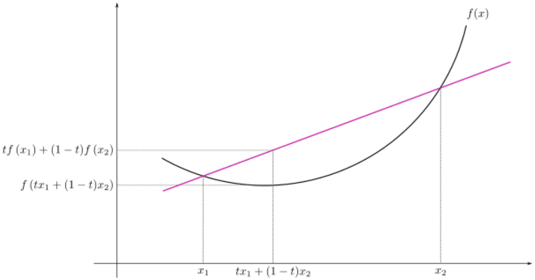

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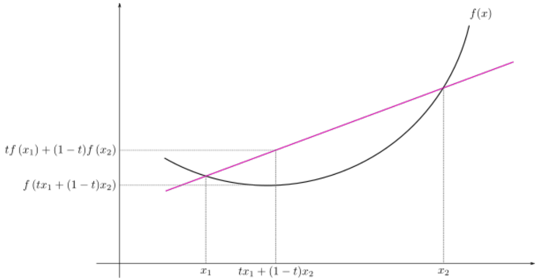

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$$\nabla \mathcal{L}(\mathbf{w}^\star) = \mathbf{0}\,, \tag{19}$$

where $\mathbf{w}^\star$ corresponds to the parameter at the optimum point.

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By taking the gradient of $\mathcal{L}(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N}\left(y_n - \mathbf{x}_n^\top \mathbf{w}\right)^2 = \frac{1}{2N}(\mathbf{y} - \mathbf{X}\mathbf{w})^\top(\mathbf{y} - \mathbf{X}\mathbf{w})$, we have

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Given the property of convexity $\nabla\mathcal{L}(\mathbf{w}^\star) = \mathbf{0}$, we can get the normal equations for linear regression:

$$\mathbf{X}^\top \underbrace{(\mathbf{y} - \mathbf{X}\mathbf{w})}_{\text{error}} = \mathbf{0}\,, \tag{23}$$

where the error $\mathbf{e} := \mathbf{y} - \mathbf{X}\mathbf{w}$ is orthogonal to all columns of $\mathbf{X}$.

Geometric Interpretation

Definition 9 (Span of a set of vectors)

The **span** of a set of vectors, $\{\mathbf{x}_1, \ldots, \mathbf{x}_k\}$, is the set of all possible linear combinations of these vectors; i.e. $\text{span}\{\mathbf{x}_1, \ldots, \mathbf{x}_k\} = \{\alpha_1 \mathbf{x}_1 + \ldots + \alpha_k \mathbf{x}_k \,|\, \alpha_1, \ldots, \alpha_k \in \mathbb{R}\}$.

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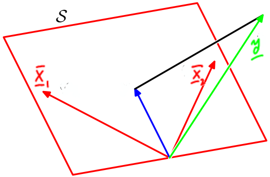

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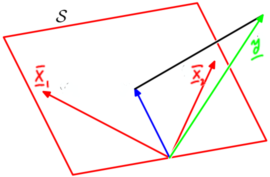

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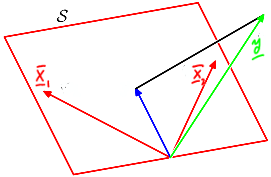

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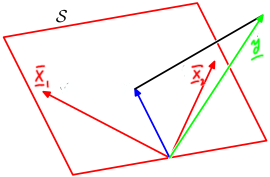

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- the optimum choice for $\mathbf{u}$, i.e. $\mathbf{u}^\star$, requires $\mathbf{y} - \mathbf{u}^\star$ to be orthogonal to $span(\mathbf{X})$.
- $\mathbf{u}^\star$ should be equal to *the projection of* $\mathbf{y}$ *onto* $span(\mathbf{X})$.

Least Squares

We need to solve the linear system of the normal equation $\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) = \mathbf{0}$, where

$$\mathbf{X}^\top y = \underbrace{\mathbf{X}^\top\mathbf{X}}_{\text{Gram matrix}} \mathbf{w} \tag{24}$$

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Remark 10

The Gram matrix $\mathbf{X}^\top\mathbf{X} \in \mathbb{R}^{D\times D}$ is invertible if and only if $\mathbf{X}$ has full column rank, or in other words $rank(\mathbf{X}) = D$.

Rank Deficiency and Ill-Conditioning

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Can we solve least squares if $\mathbf{X}$ is rank deficient?
Yes, using a linear system solver, e.g., $\text{np.linalg.solve}(\mathbf{X}, \mathbf{y})$.

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Recall: Gaussian distribution and independence

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Two random variables X and Y are called *independent* when $p(x,y) = p(x)p(y)$.

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The probabilistic view point: maximize this likelihood over the choice of model $\mathbf{w}$.

Maximum-likelihood estimator (MLE)

Instead of maximizing the likelihood, we can maximize the logarithm of the likelihood, i.e., log-likelihood (LL):

$$\mathcal{L}_{\mathsf{LL}}(\mathbf{w}) := \log p(\mathbf{y} \mid \mathbf{X}, \mathbf{w}) = -\frac{1}{2\sigma^2} \sum_{n=1}^{N} (y_n - \mathbf{x}_n^\top \mathbf{w})^2 + \text{cnst.} \tag{31}$$

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Maximizing the LL is equivalent to minimizing the MSE:

$$\arg\min_{\mathbf{w}} \mathcal{L}_{\mathsf{MSE}}(\mathbf{w}) = \arg\max_{\mathbf{w}} \mathcal{L}_{\mathsf{LL}}(\mathbf{w}). \tag{34}$$

Properties of MLE

MLE is a *sample* approximation to the *expected log-likelihood*:

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4. MLE is efficient, i.e. it achieves the Cramer-Rao lower bound.

$$\text{Covariance}(\mathbf{w}_{\mathsf{MLE}}) = \mathbf{F}^{-1}(\mathbf{w}_{\mathsf{true}}) \tag{38}$$

Another example

What if we replace the Gaussian distribution with a Laplace distribution?

$$p(y_n \mid \mathbf{x}_n, \mathbf{w}) = \frac{1}{2b} e^{-\frac{1}{b}\left|y_n - \mathbf{x}_n^\top \mathbf{w}\right|} \tag{39}$$

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we can recover the MAE cost function!

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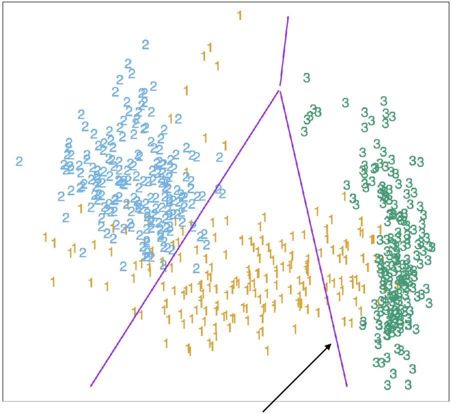

Linear Decision boundary

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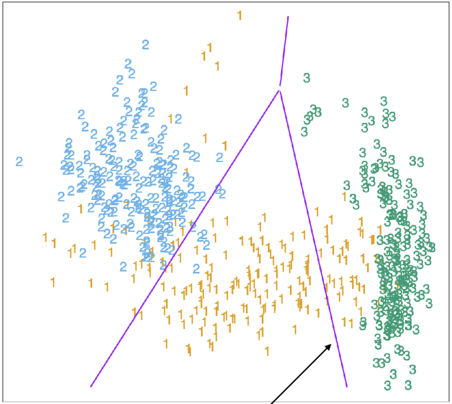

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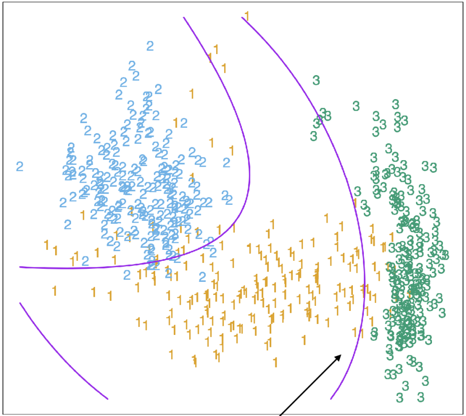

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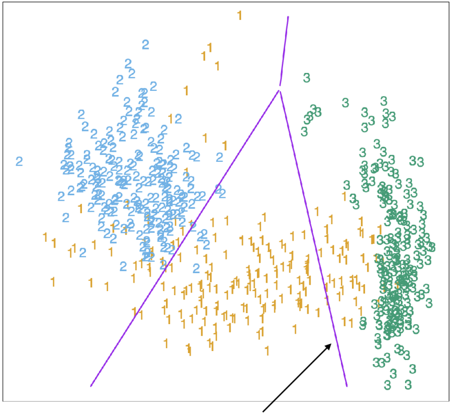

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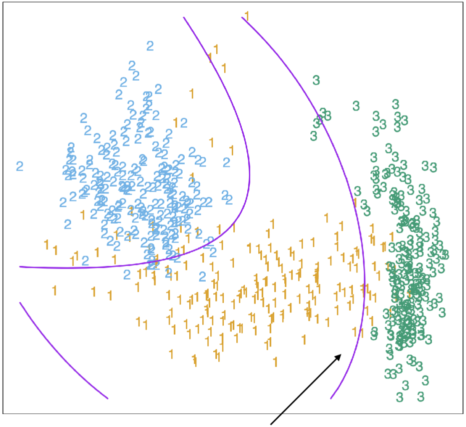

Nonlinear Decision boundary

The boundaries of these regions are called decision boundaries.

Classification: a special case of regression?

Classification is a **regression problem** with discrete labels:

$$(\mathbf{x}, y) \in \mathcal{X} \times \{0, 1\} \subset \mathcal{X} \times \mathbb{R} \tag{40}$$

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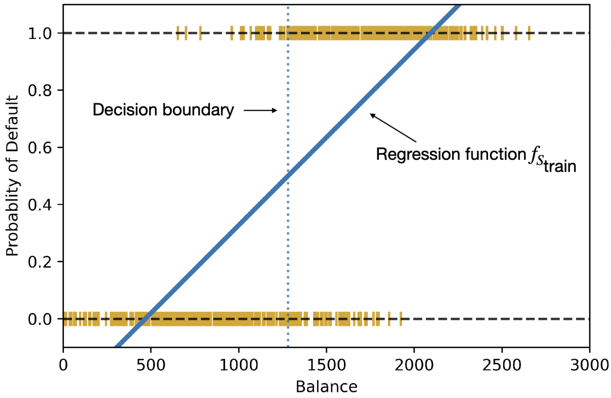
Could we use previously seen regression methods to solve it?

Is it a good idea to use some regression methods?



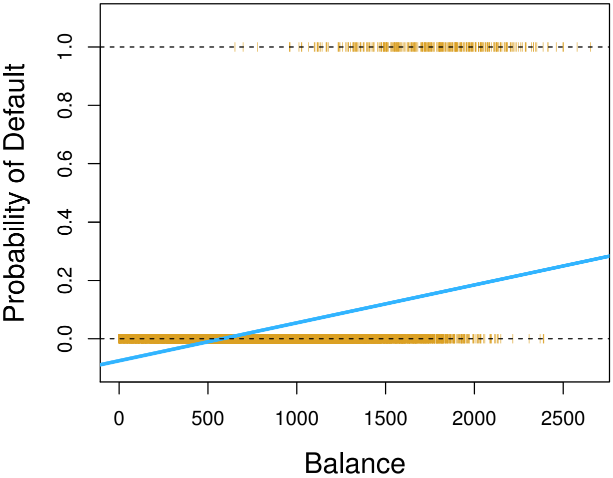
$y = 1$ **if "default"**

$y = 0$ **if "no default"**

We label the output as probability for sake of interpretation

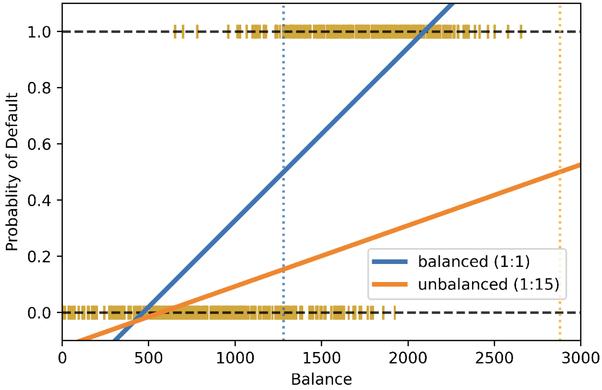
Classification is not just a special form of regression

- The predicted values are not probabilities (not in $[0, 1]$)



Classification is not just a special form of regression

- Sensitivity to unbalanced data



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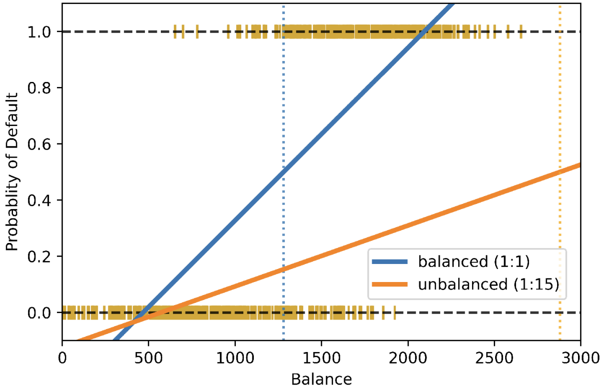

The position of the line depends crucially on how many points are in each class.

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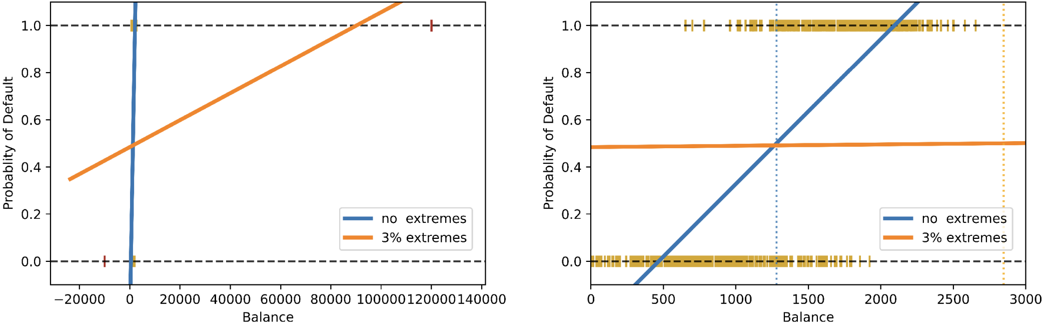

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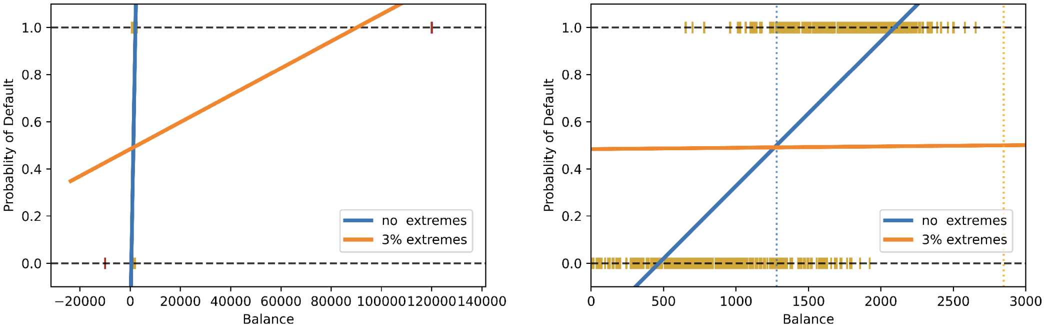

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- Maximum A-Posteriori (MAP): If we want to maximize the probability of guessing the correct label, then we should choose the decision rule

$$\hat{y}(\mathbf{x}) = \arg\max_{y \in \mathcal{Y}} p(y|\mathbf{x}) \tag{41}$$

  This classifier is also called the *Bayes classifier*.

- In practice, we do not know the joint distribution $p(\mathbf{x}, y)$, but we can use the data to learn the distribution (by assuming the data distribution).

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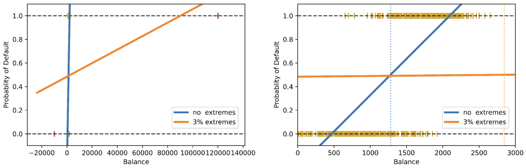

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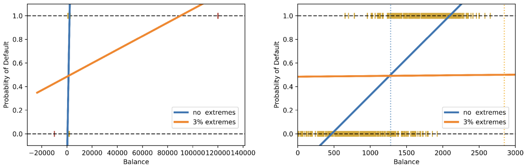

Solution: Transforming the predictions that take values in $(-\infty, \infty)$ into $[0, 1]$.

The logistic function

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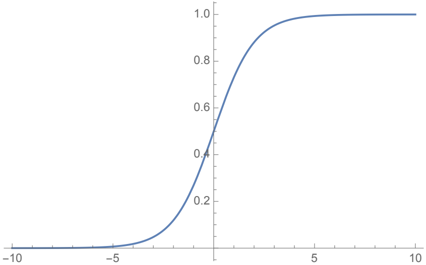

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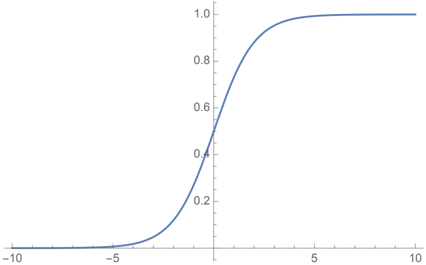

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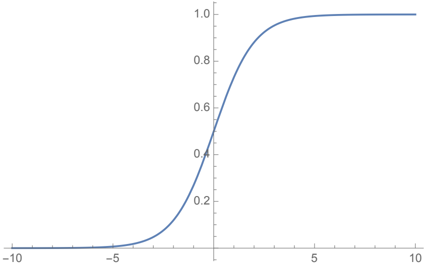

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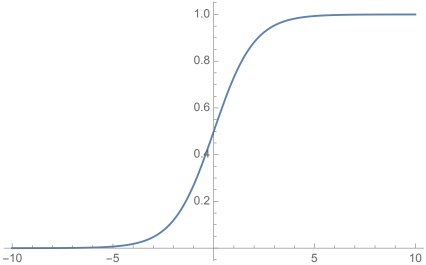

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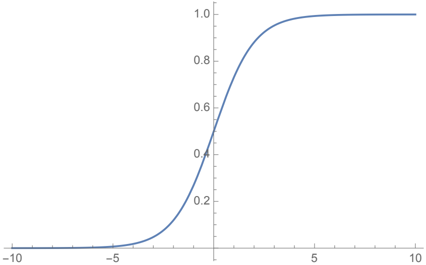

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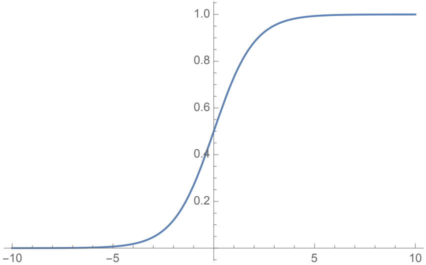

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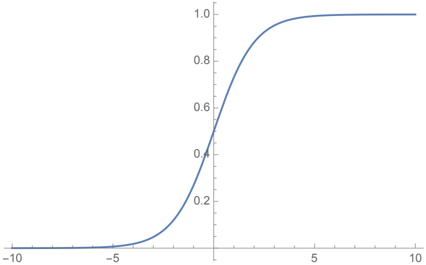

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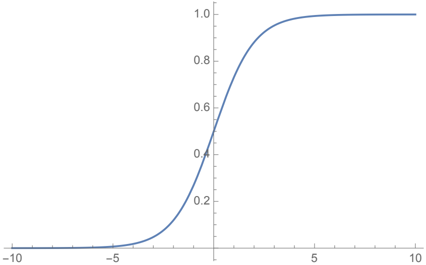

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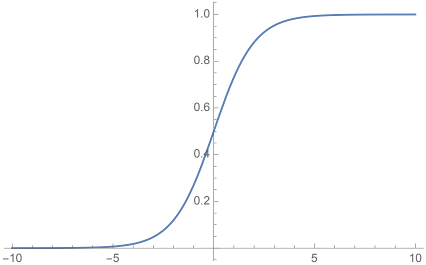

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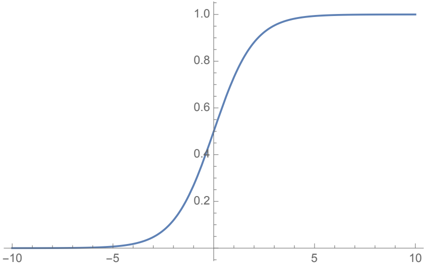

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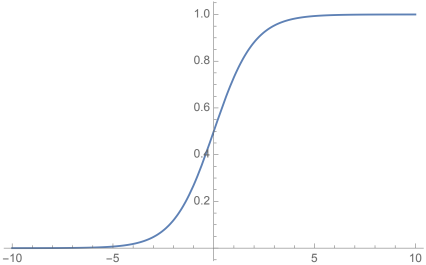

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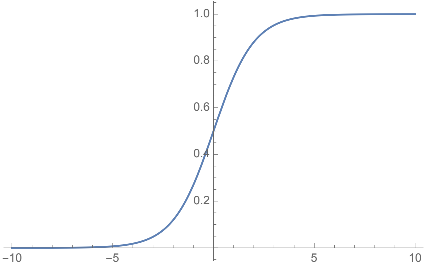

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Assume a training set S_{train}, consisting of i.i.d. samples $\{\mathbf{x}_n, y_n\}_{n=1}^{N}$ (fixed but unknown $\mathcal{D}$).

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$$p(\mathbf{y}|\mathbf{X}, \mathbf{w}) = \prod_{n=1}^{N} p(y_n|\mathbf{x}_n)$$

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As a result,

$$\mathbf{w}^\star = \arg\min_{\mathbf{w}} \mathcal{L}(\mathbf{w}) = \arg\min_{\mathbf{w}} \left(-\log p(\mathbf{y}|\mathbf{X}, \mathbf{w}) := \frac{1}{N} \sum_{n=1}^{N} -y_n \mathbf{x}_n^\top \mathbf{w} + \log(1 + e^{\mathbf{x}_n^\top \mathbf{w}}) \right) \tag{55}$$

Gradient of the negative log likelihood

Recall that

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Let's minimize $\mathcal{L}(\mathbf{w})$ through the property of stationary points.

$$\nabla \mathcal{L}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_n \left(\sigma(\mathbf{x}_n^\top \mathbf{w}) - y_n \right) \tag{57}$$

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where $\mathbf{X} \in \mathbb{R}^{N \times d}$.

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$\Rightarrow$ It has no closed-form solution to $\nabla \mathcal{L}(\mathbf{w}) = 0$.

This lecture:

- Basic concept of regression and classification
- Linear Regression
  - Definition
  - Gradient Descent (GD) optimization
  - Least Square
  - The probabilistic interpretation of Linear Regression
- Logistic Regression

Next lecture:

- Over-fitting and under-fitting
- Polynomial Regression and Ridge Regression
- Model selection
- Bias-Variance Decomposition