Lecture 2: Linear Models for Regression

Tao LIN

SoE, Westlake University

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WESTLAKE UNIVERSITY | SCHOOL OF ENGINEERING

This lecture:

- Basic concept of regression and classification
- Linear regression
  - Definition
  - Gradient Descent (GD) optimization
- Normal Equation and Least Squares (maybe?)

Next lecture:

- Normal Equation and Least Squares
- The probabilistic interpretation of Linear Regression
- Maximum Likelihood Estimation (MLE)
- Over-fitting and Under-fitting
- Polynomial Regression, Ridge Regression, and Lasso

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
- Dr. Robert M. Gower, Expected smoothness is the key to understanding minibatching for stochastic gradient methods,
  https://gowerrobert.github.io/pdf/talks/expected_smoothness.pdf

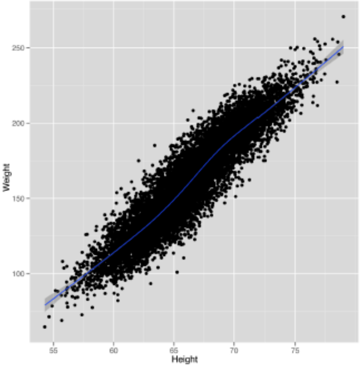
Reference

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

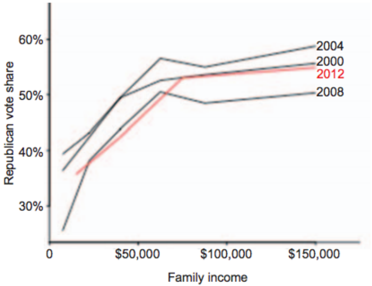
Table of Contents

Table of Contents

What is regression?



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



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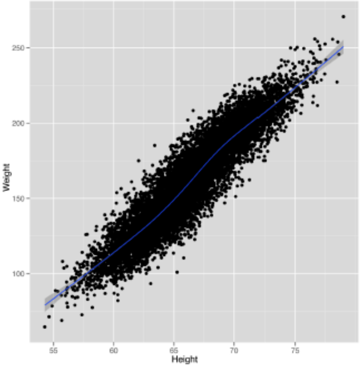

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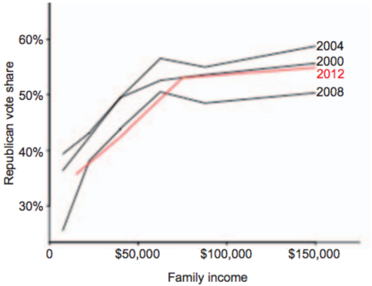

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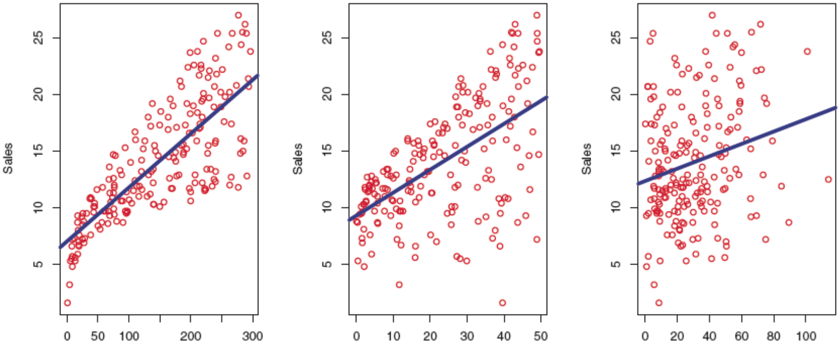
Regression is to relate input variables to the output variable.

Dataset for regression

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



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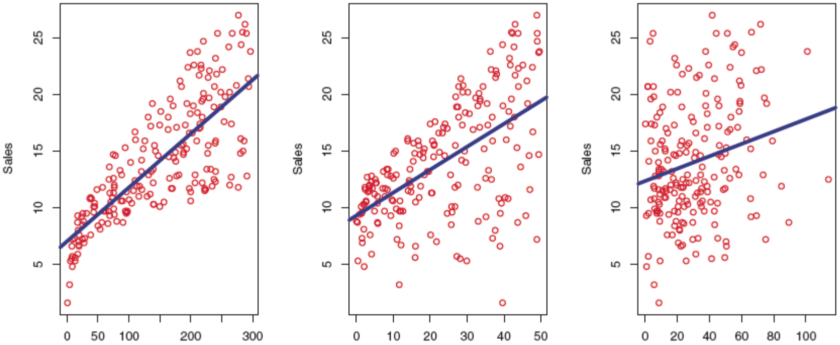

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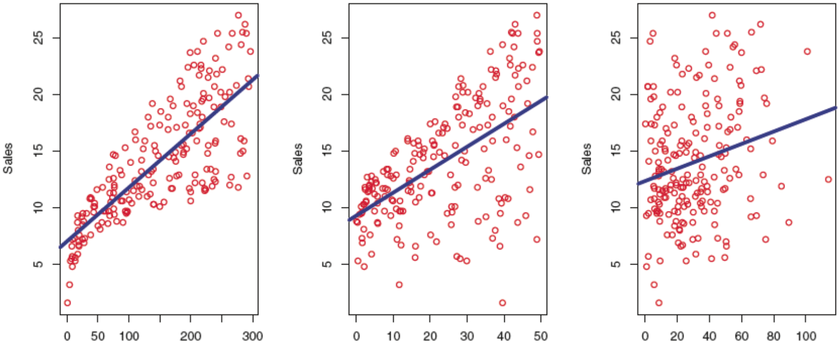
- The number of pairs N is the data-size and D is the dimensionality.



Two goals of regression

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

$$y_n \approx f(\mathbf{x}_n), \text{ for all } n \tag{2}$$

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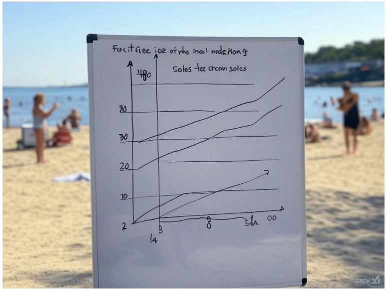
2. interpretation: understand the effect of the input on the output.

   e.g., are taller people heavier too?

Why correlation isn’t causation: spurious correlation



ice cream sales vs. drowning incidents

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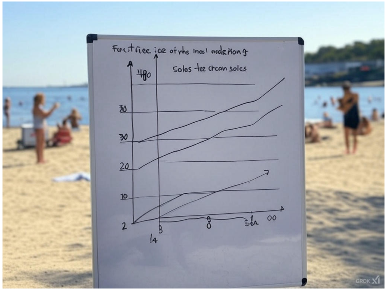

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Remark 1 (Correlation $\neq$ Causation)

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

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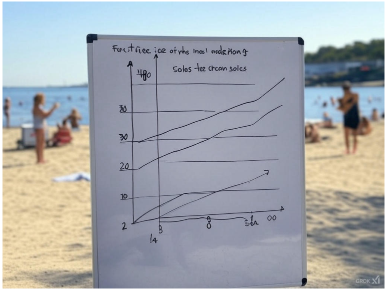

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Brainstorm other examples!

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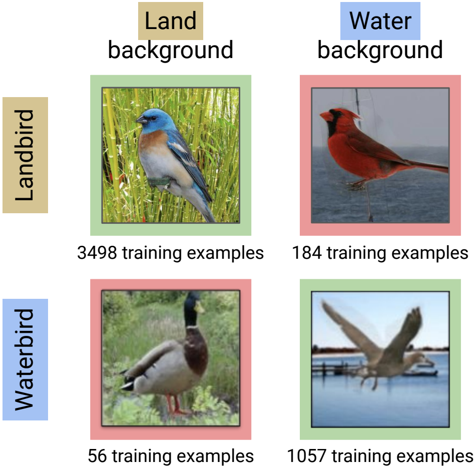
What is the concept of “spurious correlations”?



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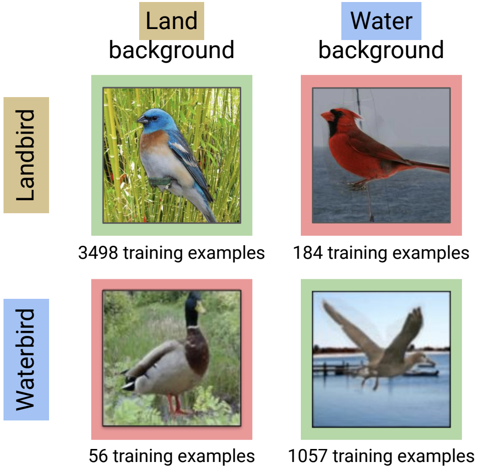

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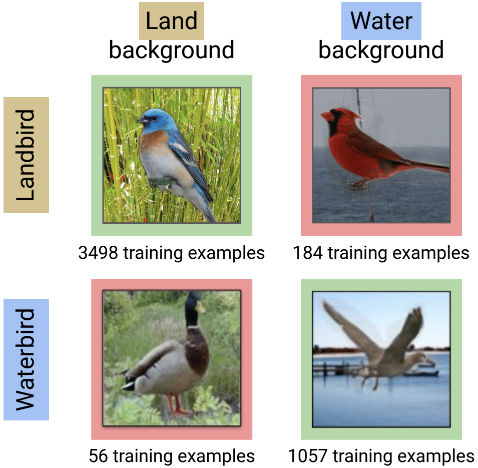

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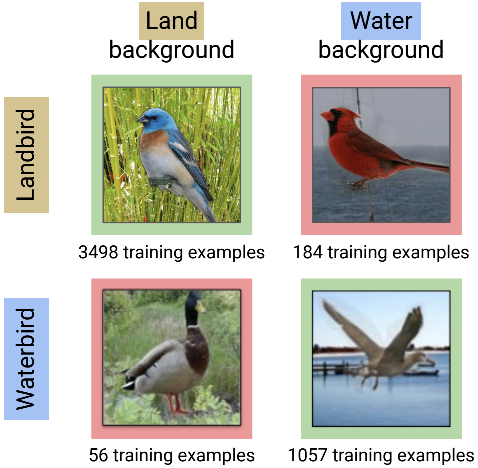
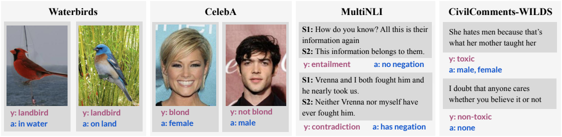
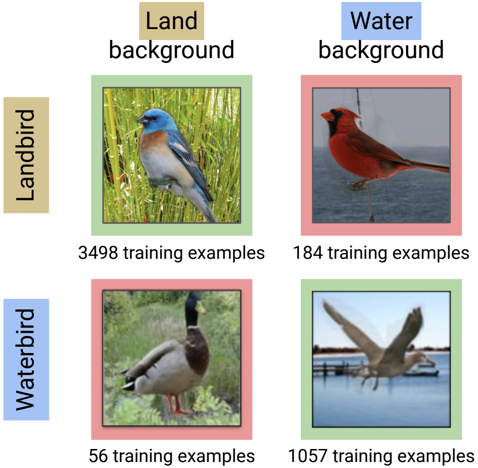
- A model trained on $\mathcal{D}_{tr}$ may simply use a to predict y, but this will result in incorrect predictions on samples with $\langle y', a \rangle$.

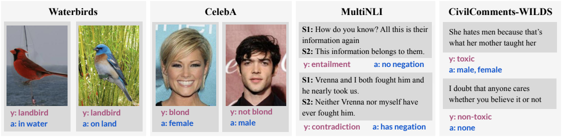


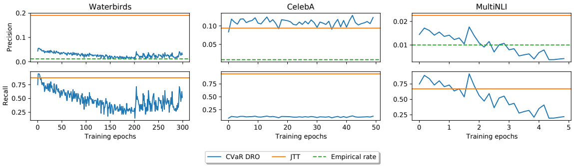


Remark 2 (Shortcut learning in Deep Learning)

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







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A formal definition of spurious correlation

Definition 3 (Spurious Correlation)

Let $\mathcal{D}_{tr} = \{(x_i, y_i)\}_{i=1}^{n}$ be the training set with $x_i \in \mathcal{X}$ and $y_i \in \mathcal{Y}$, where $\mathcal{X}$ denotes the set of all possible inputs, $\mathcal{Y}$ denotes the set of K classes.

- For each data point x_i with class label y_i, there is a spurious attribute $a_i \in \mathcal{A}$ of x_i, where a_i is non-predictive of y_i, and $\mathcal{A}$ denotes the set of all possible spurious attributes.

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- A set of data with the spurious correlation $\langle y, a \rangle$ is annotated with the group label $g = (y, a) \in \mathcal{G}$, where $\mathcal{G} := \mathcal{Y} \times \mathcal{A}$ is the set of combinations of class labels and spurious attributes.

Wait!

Wait!

What is the definition of “classes”?

Table of Contents

Classification

We observe some data

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Remark 4

no ordering between classes.

Classifier

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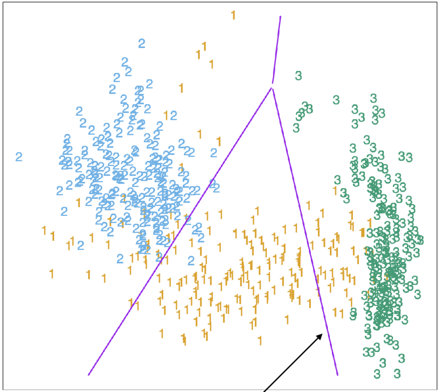

Linear Decision boundary

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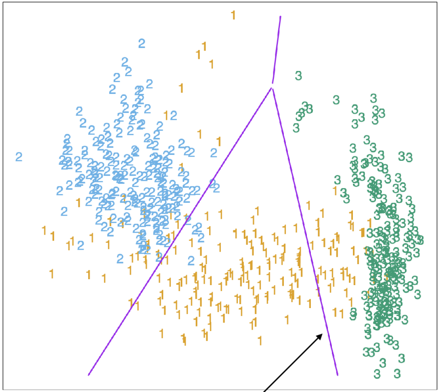

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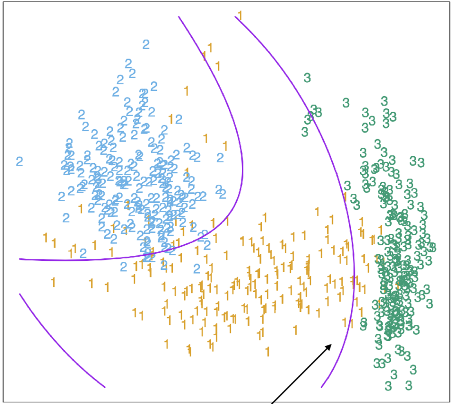

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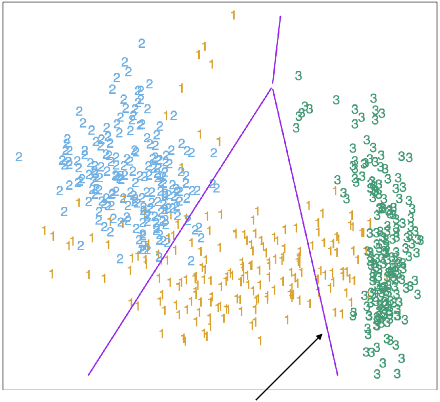

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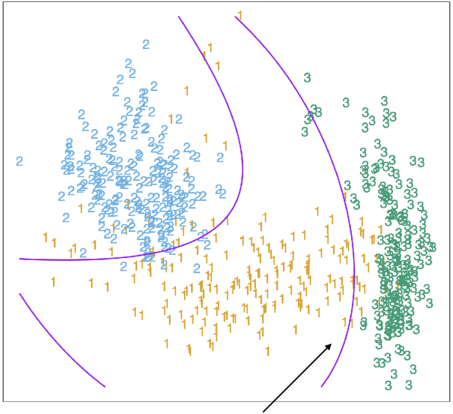

Nonlinear Decision boundary

The boundaries of these regions are called decision boundaries.

Classification: a special case of regression?

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

$$(\mathbf{x}, y) \in \mathcal{X} \times \{0, 1\} \subset \mathcal{X} \times \mathbb{R} \tag{4}$$

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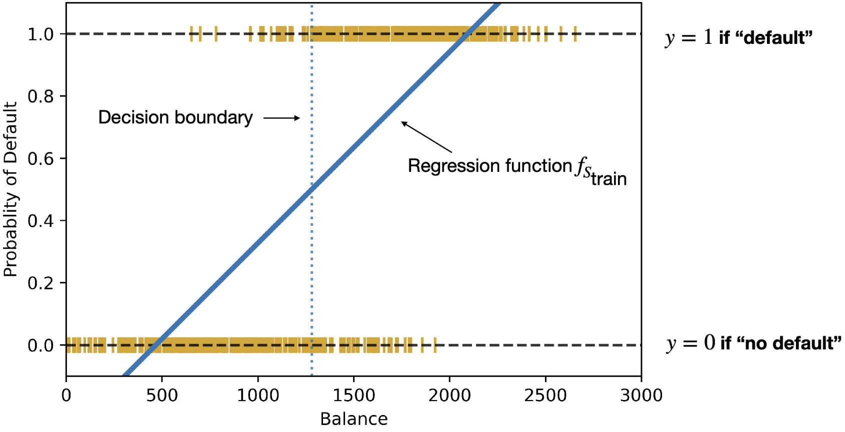
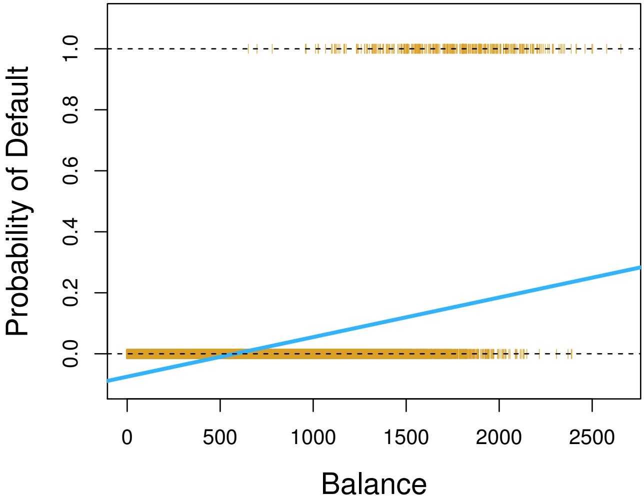
Could we use previously seen regression methods to solve it?

Is it a good idea to use regression methods for classification tasks?



We label the output as probability for sake of interpretation

Classification is not just a special form of regression



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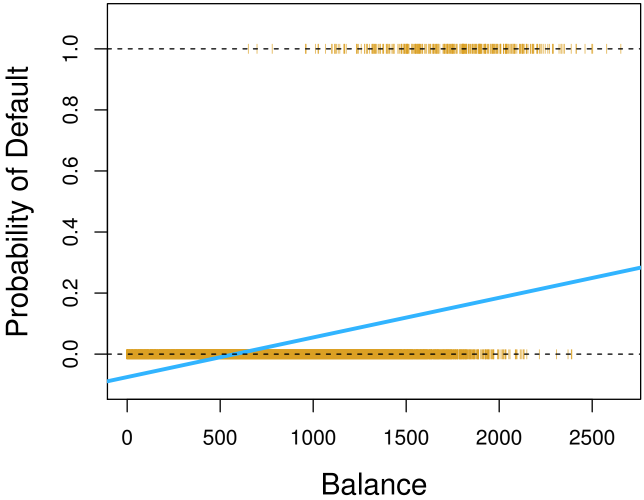
- The predicted values are not probabilities (not in $[0, 1]$).



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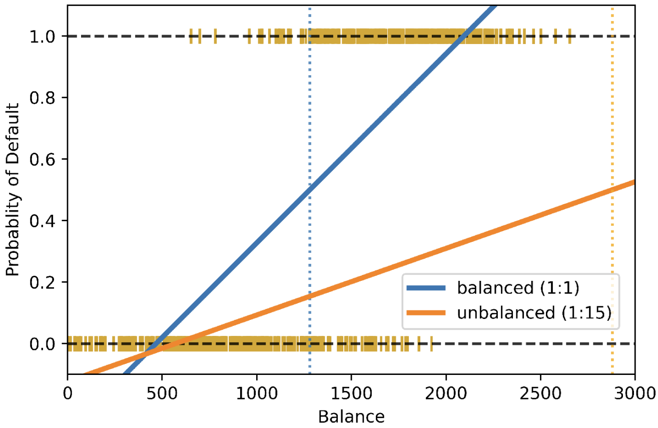
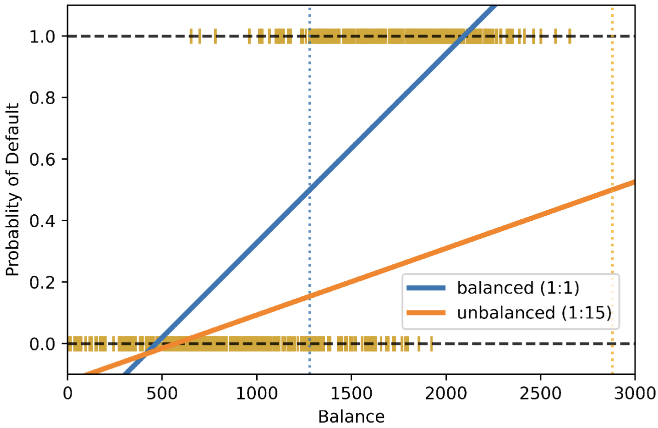


Classification is not just a special form of regression

- Sensitivity to unbalanced data.



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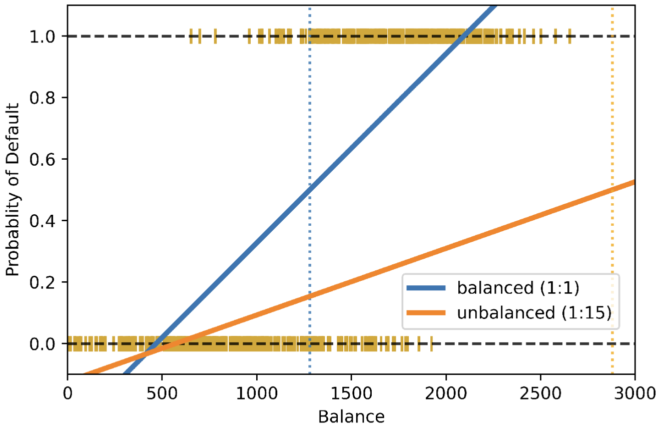
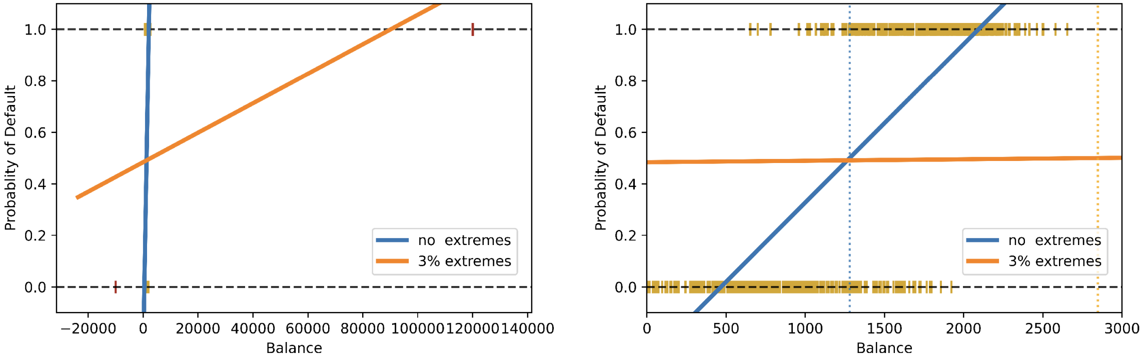


The position of the line depends crucially on how many points are in each class.

Classification is not just a special form of regression



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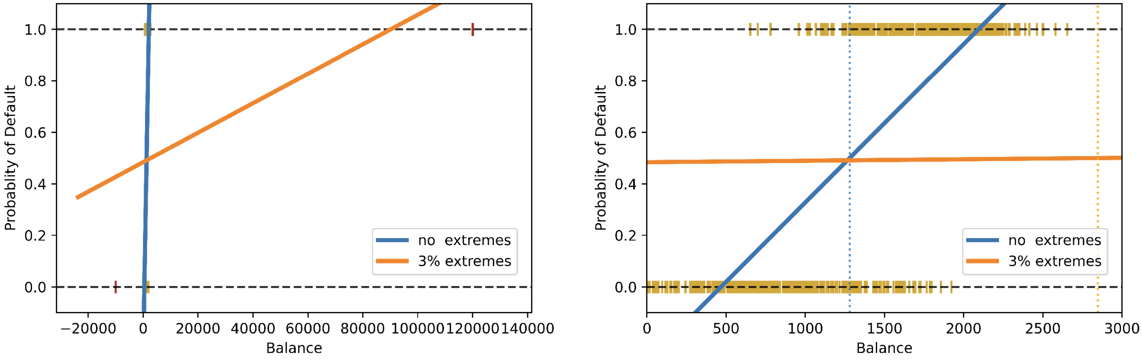

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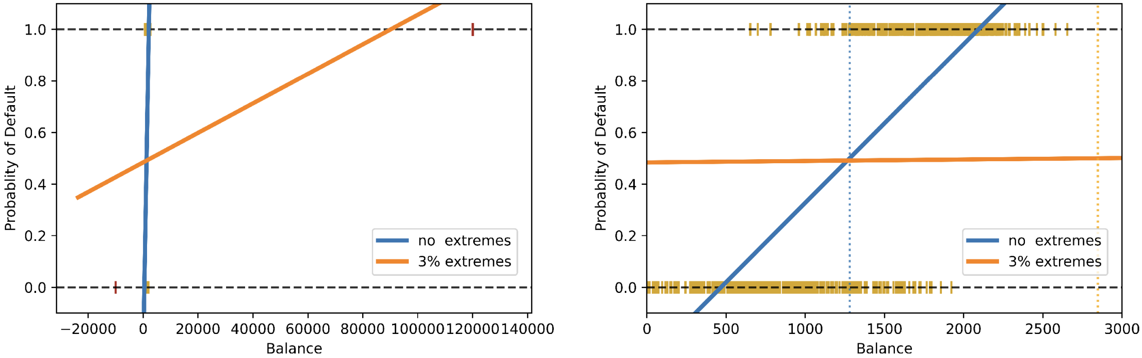

The position of the line depends crucially on where the points lie.

How to perform classification?

- A lot of different approaches have been developed

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- Fundamental task of classification:

> **separate the space into various decision regions**

Table of Contents

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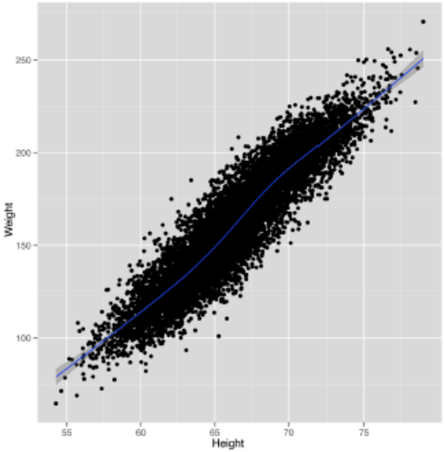

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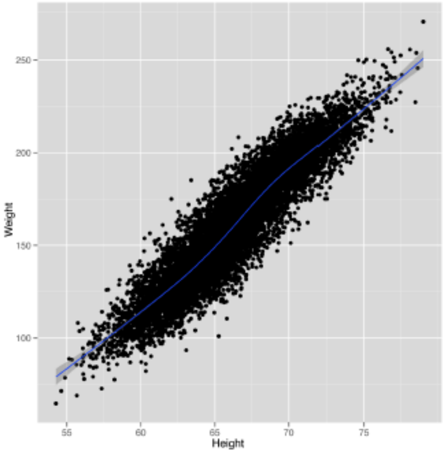

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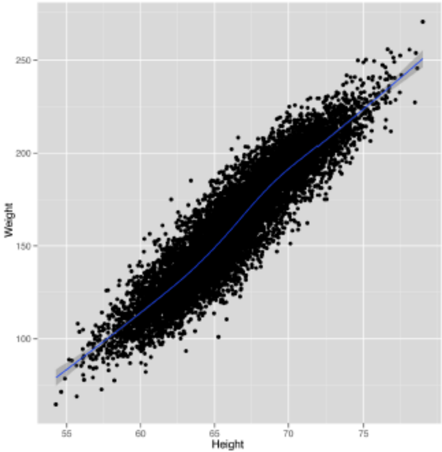

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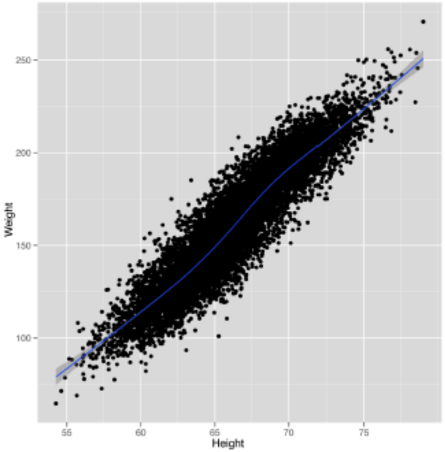
- a linear relationship is assumed for f



Detailed definition

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(8)

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We need an optimization algorithm!

Why learn about *linear* regression?

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Consider the following models.

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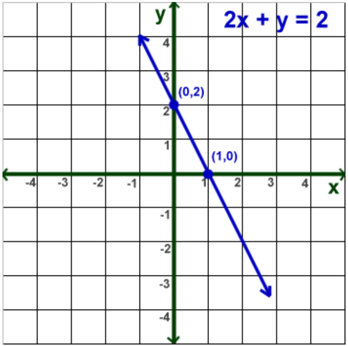
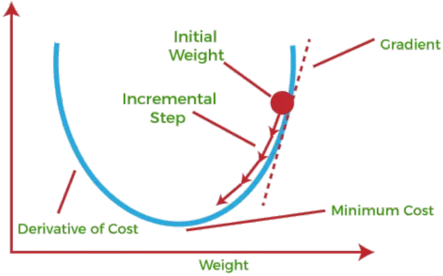
Q: How can we estimate values of $\mathbf{w}$ given the data $\mathcal{D}$?

Analytical vs. Numerical solutions

- ***Analytical solutions*** provide precise closed-form solutions but are limited to simple problems.

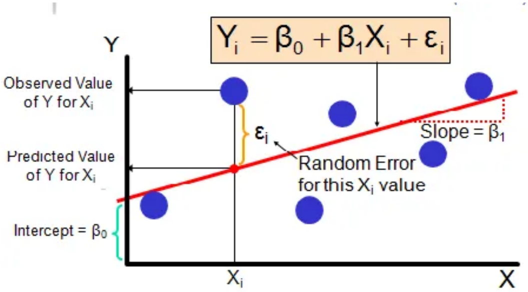
- ***Gradient Descent*** (GD) is a numerical method that approximates the optimal solution iteratively for complex problems.





https://medium.com/@msong507/gradient-descent-intuitive-overview-43e7869e1545

Approximate optimal solution $\mathbf{w}^\star$: cost function



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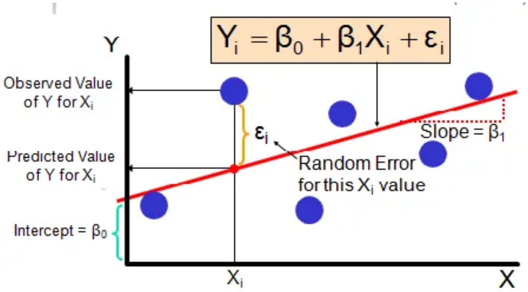

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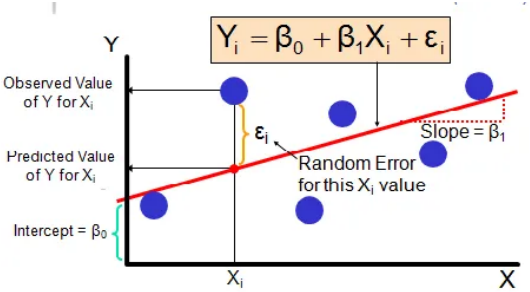

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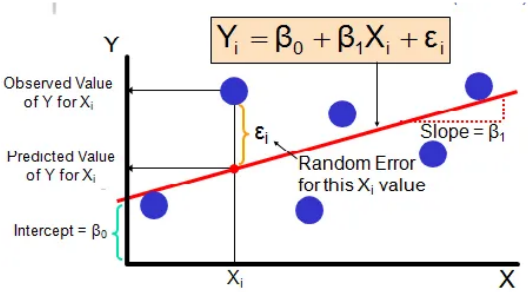

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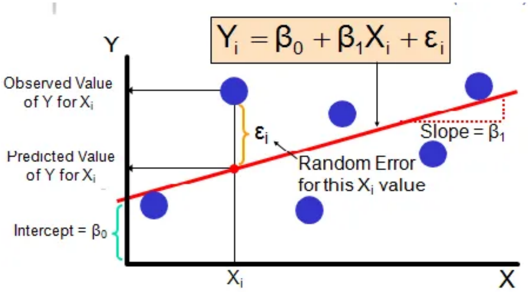

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  - the cost penalizes "large" mistakes and "very-large" mistakes similarly

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Mean Squared Error (MSE) and outliers

$$\text{MSE}(\mathbf{w}) := \frac{1}{N}\sum_{n=1}^{N}\left[y_n - f_{\mathbf{w}}(\mathbf{x}_n)\right]^2 \tag{9}$$

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

Discussion on different cost functions

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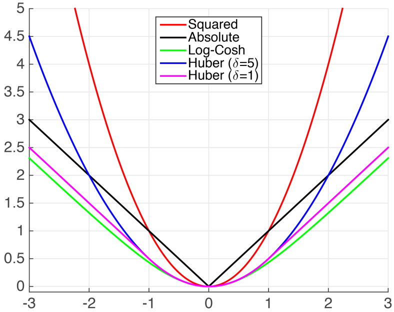

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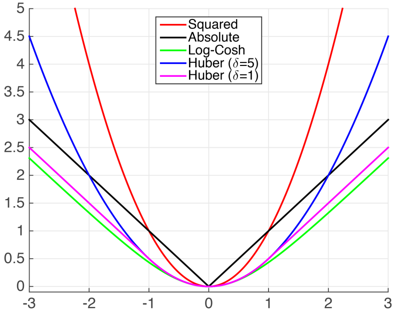
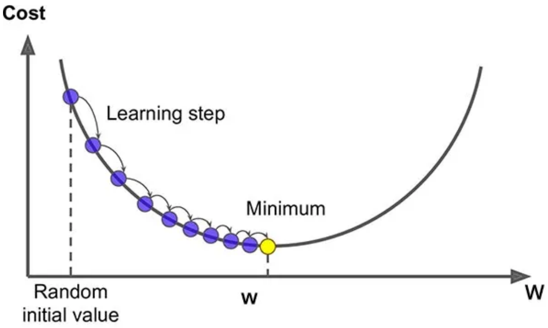
where Huber loss uses MSE logic for “small” residual values and MAE logic for “large” residual values.



Learning / Estimation / Fitting



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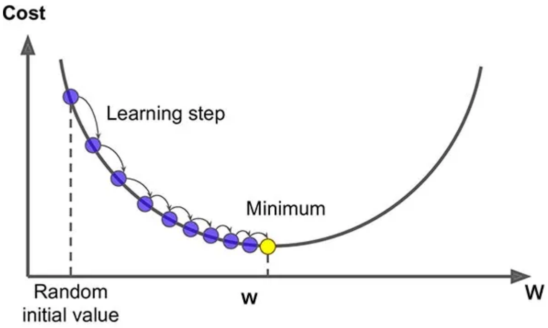

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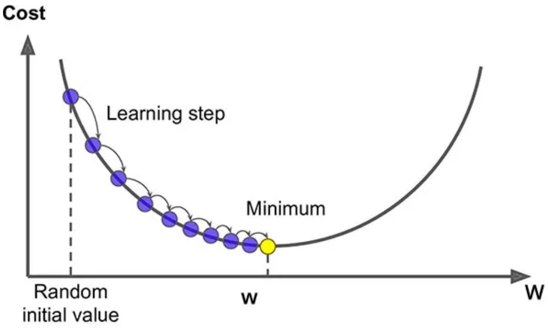

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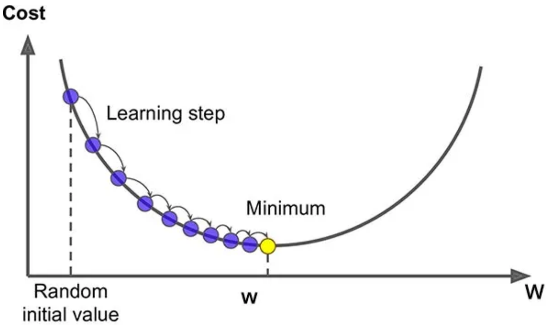

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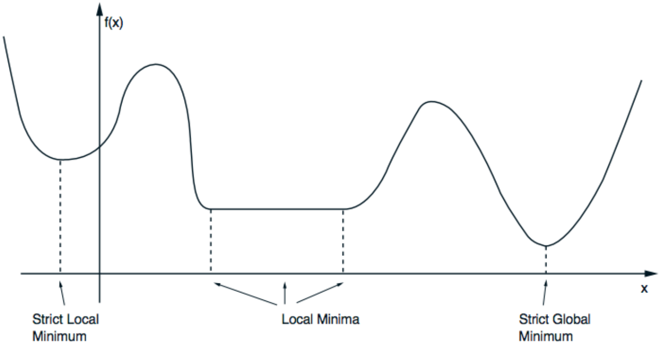
We will use an optimization algorithm like GD to solve the problem (to find a good $\mathbf{w}$).

Optimization landscapes



The above figure is taken from Bertsekas, Nonlinear programming.

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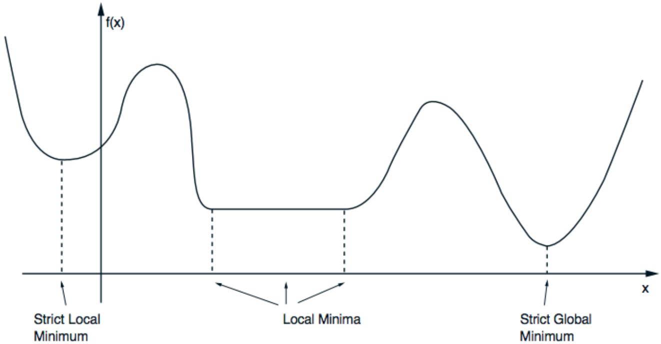

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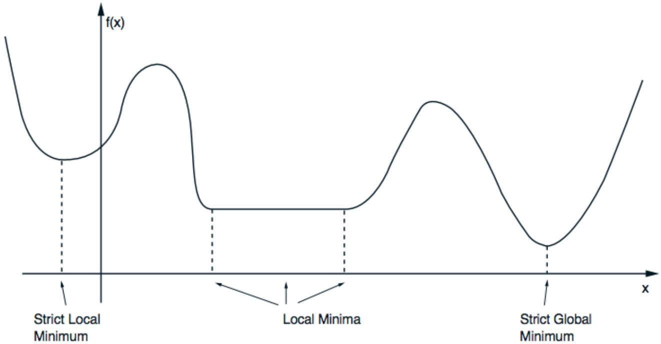

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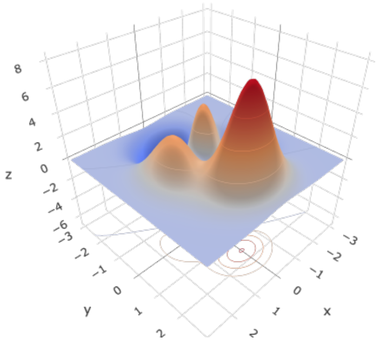

This is where gradient descent can help.

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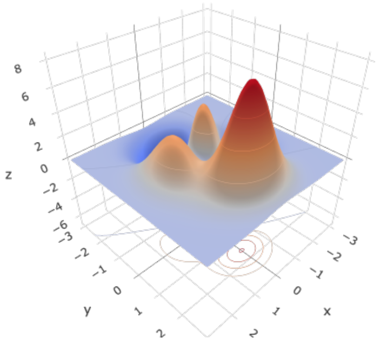

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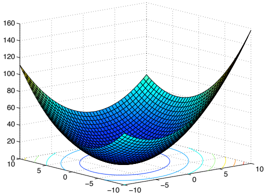
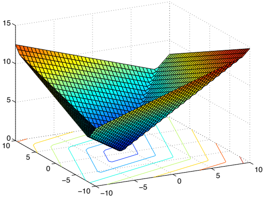
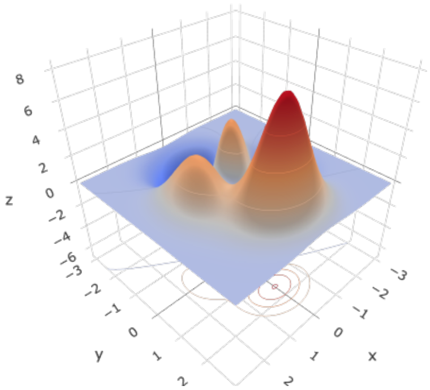
For a 2-parameter model, MSE$(\mathbf{w})$ and MAE$(\mathbf{w})$ are shown below.

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

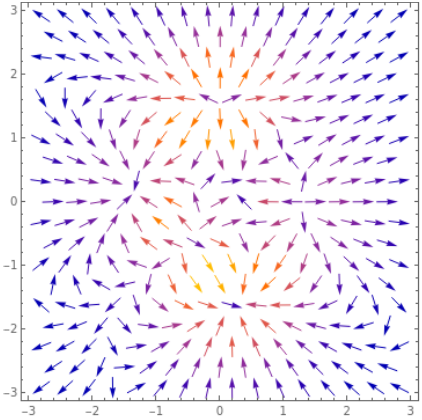




Example:



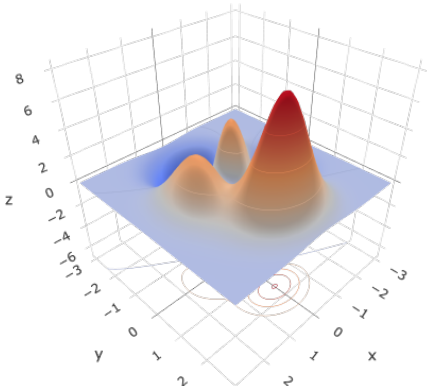
Cost function $f(x, y)$.



Gradient of f plotted as a vector field:

$$\nabla f(x, y) = \begin{bmatrix} \frac{\partial f}{\partial x}(x, y) \\ \frac{\partial f}{\partial y}(x, y) \end{bmatrix}$$

Example: revisit this link for more details.



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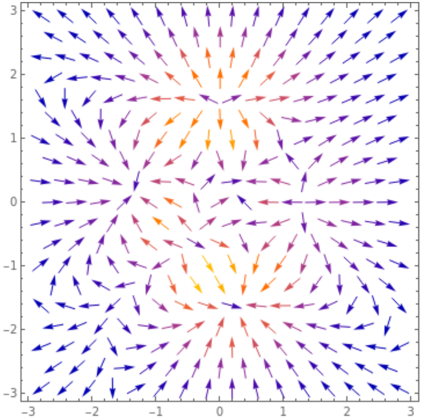

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where $\gamma > 0$ is the step-size (or learning rate). Then repeat with the next t.

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

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \in \mathbb{R}^N, \qquad \mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1D} \\ x_{21} & x_{22} & \dots & x_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \dots & x_{ND} \end{bmatrix} \in \mathbb{R}^{N \times D} \tag{15}$$

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$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \in \mathbb{R}^N, \qquad \mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1D} \\ x_{21} & x_{22} & \dots & x_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \dots & x_{ND} \end{bmatrix} \in \mathbb{R}^{N \times D} \tag{15}$$

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

$$\mathbf{e} = \mathbf{y} - \mathbf{X}\mathbf{w} = \begin{pmatrix} e_1 \\ \vdots \\ e_n \\ \vdots \\ e_N \end{pmatrix} \in \mathbb{R}^N, \tag{16}$$

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

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where $e_n := y_n - \mathbf{x}_n^\top \mathbf{w}$. The MSE is defined as $\mathcal{L}(\mathbf{w}) := \frac{1}{2N} \sum_{n=1}^{N} \left(y_n - \mathbf{x}_n^\top \mathbf{w}\right)^2$,

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$$\nabla \mathcal{L}(\mathbf{w}) = -\frac{1}{N} \mathbf{X}^\top \mathbf{e}$$

.

Stochastic Gradient Descent (SGD)

- **Sum Objectives:** In machine learning, most cost functions are formulated as a sum over the training examples, that is

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- **Theoretical Motivation:** In expectation over the random choice of n, we have
$$\mathbb{E}[\nabla \mathcal{L}_n(\mathbf{w})] = \nabla \mathcal{L}(\mathbf{w})$$
which is the true gradient direction.

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- Note that in the extreme case $B := [N]$, we obtain (batch) gradient descent, i.e. $\mathbf{g} = \nabla \mathcal{L}$.

An alternative view of SGD

Finite-sum empirical risk minimization problem:

$$f(\mathbf{x}^\star) = \min_{\mathbf{x}\in\mathbb{R}^d} \left\{ f(\mathbf{x}) := \frac{1}{N}\sum_{i=1}^{N} \left(f_i(\mathbf{x}) := \boxed{F(\mathbf{x}, \boldsymbol{\xi}_i)} \right) \right\}$$

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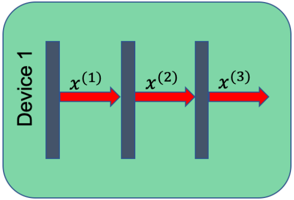

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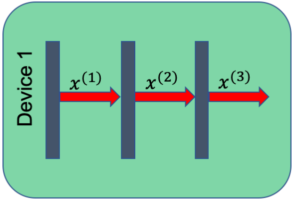

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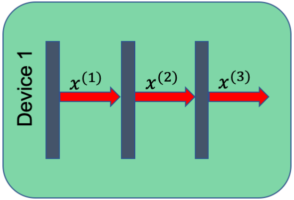

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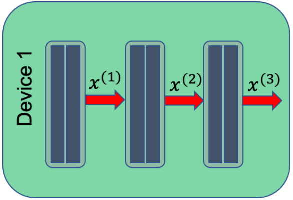

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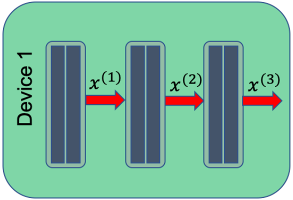
- $\mathcal{B} \in \{1, \ldots, N\}$ with $|\mathcal{B}| = B$.



Alternative view: Stochastic reformulation of finite-sum problems (SGD with arbitrary sampling)

Random sampling vector $\mathbf{v} = (v_1, \ldots, v_N) \sim \mathcal{D}$ with $\mathbb{E}[v_i] = 1 \qquad$ for $i = 1, \ldots, N$.

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Original Finite-sum problem

$$\min_{\mathbf{x}\in\mathbb{R}^d} \frac{1}{N}\sum_{i=1}^{N} f_i(\mathbf{x})$$

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Stochastic Reformulation

$$\min_{\mathbf{x}\in\mathbb{R}^d} \mathbb{E}\left[f_v(\mathbf{x})\right]$$

Minimizing the expectation of **random linear combinations** of original function

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$\downarrow$

Sample $v_i^{(t)} \sim \mathcal{D}$

$$\mathbf{x}^{(t+1)} \leftarrow \mathbf{x}^{(t)} - \eta \nabla f_{v_i^{(t)}}(\mathbf{x}^{(t)})$$

The distribution $\mathcal{D}$ encodes any form of mini-batching/non-uniform sampling. Our analysis is done for any distribution $\mathcal{D}$.

Examples of arbitrary sampling: uniform single element

Random set $\mathcal{S} \subset \{1, \ldots, N\}$, $|\mathcal{S}| = 1$,
$\Pr[i \in \mathcal{S}] = \frac{1}{N}$, for $i = 1, \ldots, N$

$$\begin{aligned} \mathbb{E}[v_i] &= 1 \\ v_i = &\begin{cases} N & i \in \mathcal{S} \\ 0 & i \notin \mathcal{S} \end{cases} \end{aligned} \tag{17}$$

$$\nabla f_v(\mathbf{x}) = \nabla f_i(\mathbf{x}),$$

where $\mathbb{E}[\nabla f_v(\mathbf{x})] = \nabla f(\mathbf{x})$

Single element SGD

Sample $v^{(t)} \sim \mathcal{D}$

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Examples of arbitrary sampling: uniform mini-batching

Random set $\mathcal{S} \subset \{1, \ldots, N\}$, $|\mathcal{S}| = B$,
$\Pr[i \in \mathcal{S}] = \frac{B}{N}$, for $i = 1, \ldots, N$

$$\mathbb{E}[v_i] = 1$$

$$v_i = \begin{cases} \frac{N}{B} & i \in \mathcal{S} \\ 0 & i \notin \mathcal{S} \end{cases} \quad (18)$$

$$\nabla f_v(\mathbf{x}) = \frac{1}{B} \sum_{i \in \mathcal{S}} \nabla f_i(\mathbf{x}),$$

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Mini-batch SGD w/o replacement

Sample $v^{(t)} \sim \mathcal{D}$

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \eta \nabla f_{v^{(t)}}(\mathbf{x}^{(t)})$$

Examples of arbitrary sampling: non-uniform mini-batching

Random set $\mathcal{S} \subset \{1, \ldots, N\}$, $|\mathcal{S}| = B$,
$\Pr[i \in \mathcal{S}] = p_i$, for $i = 1, \ldots, N$

$$\mathbb{E}[v_i] = 1$$

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$$\nabla f_v(\mathbf{x}) = \frac{n}{p_i} \sum_{i \in \mathcal{S}} \nabla f_i(\mathbf{x}),$$

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Arbitrary sampling SGD

Sample $v^{(t)} \sim \mathcal{D}$

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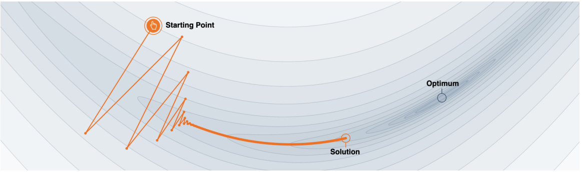
Includes all forms of SGD (and GD)

$$\min_{\mathbf{x} \in \mathbb{R}^d} \mathbb{E}\left[f_v(\mathbf{x}) := \frac{1}{N} \sum_{i=1}^{N} v_i f_i(\mathbf{x})\right]$$

Table of Contents

Motivation

Recall that *GD for Linear Regression with MSE loss* is an iterative optimization algorithm, computationally flexibility for handling large datasets.



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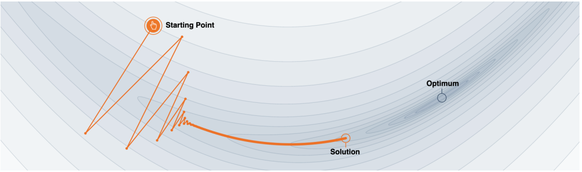
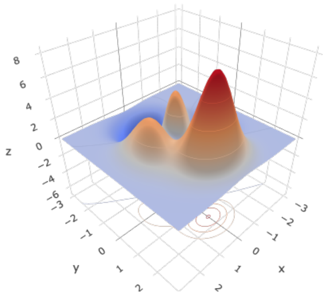
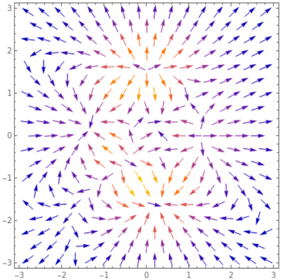


Can we compute the optimum of the cost function analytically?

- Linear regression using an MSE cost function is one such case.



Cost function $f(x, y)$.



Gradient of f plotted as a vector field.

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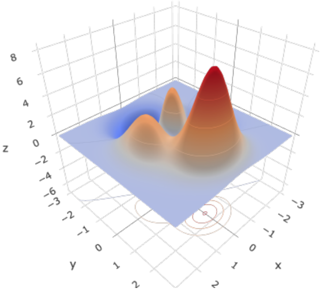

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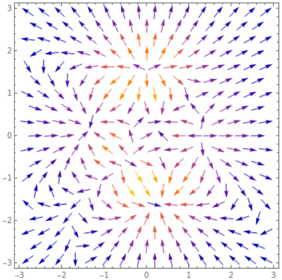

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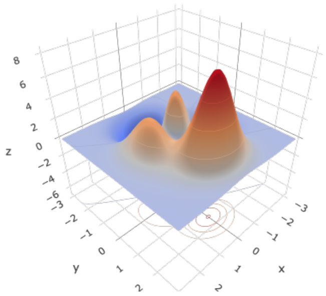

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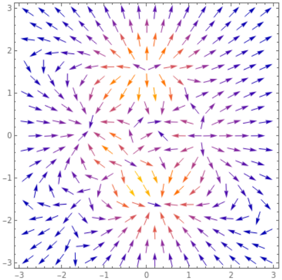
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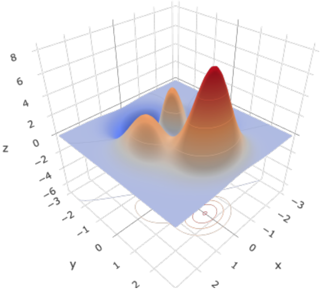
$\Rightarrow$ These equations are sometimes called the normal equations.



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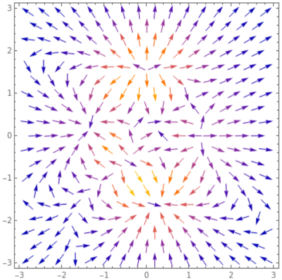

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$\Rightarrow$ Solving the normal equations is called the least squares.

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$$\mathcal{L}(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N}\left(y_n - \mathbf{x}_n^\top \mathbf{w}\right)^2 = \frac{1}{2N}(\mathbf{y} - \mathbf{X}\mathbf{w})^\top(\mathbf{y} - \mathbf{X}\mathbf{w}), \tag{20}$$

where

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

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

$$\mathcal{L}(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N}\left(y_n - \mathbf{x}_n^\top \mathbf{w}\right)^2 = \frac{1}{2N}(\mathbf{y} - \mathbf{X}\mathbf{w})^\top(\mathbf{y} - \mathbf{X}\mathbf{w}), \tag{20}$$

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What is the meaning of finding the analytical solution?

Steps to form normal equations

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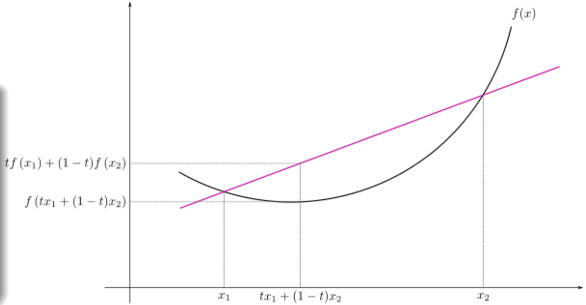

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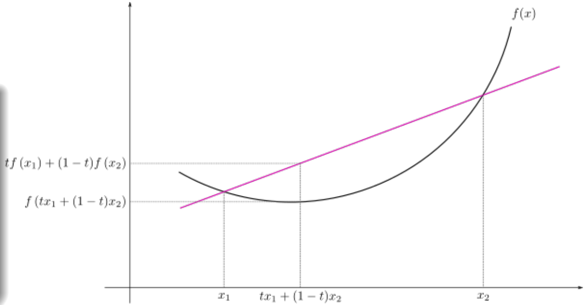

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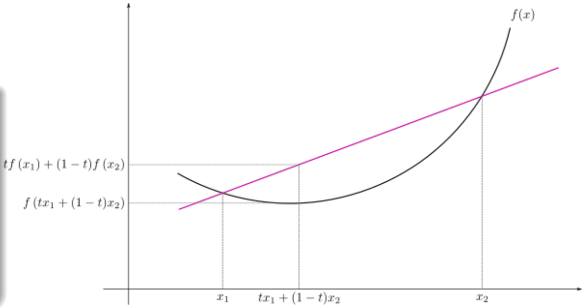

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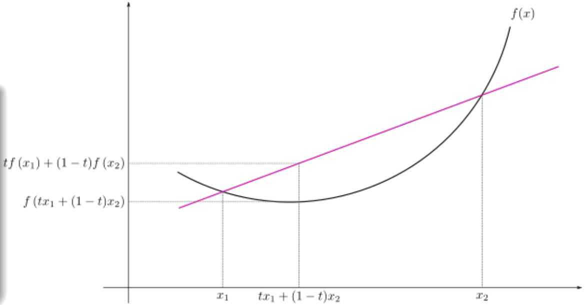

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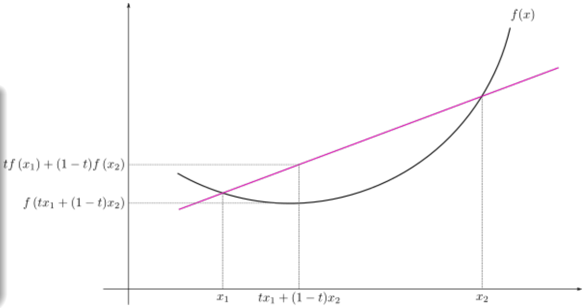

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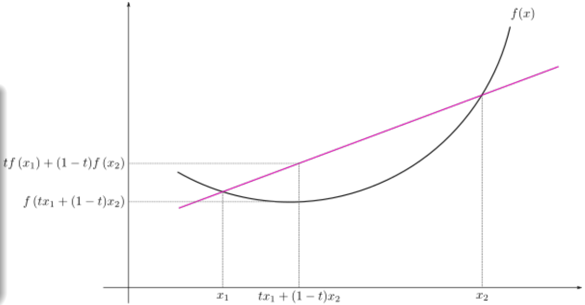

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$$\nabla \mathcal{L}(\mathbf{w}^\star) = \mathbf{0}\,, \qquad (23)$$

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

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There are several ways of proving this:

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   $\Rightarrow$ its non-zero eigenvalues are the squares of the non-zero singular values of the matrix $\mathbf{X}$.

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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:

$$\mathbf{X}^\top \underbrace{(\mathbf{y} - \mathbf{X}\mathbf{w})}_{\text{error}} = \mathbf{0}\,, \tag{27}$$

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

Geometric interpretation of Normal Equations

Definition 10 (Span of a set of vectors)

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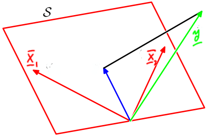

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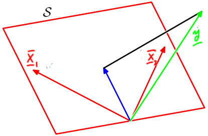

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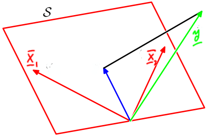

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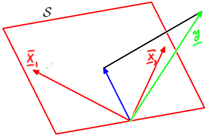

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- $\mathbf{u}^\star$ should be equal to *the projection of* $\mathbf{y}$ *onto* $span(\mathbf{X})$.

Least Squares

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Remark 11

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 $rank(\mathbf{X}) = D$.

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

This lecture:

- Basic concept of regression and classification
- Linear regression
  - Definition
  - Gradient Descent (GD) optimization
- Normal Equation and Least Squares

Next lecture:

- The probabilistic interpretation of Linear Regression
- Maximum Likelihood Estimation (MLE)
- Over-fitting and Under-fitting
- Polynomial Regression, Ridge Regression, and Lasso