

B1:Engineering Computation – Project MT23

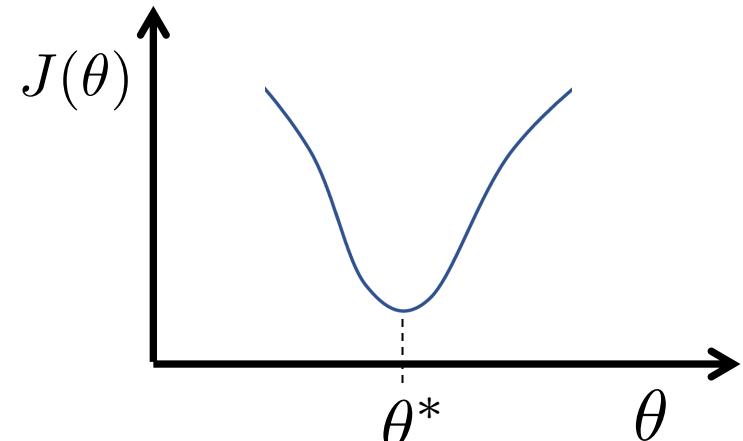
# Optimization for Regression and Classification models

# Optimization:

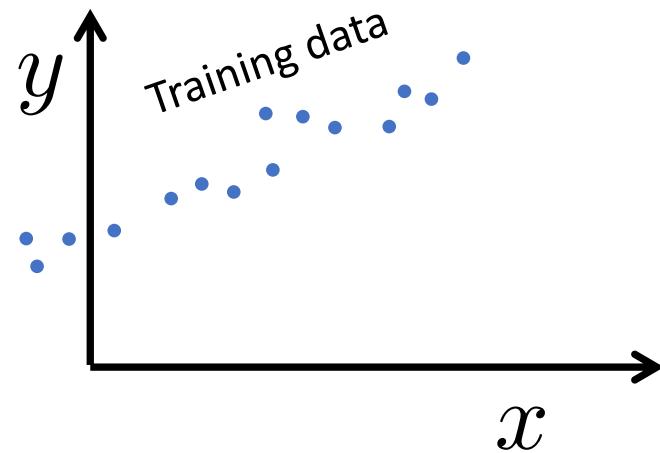
Methods for finding the minimum or maximum value of a function  
(and the parameters  $\theta$  that min/maximize it)

$$\min_{\theta} \mathcal{J}(\theta)$$

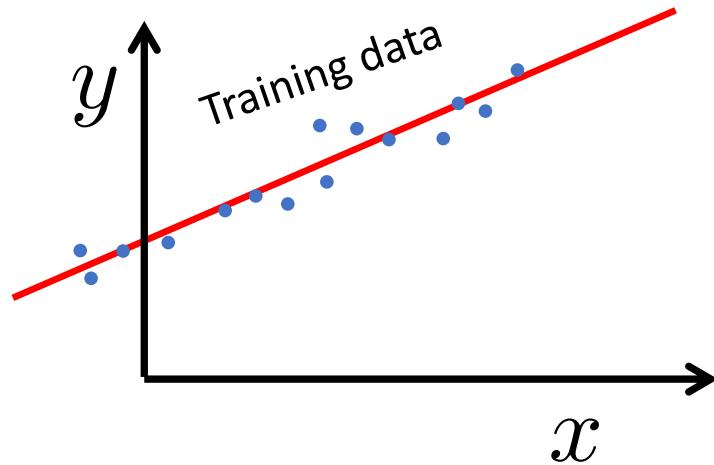
Cost function,  
a.k.a. Objective function  
(sometimes “Loss” function)



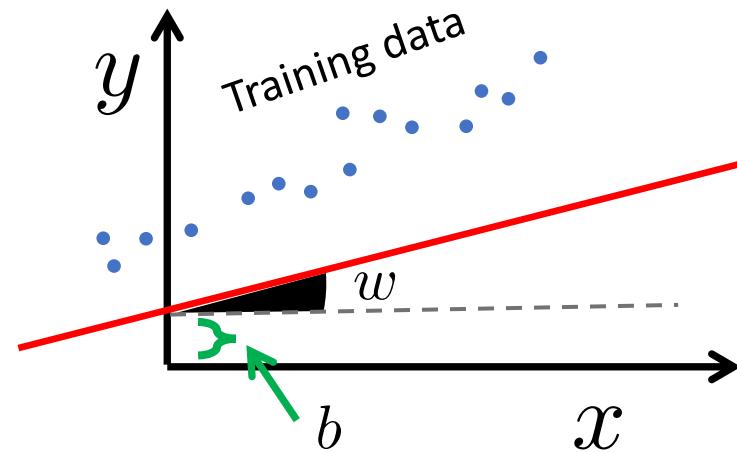
# Example: Optimization of a Regression model



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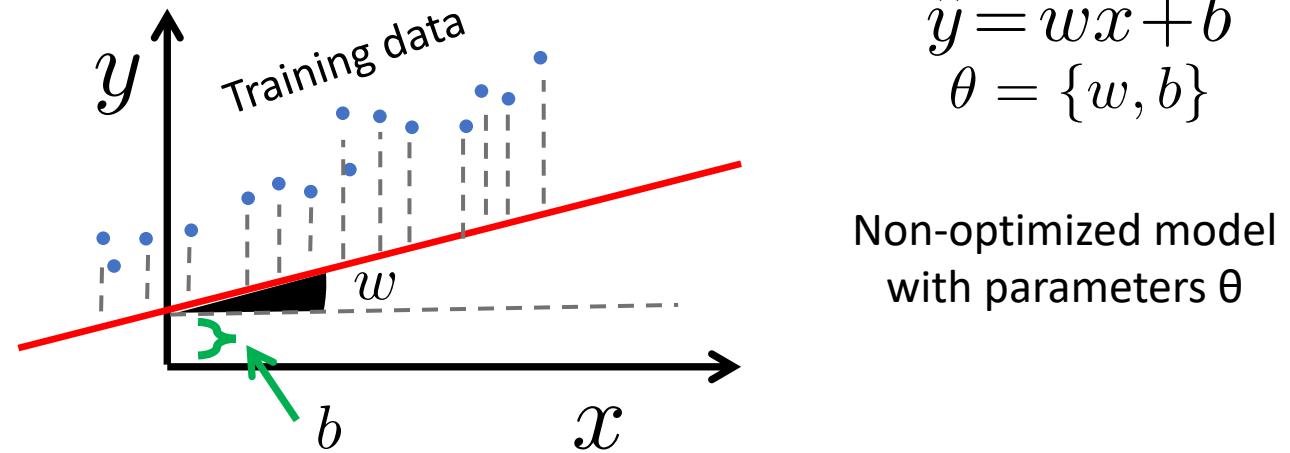
# Example: Optimization of a Regression model



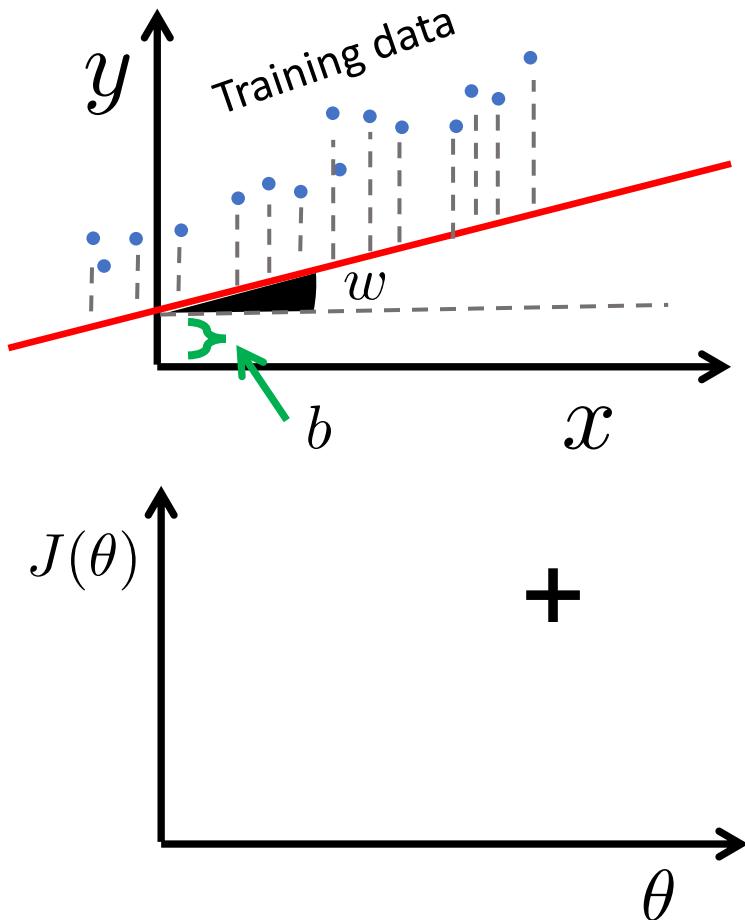
$$\hat{y} = wx + b$$
$$\theta = \{w, b\}$$

Non-optimized model  
with parameters  $\theta$

# Example: Optimization of a Regression model



# Example: Optimization of a Regression model



$$\hat{y} = wx + b$$

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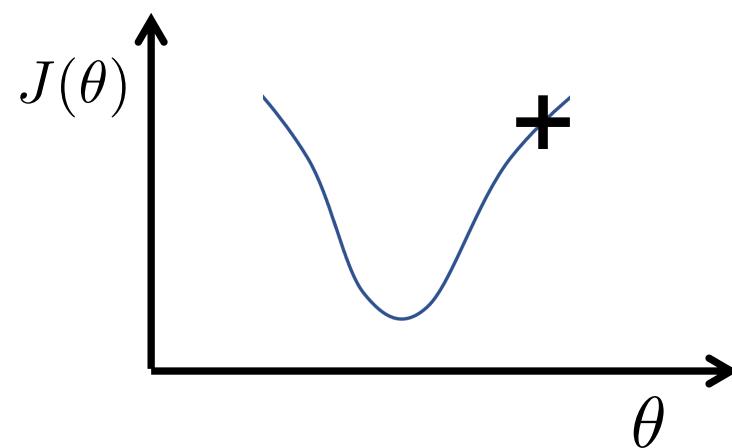
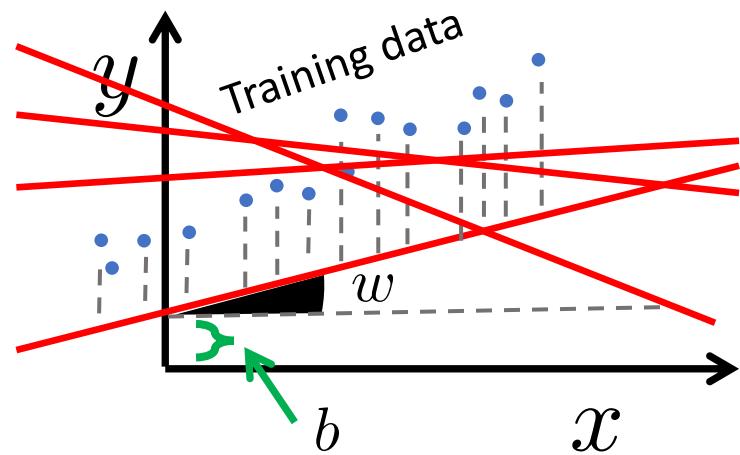
## Non-optimized model with parameters $\theta$

$$J(\theta) = \frac{1}{N} \sum_{x,y} \mathcal{L}(\hat{y}_\theta(x), y)$$

**Cost**                                   **Loss**

$$= \frac{1}{N} \sum_{x,y} (\hat{y}_\theta(x) - y)^2 \quad \textit{Mean Squared Error (MSE)} \textit{ loss}$$

# Example: Optimization of a Regression model



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Non-optimized model  
with parameters  $\theta$

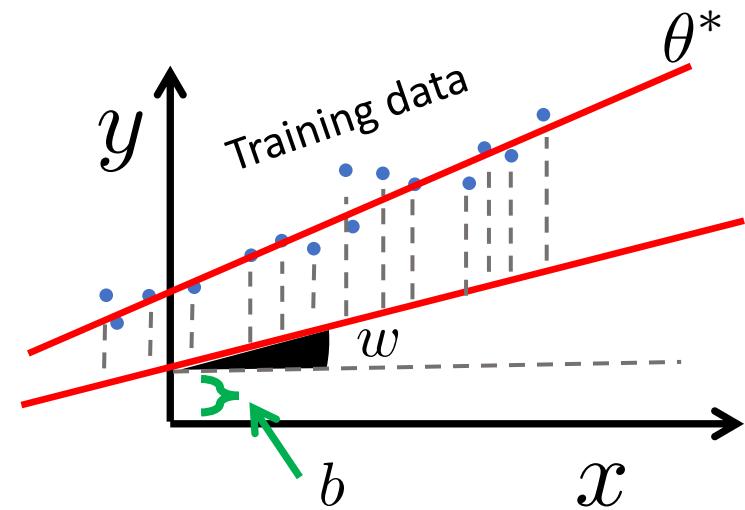
Cost

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Loss

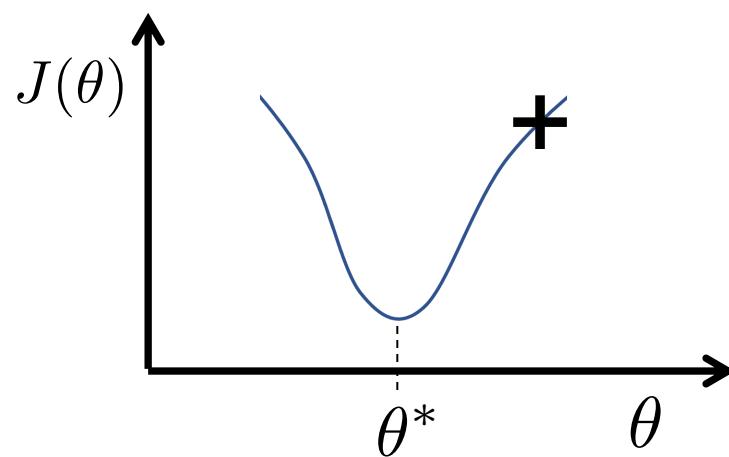
Mean Squared Error (MSE)  
loss

# Example: Optimization of a Regression model



$$\hat{y} = wx + b$$
$$\theta = \{w, b\}$$

Non-optimized model  
with parameters  $\theta$



Cost

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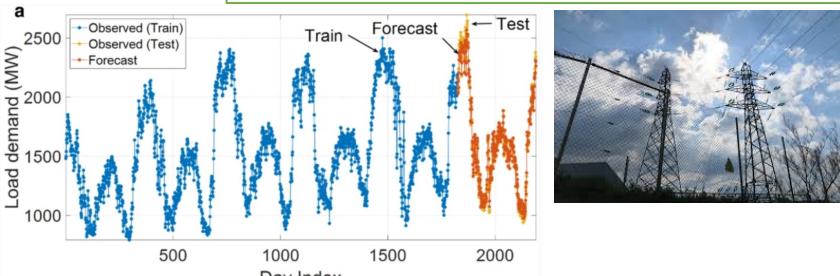
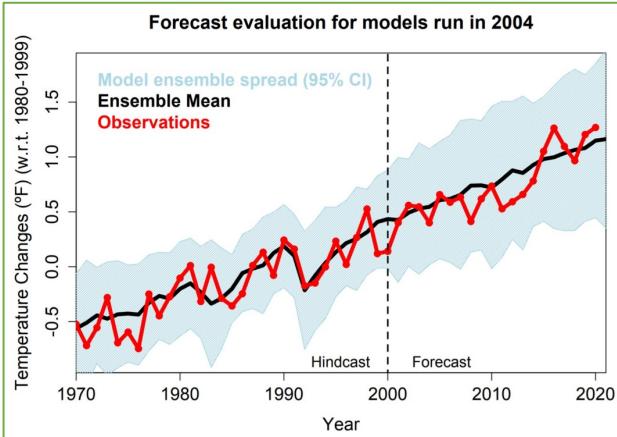
Loss

Mean Squared Error (MSE) loss

# Optimization: Statistics, Machine Learning, Control, Robotics, AI...



[1]



[2]

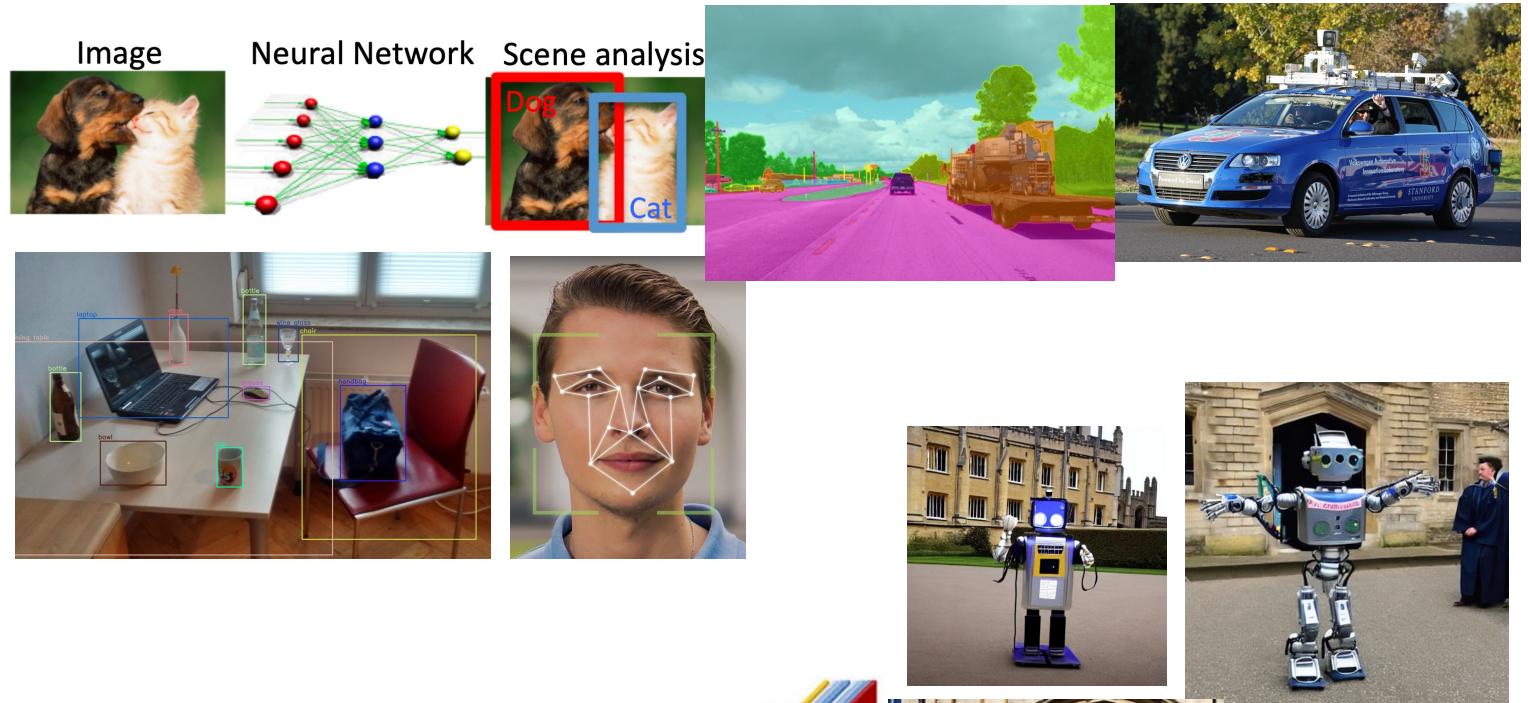
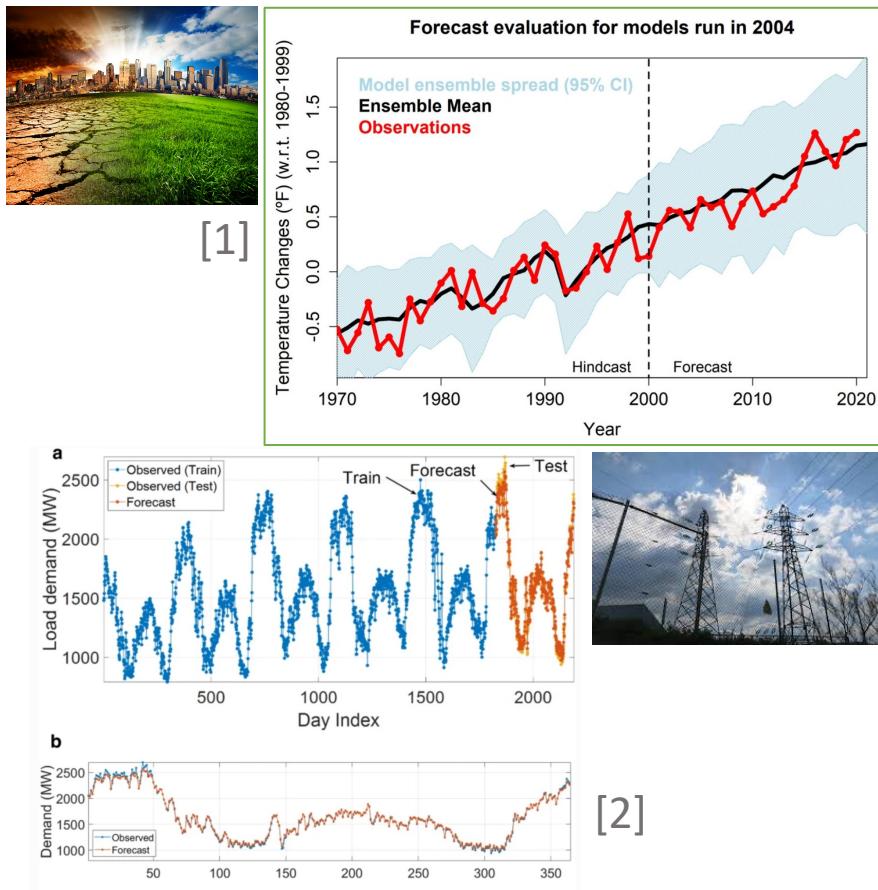
[1] <https://climate.nasa.gov/news/2943/study-confirms-climate-models-are-getting-future-warming-projections-right/>

<https://climate.nasa.gov/solutions/adaptation-mitigation/>

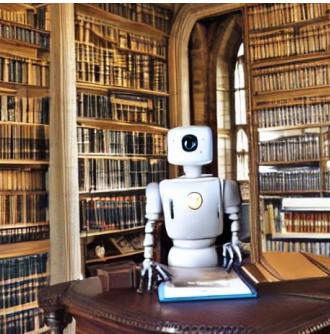
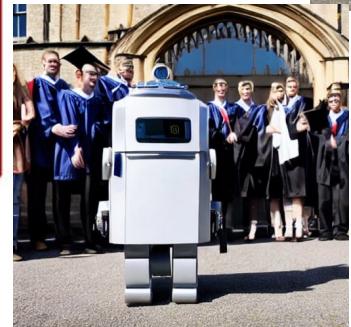
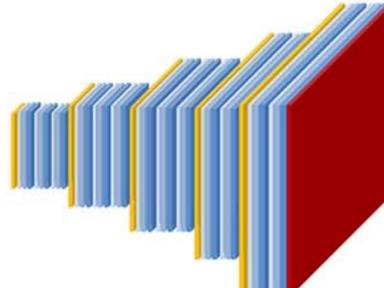
B1: Engineering Computation - Optimization Project

[2] Hamad et al, Deep learning-based load forecasting considering data reshaping using MATLAB\Simulink

# Optimization: Statistics, Machine Learning, Control, Robotics, AI...



*"A robot studying at  
University of Oxford"*



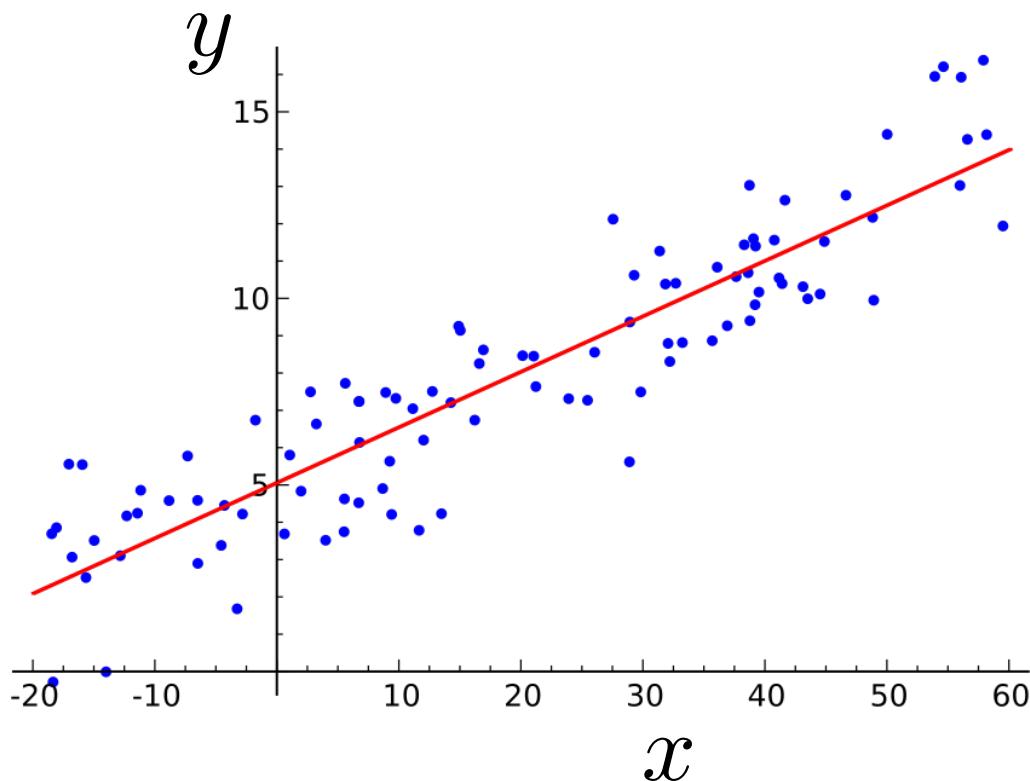
[1] <https://climate.nasa.gov/news/2943/study-confirms-climate-models-are-getting-future-warming-projections-right/>  
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B1: Engineering Computation - Optimization Project

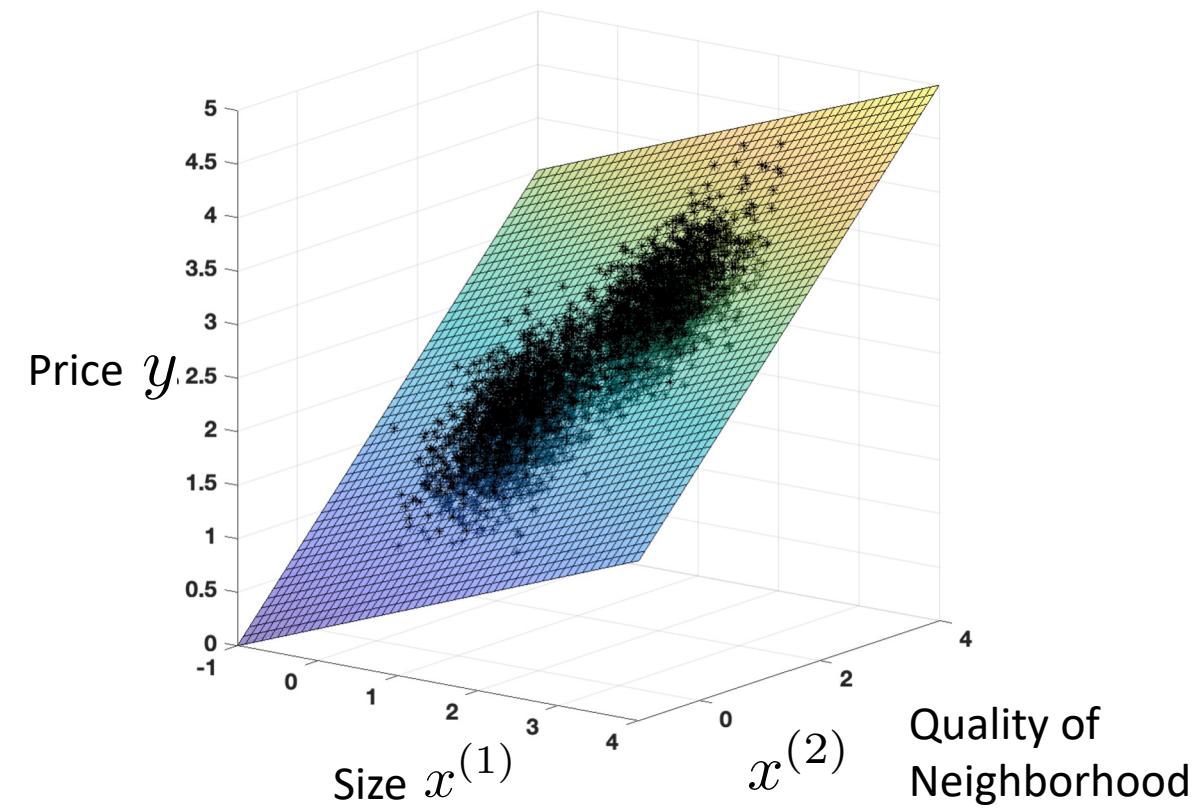
[2] Hamad et al, Deep learning-based load forecasting considering data reshaping using MATLAB\Simulink

# Tasks

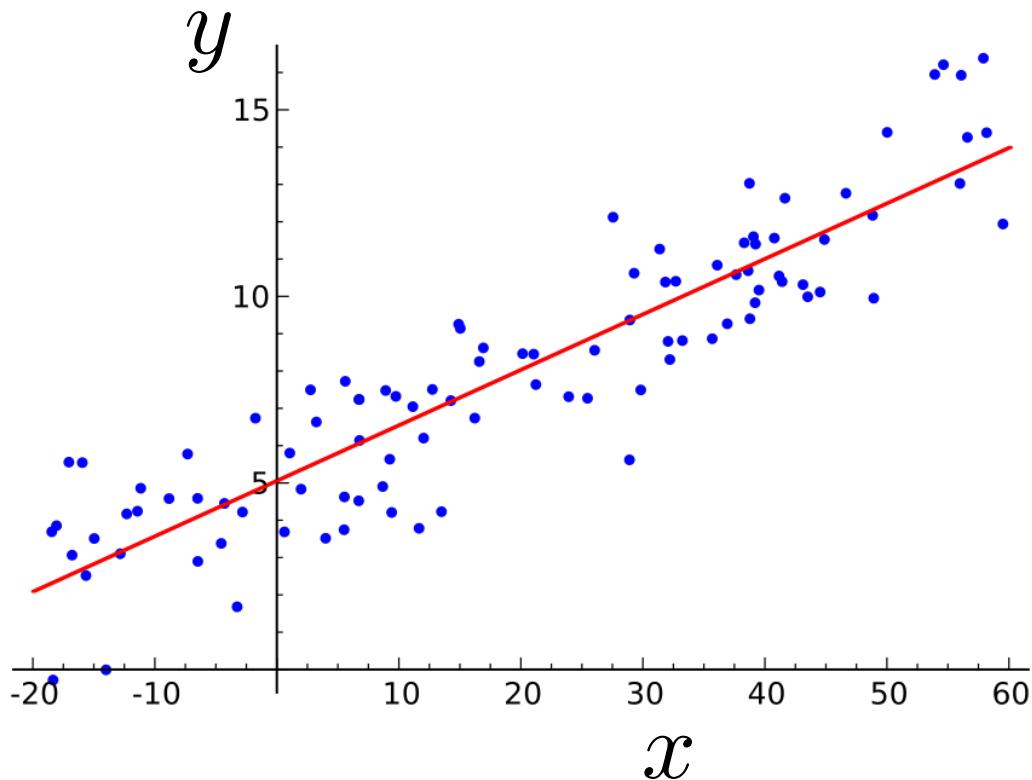
# Linear Regression



Example: Price of a house



# Closed form solution for MSE



$$\min_{\theta} J(\theta) = \min_{\theta} \frac{1}{N} \sum_{x,y} (\hat{y}_{\theta}(x) - y)^2$$

**Solution given by:**

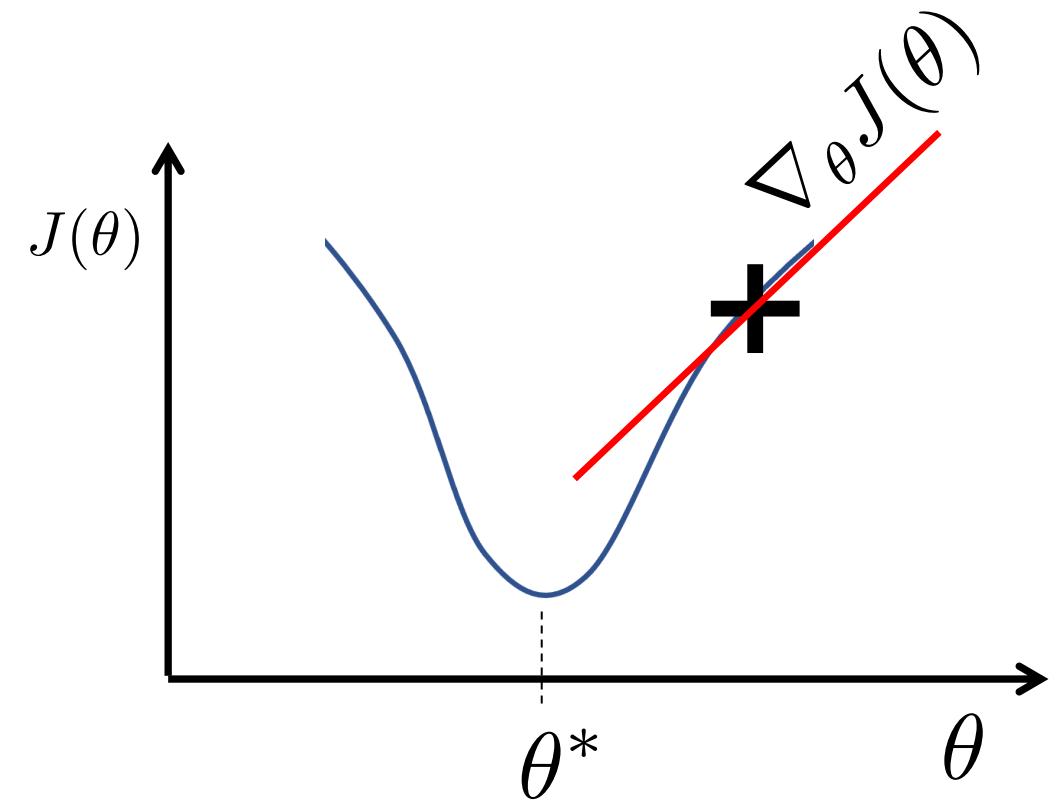
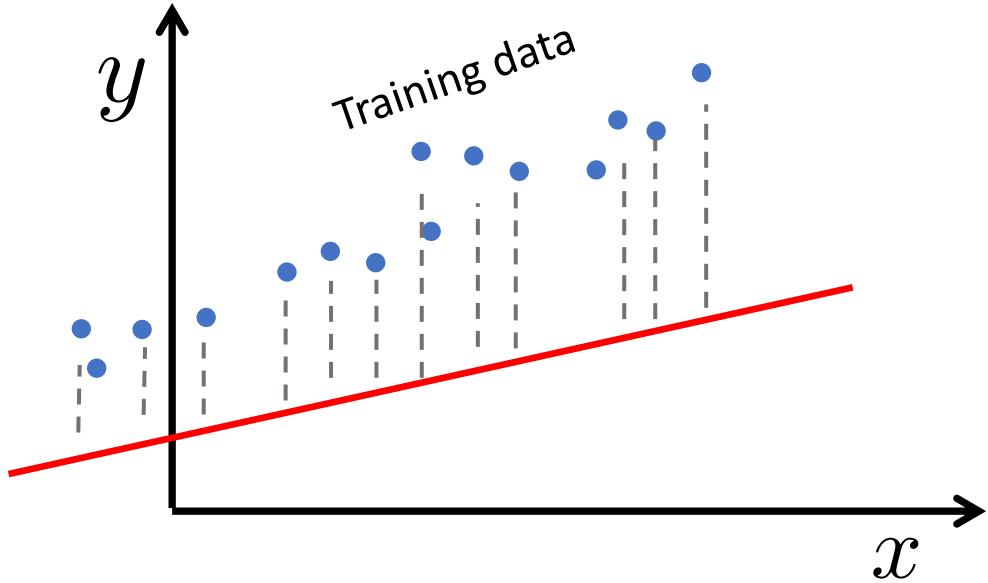
$$\theta^* = (X^T X)^{-1} X^T Y$$

Where:

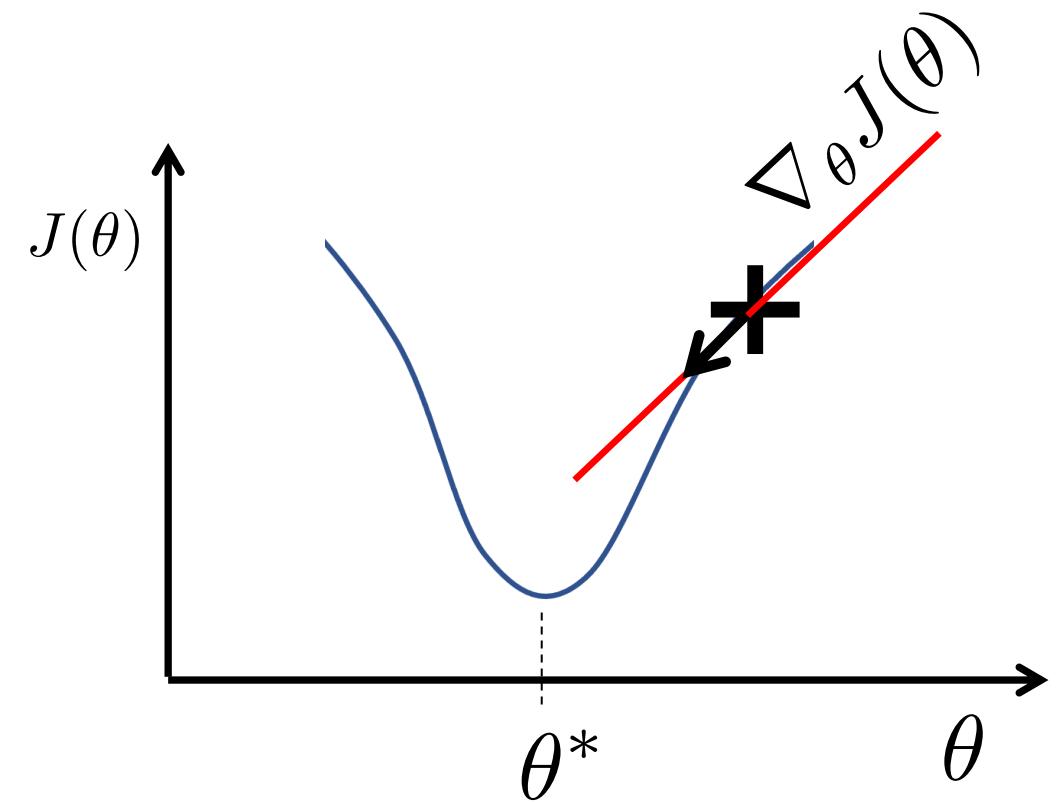
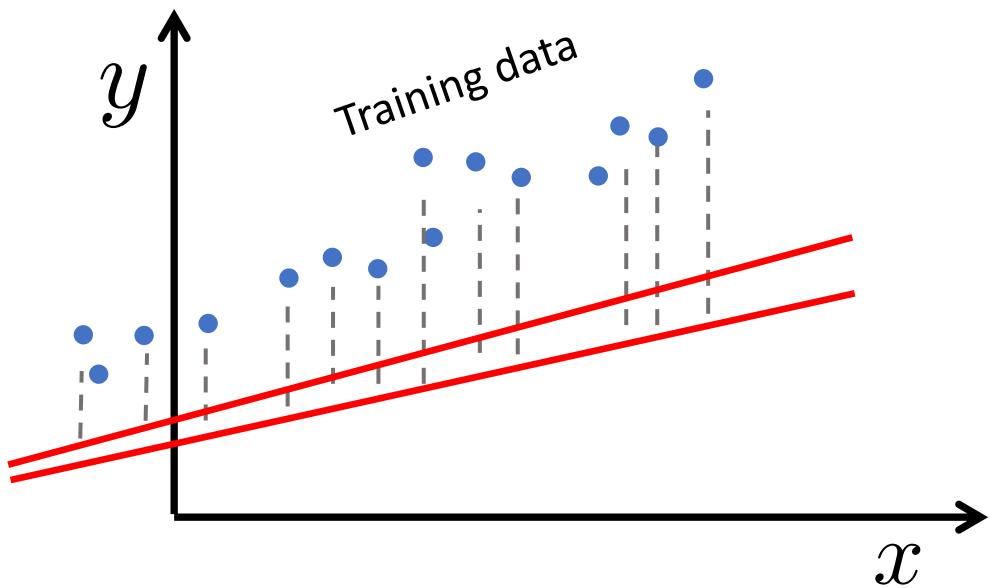
$$X = [x^{(1)}, x^{(2)}, \dots, x^{(D)}, 1]$$

$$\theta = [w^{(1)}, w^{(2)}, \dots, w^{(D)}, b]^T$$

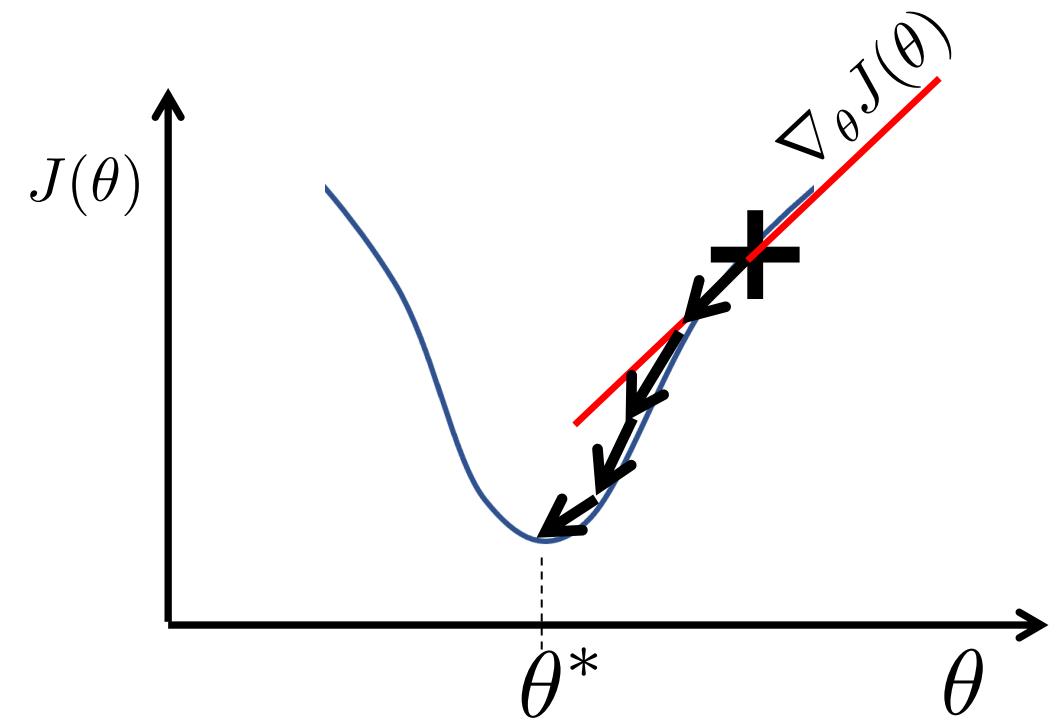
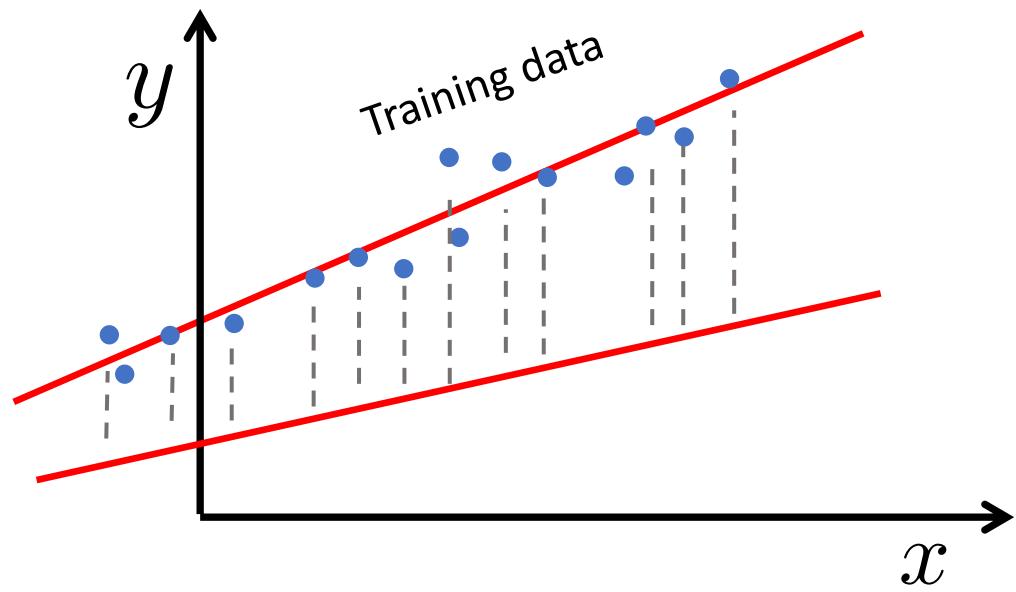
# Gradient Descent for Optimization



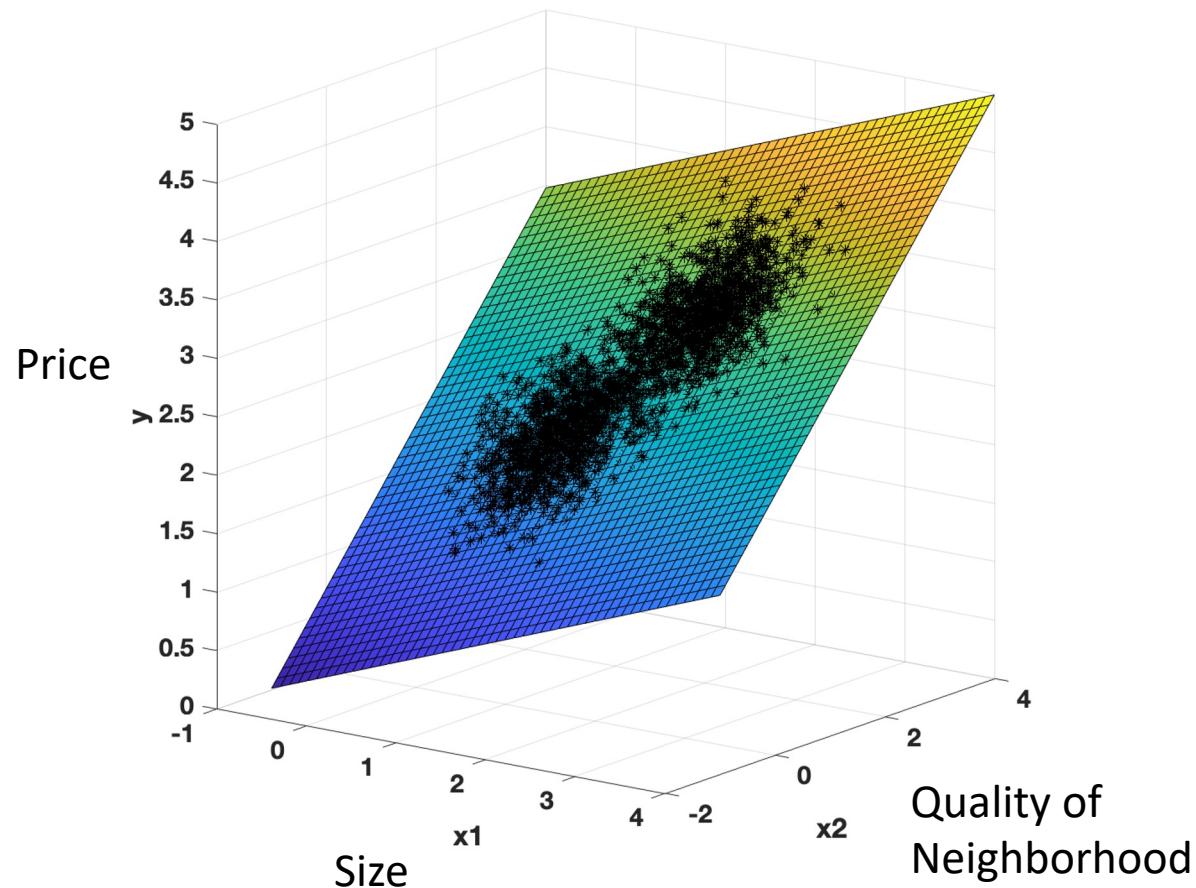
# Gradient Descent for Regression



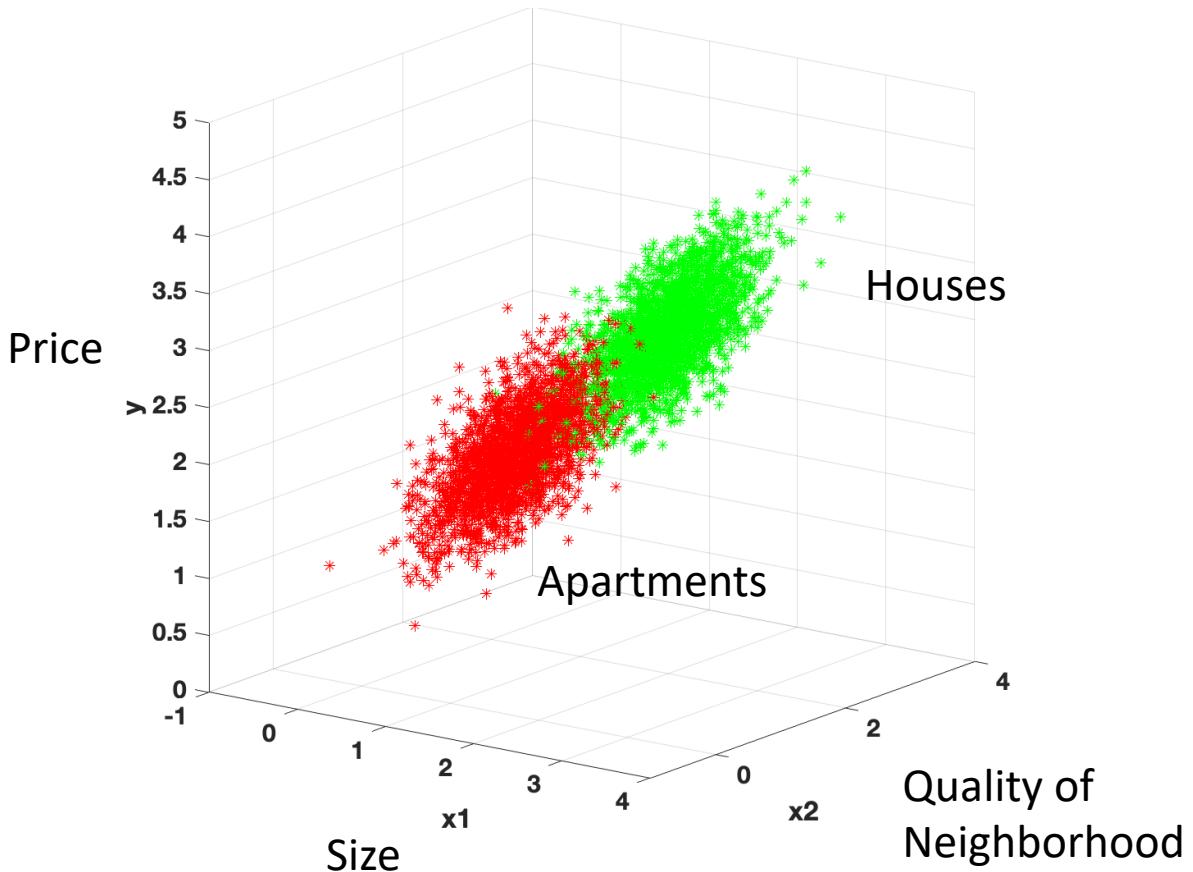
# Gradient Descent for Regression



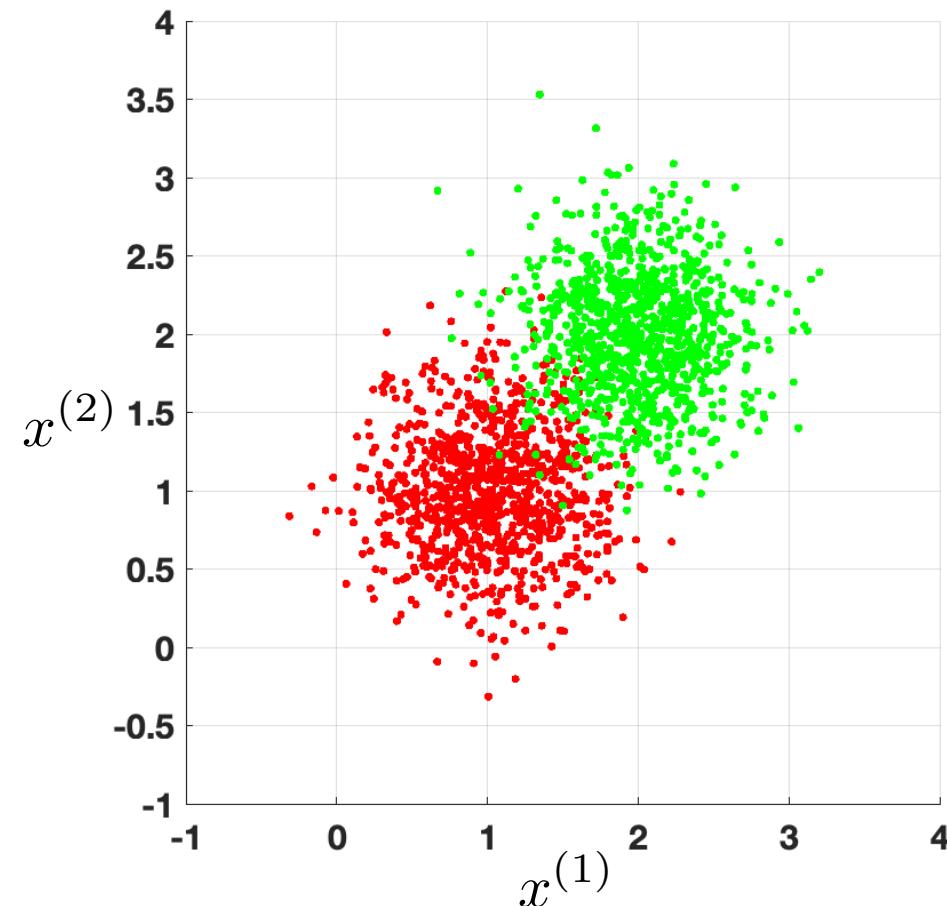
# Regression



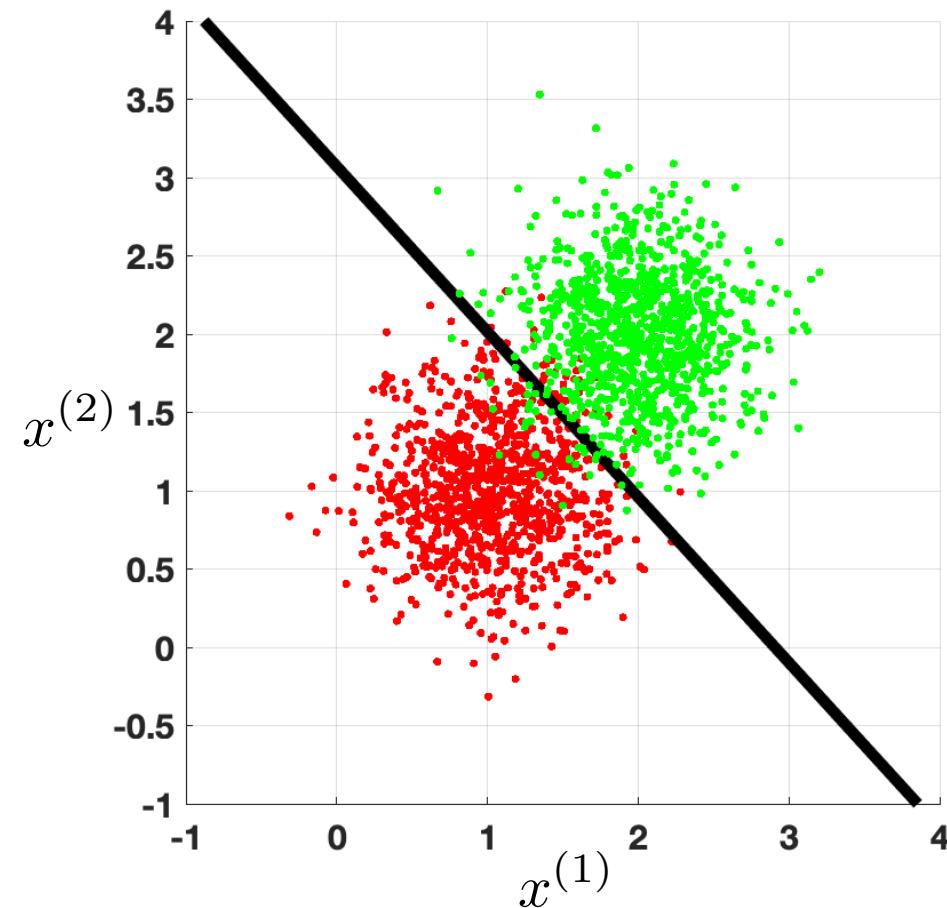
# Classification



# Classification



# Classification



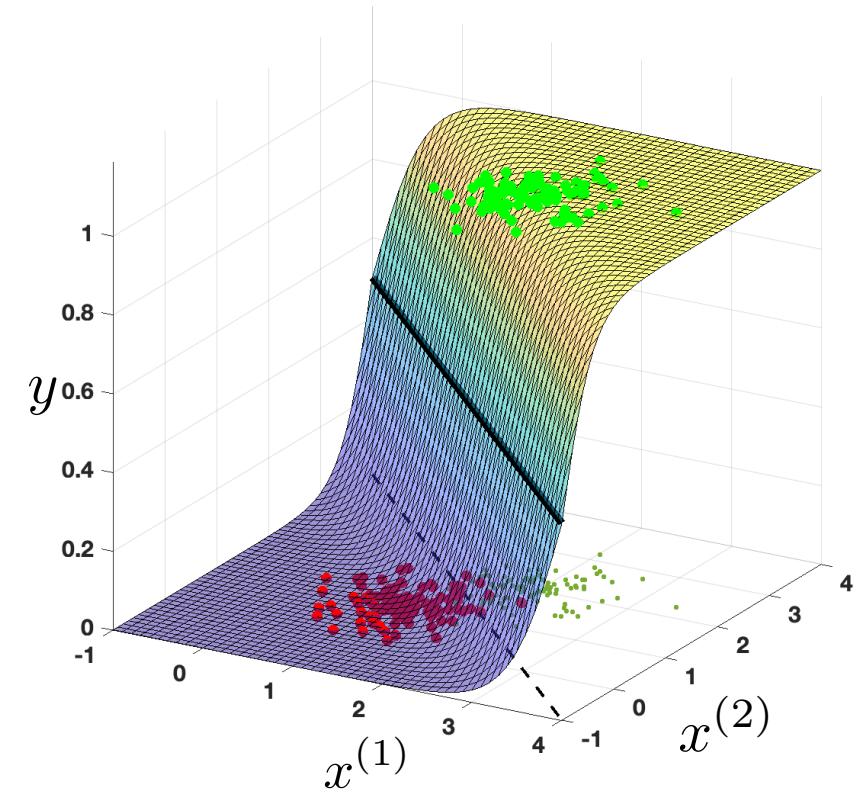
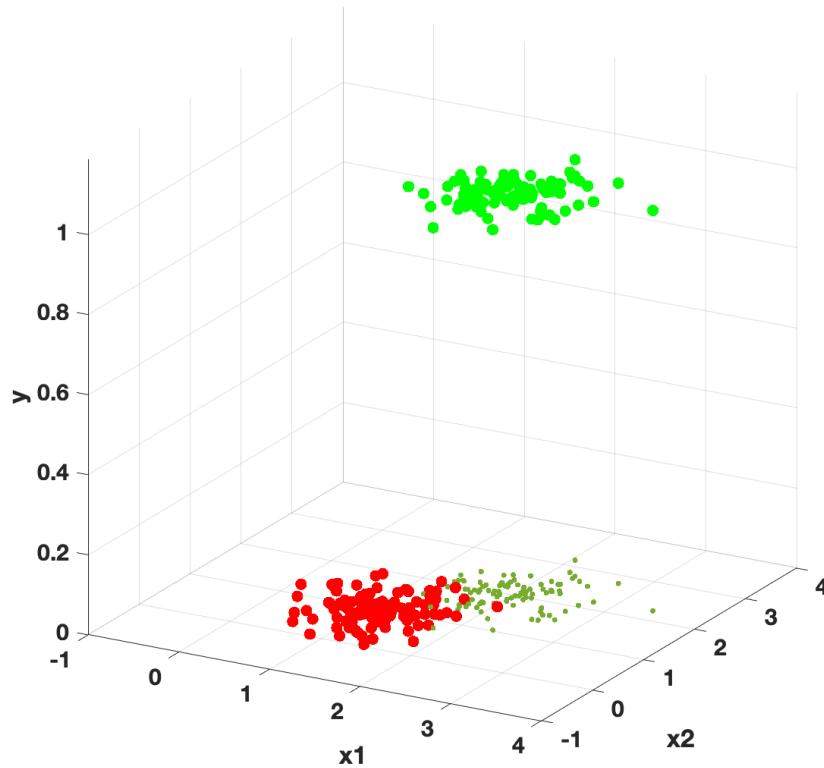
# Classification with Logistic Regression

We fit a **non-linear function** to the data.

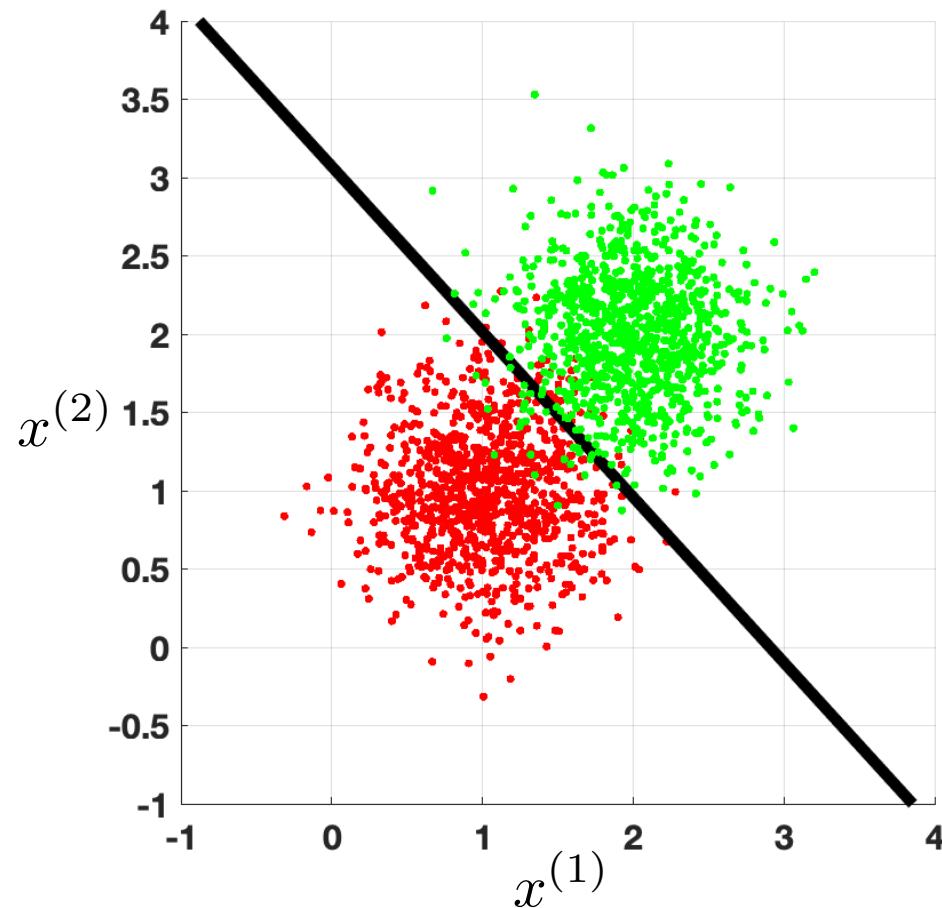
No closed form solution.

Fit with Grad Descent similar to Linear Regression.

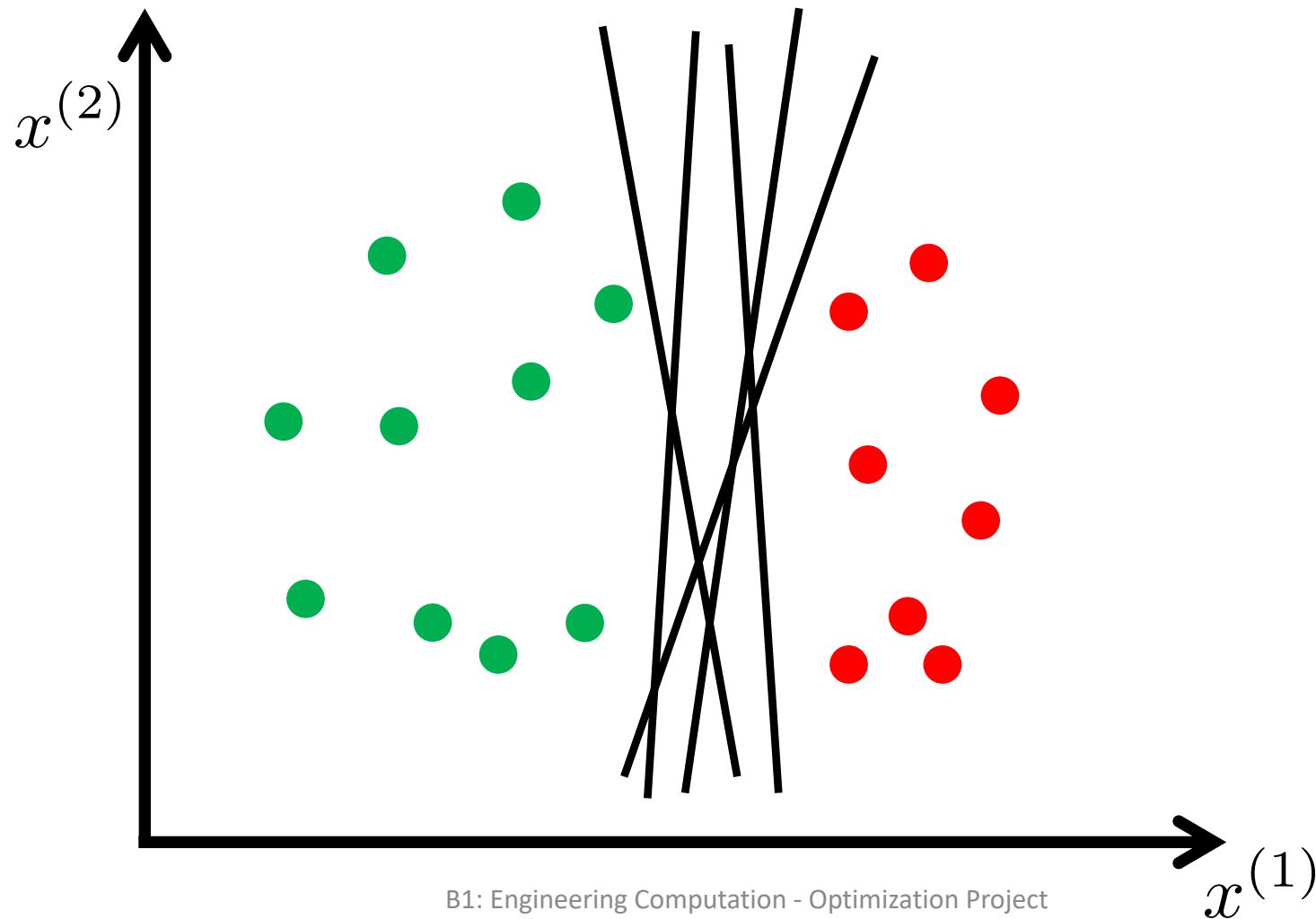
**y** is Probability  
that a sample is  
of the “green”  
class



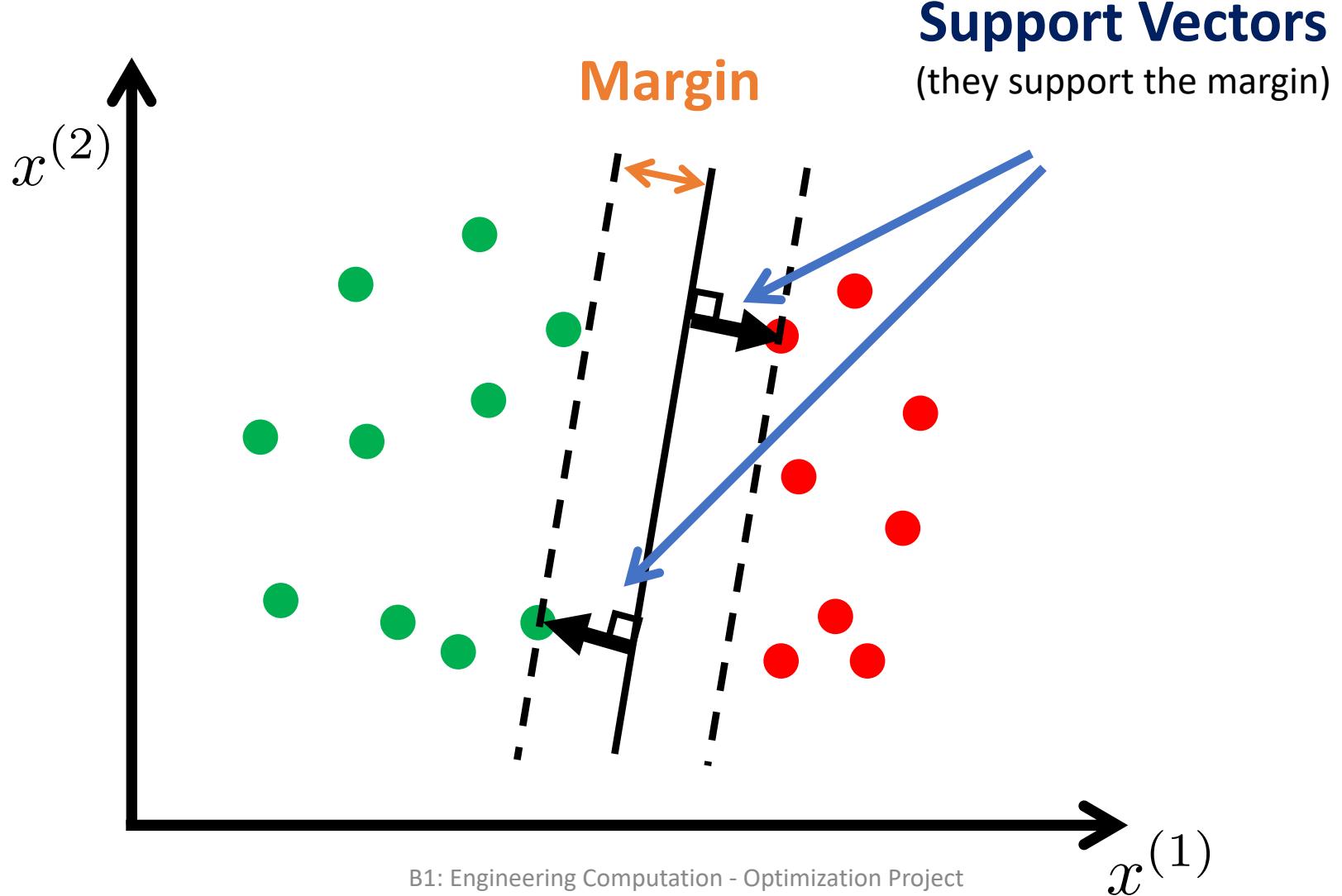
# Decision boundary of LogRegr (“from up top”)



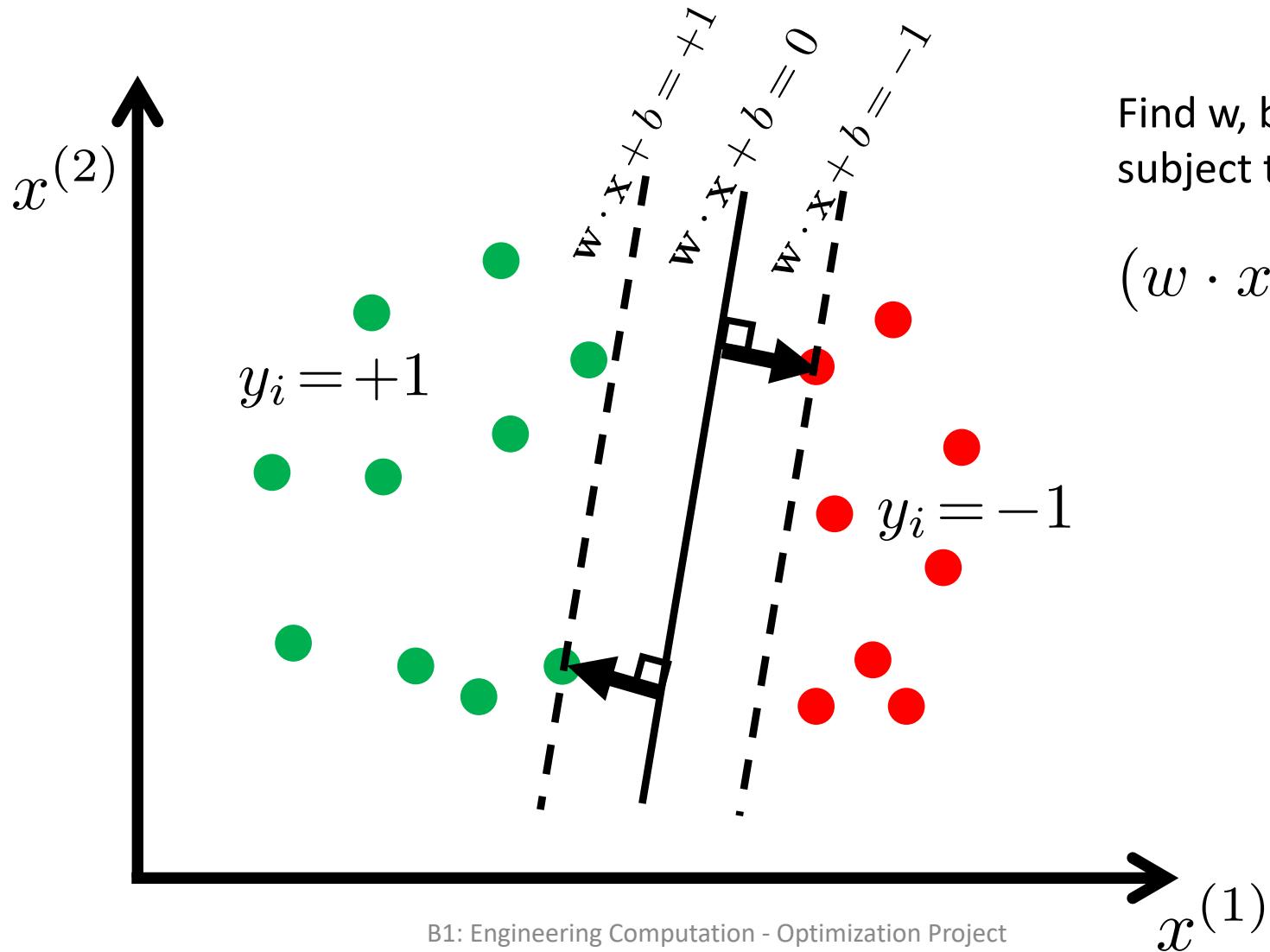
# Which Decision Boundary is Best?



# Support Vector Machine



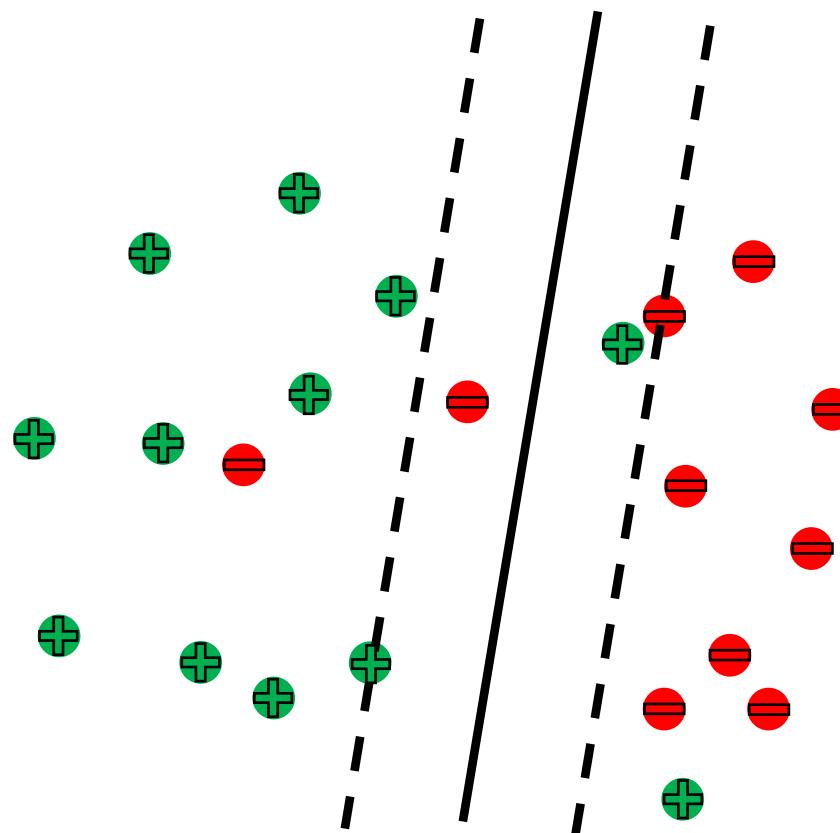
# Support Vector Machine



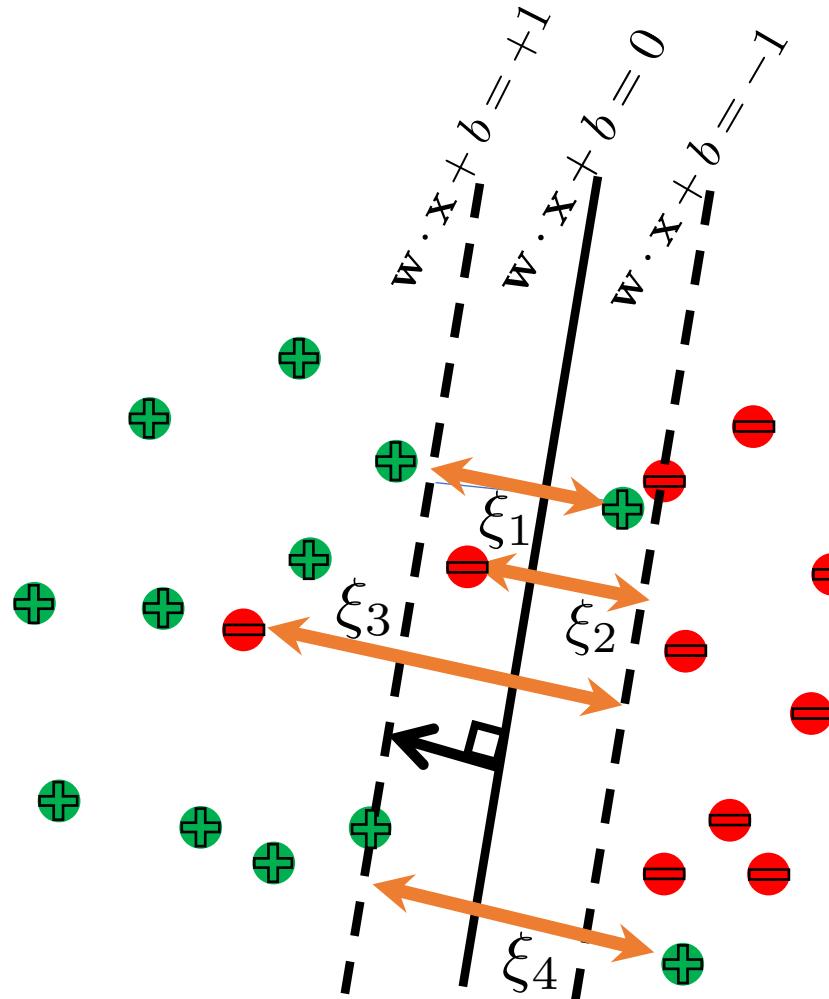
Find  $w, b$  (line)  
subject to (constraints):

$$(w \cdot x_i + b)y_i \geq 1, \forall i$$

# What if perfect linear boundary doesn't exist?

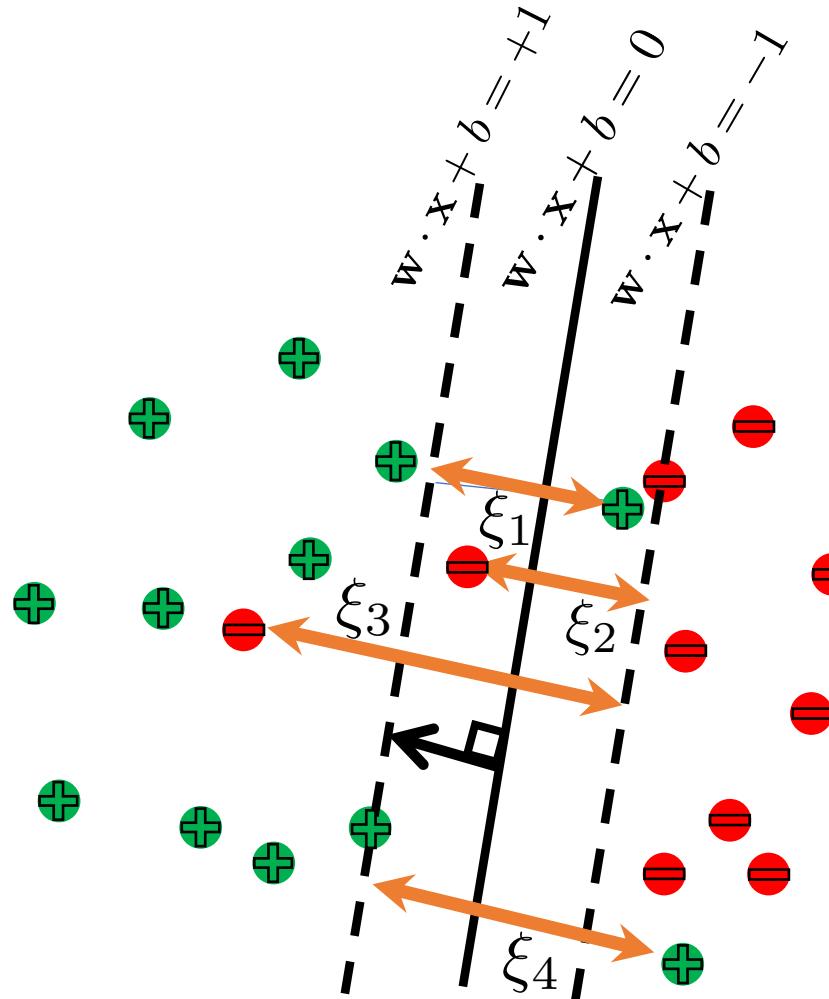


# Support Vector Machine



s.t. (subject to)  
 $(w \cdot x_i + b)y_i \geq 1 - \xi_i, \forall i$   
 $\xi_i \geq 0, \forall i$

# Support Vector Machine - Optimization



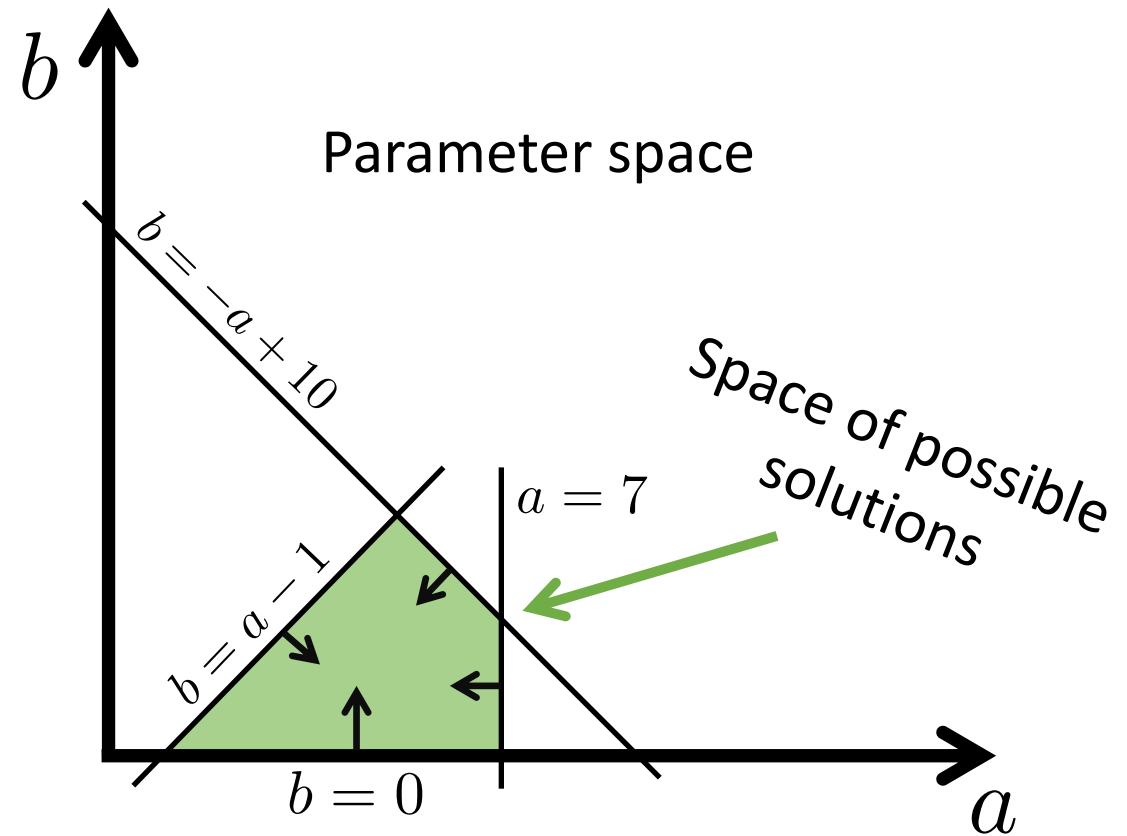
$$\begin{aligned} & \min_{w,b,\xi} \sum_i \xi_i \\ \text{s.t. (subject to)} \\ & (w \cdot x_i + b)y_i \geq 1 - \xi_i, \quad \forall i \\ & \xi_i \geq 0, \quad \forall i \end{aligned}$$

# SVM optimized with *Linear Programming*

Example of  
Linear Programming  
in 2-dimensions  
(2 parameters)

Space for feasible solutions  
from the constraints

$$\begin{aligned} & \min_{a,b} f(a,b) \\ \text{s.t. (subject to)} \\ & b < -x + 10 \\ & b < x - 1 \\ & b > 0 \\ & a < 7 \end{aligned}$$



# SVM optimized with *Linear Programming*

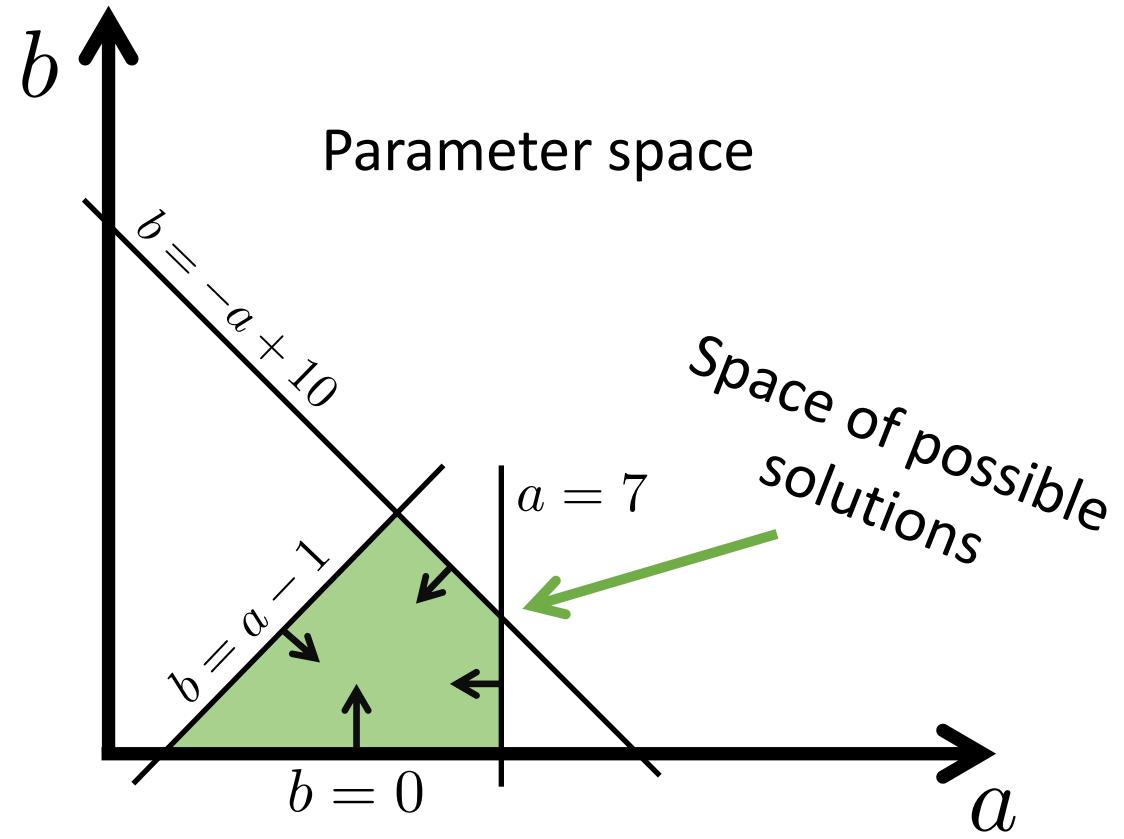
Example of  
Linear Programming  
in 2-dimensions  
(2 parameters)

Space for feasible solutions  
from the constraints

For SVMs, each data point  
gives one inequality:

$$\begin{aligned} & \min_{a,b} f(a,b) \\ \text{s.t. (subject to)} \\ & b < -x + 10 \\ & b < x - 1 \\ & b > 0 \\ & a < 7 \end{aligned}$$

$$\begin{aligned} & \min_{w,b,\xi} \sum_i \xi_i \\ \text{s.t. (subject to)} \\ & (w \cdot x_i + b)y_i \geq 1 - \xi_i, \quad \forall i \\ & \xi_i \geq 0, \quad \forall i \end{aligned}$$



# SVM via Gradient Descent

*Equivalent formulation of SVM (will be explained):*

$$\min_{w,b} \underbrace{\frac{1}{N} \sum_i^N}_{\text{Cost function}} \max(0, 1 - (wx_i + b)y_i)$$

*Hinge Loss*

*Solve with **Gradient Descent!***

# SVM via Gradient Descent

*Equivalent formulation of SVM (will be explained):*

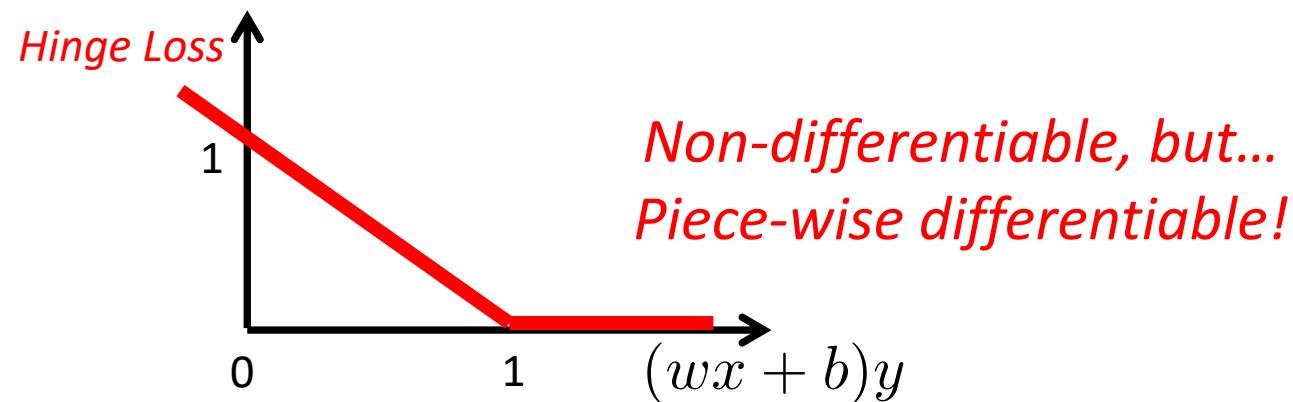
$$\min_{w,b} \frac{1}{N} \sum_i^N \max(0, 1 - (wx_i + b)y_i)$$

Cost function

*Hinge Loss*

*Solve with Gradient Descent!*

*Gradient of max(0,...) ?!?*



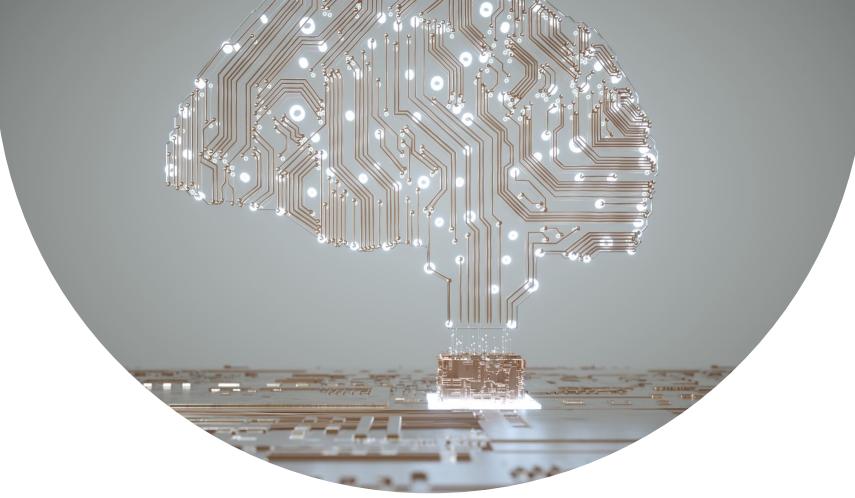
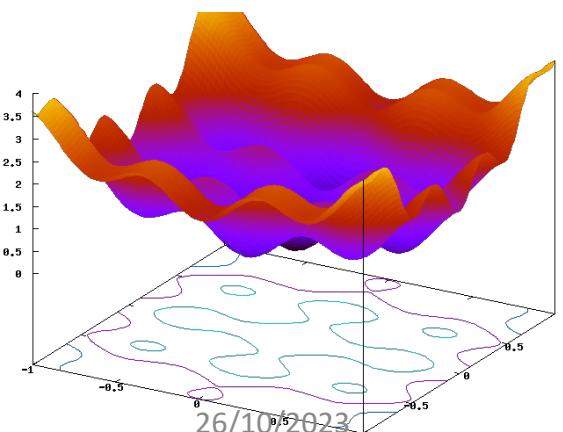
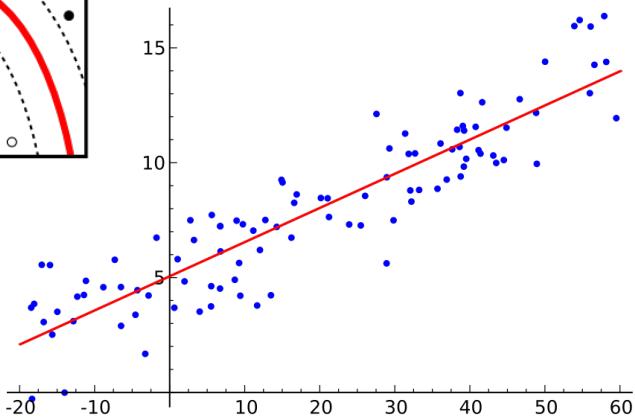
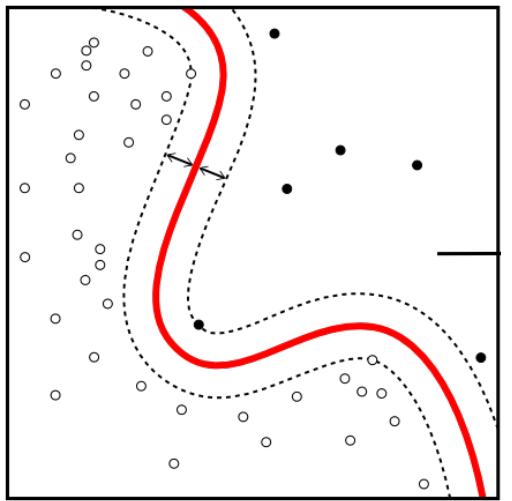
# Overview

## Regression

- Linear Regression with MSE ([B1 Numerical Algorithms](#))

## Classification

- Logistic Regression ([explained in project](#))
- Support Vector Machines ([explained in project](#))
- Optimizing with Closed-Form solution ([B1 Numerical Algorithms](#))
- Gradient Descent (and stochastic variant) ([B1 Numerical Algorithms](#))
- GD using Sub-gradients for piecewise linear cost functions ([B1 Optimization](#))
- Linear Programming ([B1 Optimization](#))
- Overfitting and generalization ([B1 Numerical Algorithms](#))
- Analysis of properties of algorithms



B1:Engineering Computation – Project MT22

# Optimization for Regression and Classification models