Linear and Logistic regression

CS21206: Foundations of AI and ML

Abir Das & Ayan Chaudhury

IIT Kharagpur

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Agenda

- Understand regression and classification with linear models.
- Understand Gradient Descent and its few variants.
- Using MLE to understand linear regression.
- Using logistic function for binary classification and estimating logistic regression parameters.

Resources

- The Elements of Statistical Learning by T Hastie, R Tibshirani, J Friedman. [Link] [Chapter 3 and 4]
- Artificial Intelligence: A Modern Approach by S Russell and P Norvig. [Link] [Chapter 19]

Linear Regression

- In a regression problem we want to find the relation between some input variables $\mathbf{x}$ and output variables y, where $\mathbf{x} \in \mathbb{R}^d$ and $y \in \mathbb{R}$.
- Inputs are also often referred to as covariates, predictors and features; while outputs are known as variates, targets and labels.
- Examples of such input-output pairs can be
  - {Outside temperature, People inside classroom, target room temperature | Energy requirement}
  - {Size, Number of Bedrooms, Number of Floors, Age of the Home | Price}

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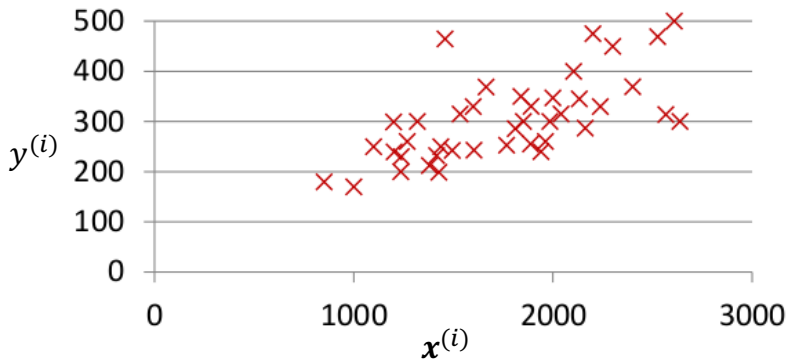
- We have a set of N observations of y as $\{y^{(1)}, y^{(2)}, \cdots, y^{(N)}\}$ and the corresponding input variables $\{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \cdots, \mathbf{x}^{(N)}\}$.



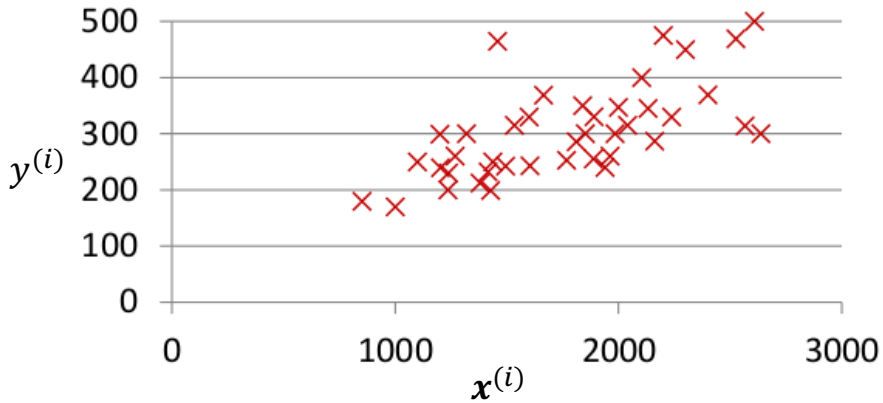
Linear Regression

- The input and output variables are assumed to be related via a relation, known as hypothesis. $\widehat{y} = h_{\boldsymbol{\theta}}(\mathbf{x})$, where $\boldsymbol{\theta}$ is the parameter vector.
- The goal is to predict the output variable $\widehat{y^*} = f(\mathbf{x}^*)$ for an arbitrary value of the input variable $\mathbf{x}^*$.
- However, let us start with scalar inputs (x) and scalar outputs (y).

Univariate Linear Regression

- hypothesis: $h_{\boldsymbol{\theta}}(x) = \theta_0 + \theta_1 x$.
- Cost Function: Sum of squared errors.

$$J(\theta_0, \theta_1) = \frac{1}{2N} \sum_{i=1}^{N} \left(h_{\boldsymbol{\theta}}(x^{(i)}) - y^{(i)} \right)^2$$



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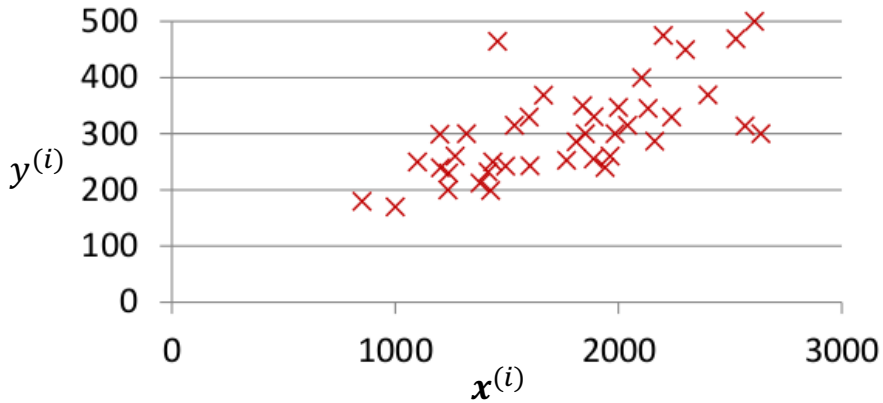

- Optimization objective: find model parameters (θ_0, θ_1) that will minimize the sum of squared errors.
- Machine learning involves optimization (minimization/maximization) in many contexts.
- The goal is to find parameters $\boldsymbol{\theta}$ of a hypothesis that significantly reduce a cost function or objective function $J(\boldsymbol{\theta})$.
- Its easy to spend a semester on optimization. Thus, we will very briefly scratch the surface to the level we need it here.

Machine Learning and Optimization

- In learning we care about some performance measure P (*e.g.*, image classification accuracy, language translation accuracy *etc.*) on test set, but we minimize a different cost function $J(\boldsymbol{\theta})$ on training set, with the hope that doing so will improve P.
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- Gradient based optimization is the most popular way for training Machine Learning Models.
- But before going there, a quick brush-up of Vector/Matrix Calculus.

Vector/Matrix Calculus

§ **Gradient:** If $f(\mathbf{x}) \in \mathbb{R}$ and $\mathbf{x} \in \mathbb{R}^n$, then the gradient of $f(\mathbf{x})$ is defined as:

$$\nabla_{\mathbf{x}} f \triangleq \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \cdots & \frac{\partial f}{\partial x_n} \end{bmatrix}^T$$

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- **Jacobian Matrix:** If $\mathbf{f}(\mathbf{x}) = [f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_m(\mathbf{x})]^T \in \mathbb{R}^m$ and $\mathbf{x} \in \mathbb{R}^n$, then the Jacobian matrix of $\mathbf{f}(\mathbf{x})$ w.r.t. $\mathbf{x}$ is:

$$\nabla_{\mathbf{x}} \mathbf{f} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \dots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \dots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & \dots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}_{m \times n}$$

Vector/Matrix Calculus

- If $f(\mathbf{x}) \in \mathbb{R}$ and $\mathbf{x} \in \mathbb{R}^n$, then the **Hessian matrix** of $f(\mathbf{x})$ w.r.t. $\mathbf{x}$ is defined as:

$$\nabla^2_{\mathbf{x}} f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}_{n \times n}$$

- Note: The Hessian captures the second-order curvature of the function.

Standard Results: Linear & Quadratic Forms

Here are some standard derivative results you will use frequently:

- **Derivative of Dot Product:**

$$\frac{\partial}{\partial \mathbf{x}}(\mathbf{b}^T\mathbf{x}) = \frac{\partial}{\partial \mathbf{x}}(\mathbf{x}^T\mathbf{b}) = \mathbf{b}$$

- **Derivative of Linear Transformation:**

$$\frac{\partial}{\partial \mathbf{x}}(\mathbf{A}\mathbf{x}) = \mathbf{A}$$

- **Derivative of Quadratic Form:**

$$\frac{\partial}{\partial \mathbf{x}}(\mathbf{x}^T\mathbf{A}\mathbf{x}) = (\mathbf{A} + \mathbf{A}^T)\mathbf{x}$$

- **Special Case (Symmetric A):**

$$\text{If } \mathbf{A} = \mathbf{A}^T, \quad \frac{\partial}{\partial \mathbf{x}}(\frac{1}{2}\mathbf{x}^T\mathbf{A}\mathbf{x}) = \mathbf{A}\mathbf{x}$$

Standard Results: Product and Chain Rules

Product Rule: For $\mathbf{u} \in \mathbb{R}^m, \mathbf{v} \in \mathbb{R}^m, \mathbf{x} \in \mathbb{R}^n$:

$$\left[\frac{\partial(\mathbf{u}^T\mathbf{v})}{\partial \mathbf{x}}\right]^T_{1\times n} = [\mathbf{u}^T]_{1\times m}\left[\frac{\partial \mathbf{v}}{\partial \mathbf{x}}\right]_{m\times n} + [\mathbf{v}^T]_{1\times m}\left[\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\right]_{m\times n}$$

Chain rule - Scalar Function of Scalar Function: If $F(f(\mathbf{x})) \in \mathbb{R}$, $f(\mathbf{x}) \in \mathbb{R}$, and $\mathbf{x} \in \mathbb{R}^n$:

$$\left[\frac{\partial F}{\partial \mathbf{x}}\right]_{n\times 1} = \left[\frac{\partial f}{\partial \mathbf{x}}\right]_{n\times 1}\left[\frac{\partial F}{\partial f}\right]_{1\times 1}$$

Chain rule - Scalar Function of Vector Function: If $F(\mathbf{f}(\mathbf{x})) \in \mathbb{R}$, $\mathbf{f}(\mathbf{x}) \in \mathbb{R}^m$, and $\mathbf{x} \in \mathbb{R}^n$:

$$\left[\frac{\partial F}{\partial \mathbf{x}}\right]_{n\times 1} = \left[\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right]^T_{n\times m}\left[\frac{\partial F}{\partial \mathbf{f}}\right]_{m\times 1}$$

This vector chain rule is the foundation of Backpropagation!

Derivatives of Norms

These results are crucial for understanding Regularization (L2 norm) and Matrix Factorization.

Squared L2 Norm (Vector)

$$\frac{\partial}{\partial \mathbf{x}}||\mathbf{x}||_2^2 = \frac{\partial}{\partial \mathbf{x}}(\mathbf{x}^T\mathbf{x}) = 2\mathbf{x}$$

Squared Frobenius Norm (Matrix)

$$\frac{\partial}{\partial \mathbf{X}}||\mathbf{X}||_F^2 = \frac{\partial}{\partial \mathbf{X}}\text{tr}(\mathbf{X}\mathbf{X}^T) = 2\mathbf{X}$$

Finding Optimum

- Optimization Problem Statement:

$$\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \quad \text{subject to } \boldsymbol{\theta} \in \boldsymbol{\Theta}$$

- We are after that $\boldsymbol{\theta}$ which gives the minimum value of the cost function $J(\boldsymbol{\theta})$.

Finding Optimum

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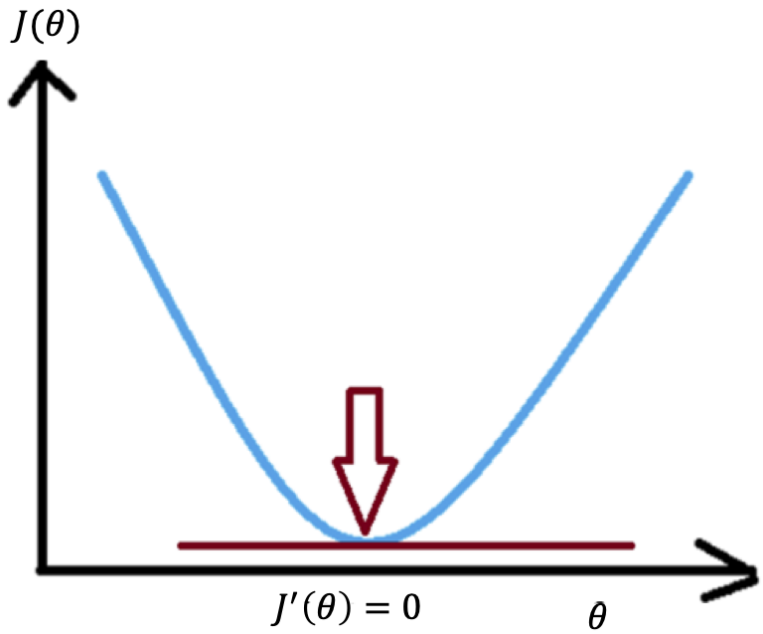
- We are after that $\boldsymbol{\theta}$ which gives the minimum value of the cost function $J(\boldsymbol{\theta})$.
- For scalar θ, the condition boils down to $\frac{\partial J}{\partial \theta} = 0$.
- For higher dimensional $\boldsymbol{\theta}$, the condition boils down to,



$$\nabla_{\boldsymbol{\theta}} J = \mathbf{0}$$

$$\begin{bmatrix} \frac{\partial J}{\partial \theta_1} & \frac{\partial J}{\partial \theta_2} & \cdots & \frac{\partial J}{\partial \theta_n} \end{bmatrix}^T = \mathbf{0}$$

One Way to Find Minima – Gradient Descent

- This is helpful but not always useful.
- For example $J(\boldsymbol{\theta}) = \log \sum_{i=1}^{m} e^{(\mathbf{a}_i^T \boldsymbol{\theta} + b_i)}$ is a convex function with clear minima.
- But finding analytical solution is not easy.

$$\nabla_{\boldsymbol{\theta}} J = \mathbf{0}$$

$$\frac{1}{\sum_{i=1}^{m} e^{(\mathbf{a}_i^T \boldsymbol{\theta} + b_i)}} \sum_{i=1}^{m} e^{(\mathbf{a}_i^T \boldsymbol{\theta} + b_i)} \mathbf{a}_i = \mathbf{0}$$

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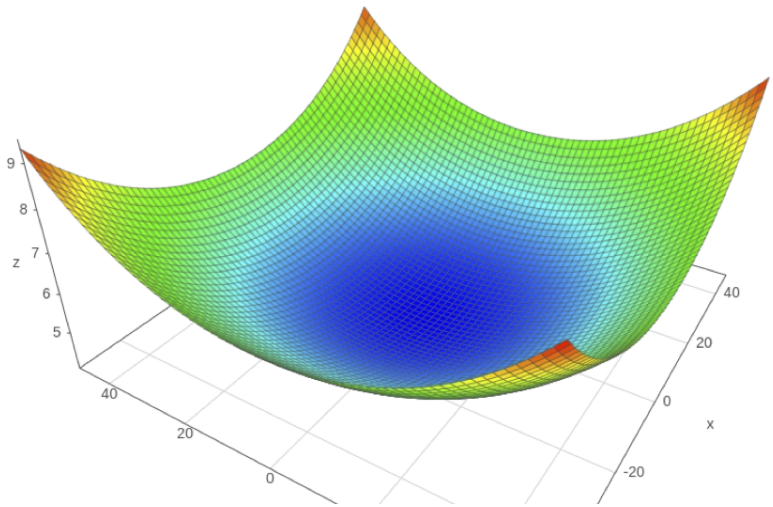

- So, a numerical iterative solution is sought for.

One Way to Find Minima – Gradient Descent

- Start with an initial guess $\boldsymbol{\theta}^0$.
- Repeatedly update $\boldsymbol{\theta}$ by taking a small step: $\boldsymbol{\theta}^k = \boldsymbol{\theta}^{k-1} + \eta\Delta\boldsymbol{\theta} \quad \cdots$ (a)
- so that $J(\boldsymbol{\theta})$ gets smaller with each update: $J(\boldsymbol{\theta}^k) \leq J(\boldsymbol{\theta}^{(k-1)}) \quad \cdots$ (b)

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\begin{aligned}
J(\boldsymbol{\theta}^k) &= J(\boldsymbol{\theta}^{k-1} + \eta\Delta\boldsymbol{\theta}) \\
&= J(\boldsymbol{\theta}^{k-1}) + \eta(\Delta\boldsymbol{\theta})^T J'(\boldsymbol{\theta}^{k-1}) + h.o.t. \text{ [Using Taylor series expansion]} \\
&\approx J(\boldsymbol{\theta}^{k-1}) + \eta(\Delta\boldsymbol{\theta})^T J'(\boldsymbol{\theta}^{k-1}) \text{ [neglecting h.o.t.]} \quad \cdots \text{(c)}
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- Combining (b) and (c), $\eta(\Delta\boldsymbol{\theta})^T J'(\boldsymbol{\theta}^{k-1}) \leq 0$ *i.e.*, $(\Delta\boldsymbol{\theta})^T J'(\boldsymbol{\theta}^{k-1}) \leq 0$, as η is positive.

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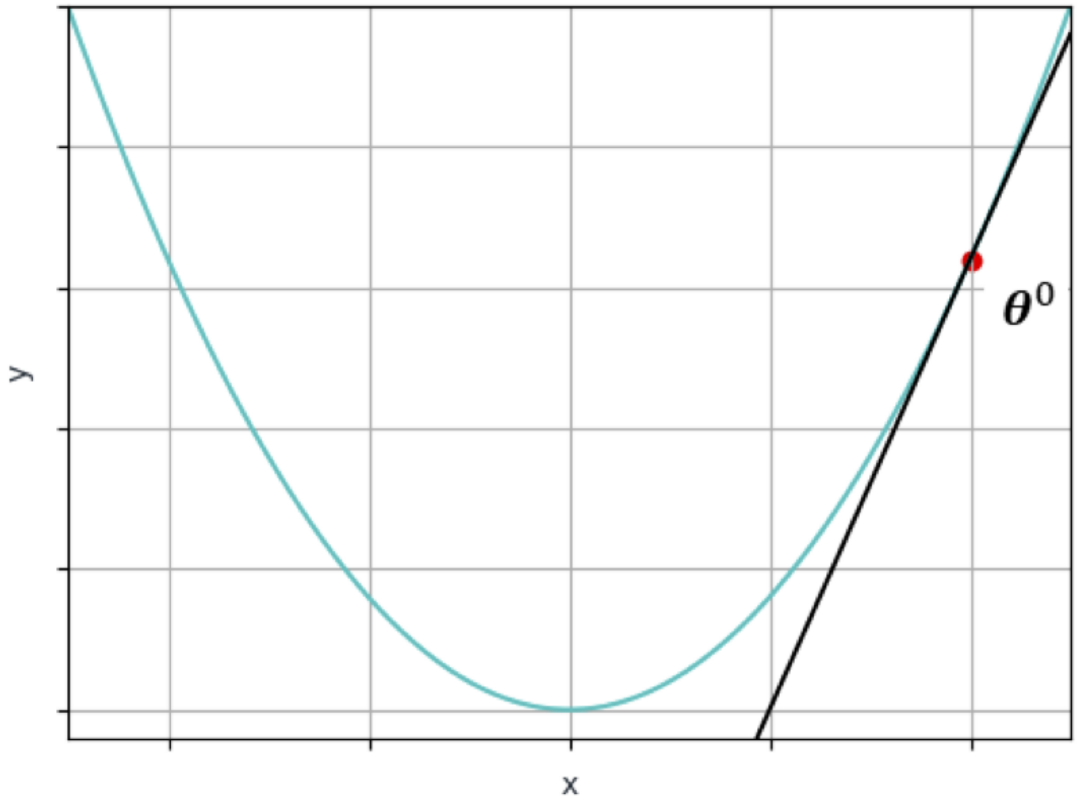
- So, for $\boldsymbol{\theta}$ to minimize $J(\boldsymbol{\theta})$, *i.e.*, to satisfy (b) we have to choose some $\Delta\boldsymbol{\theta}$ that gives a negative dot product when multiplied with $J'(\boldsymbol{\theta}^{k-1})$.
- Then why not choose, $\Delta\boldsymbol{\theta} = -J'(\boldsymbol{\theta}^{k-1})$.
- Then, $(\Delta\boldsymbol{\theta})^T J'(\boldsymbol{\theta}^{k-1}) = -||J'(\boldsymbol{\theta}^{k-1})||_2^2$ surely is a negative quantity and satisfies the condition.

Gradient Descent

- Start with an initial guess $\boldsymbol{\theta}^0$.
- Repeatedly update $\boldsymbol{\theta}$ by taking a small step: $\boldsymbol{\theta}^k = \boldsymbol{\theta}^{k-1} - \eta J'(\boldsymbol{\theta}^{k-1})$, until convergence [$J'(\boldsymbol{\theta}^{k-1})$ is very small].



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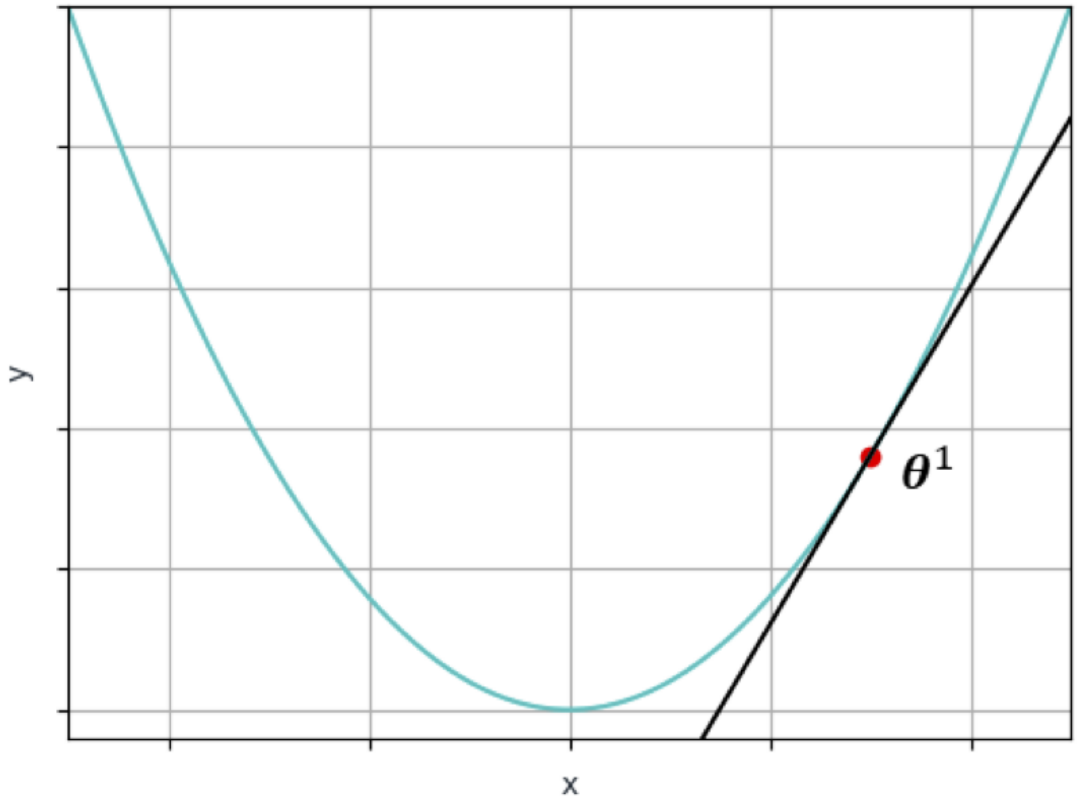

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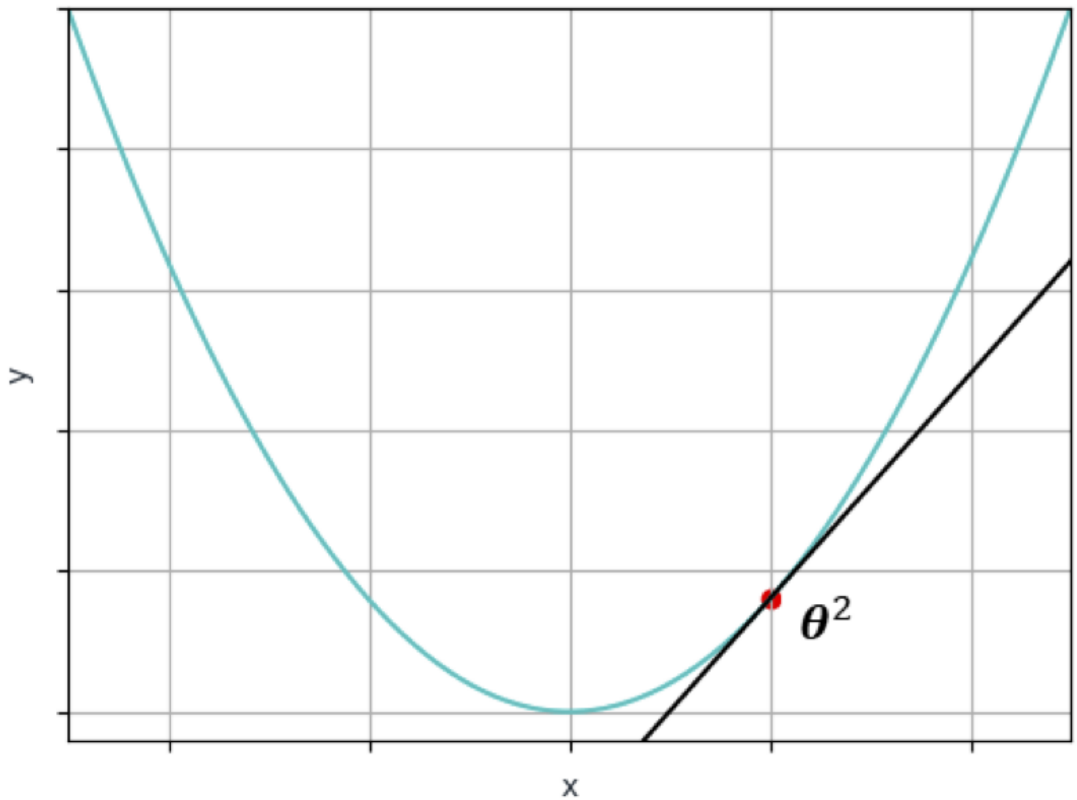

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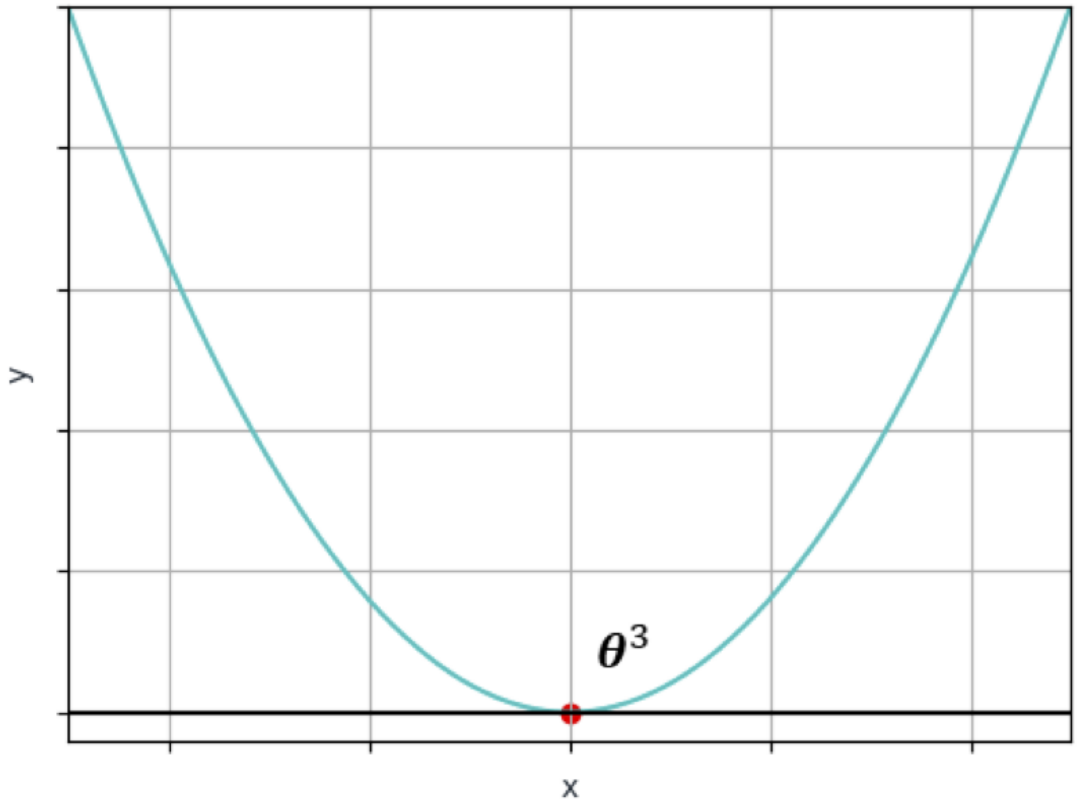
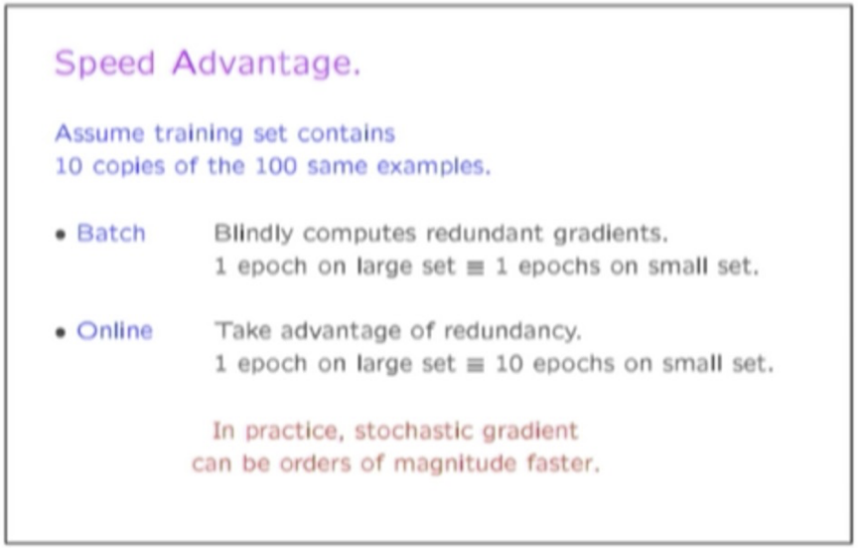


But Imagine This



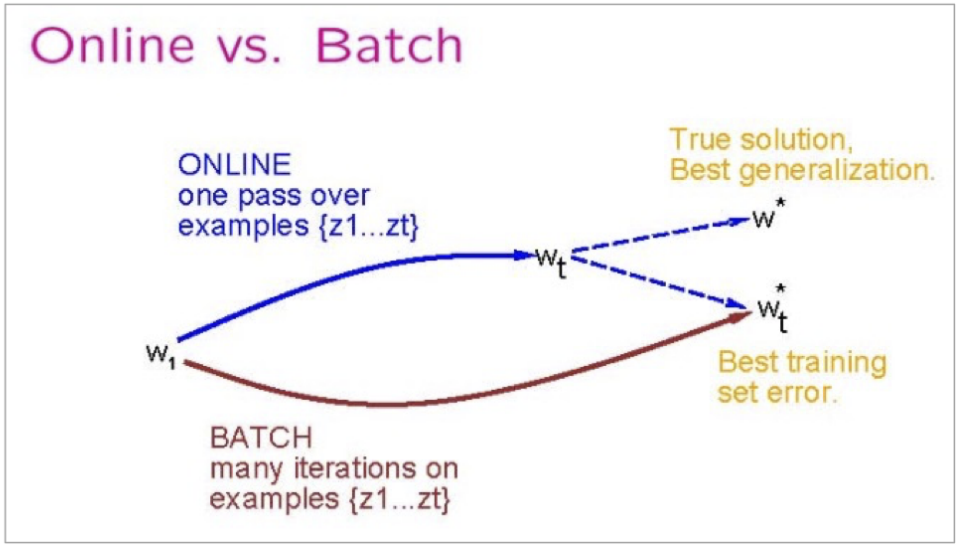


Figure credit: *Olivier Bousquet's talk at NeurIPS 2018 after winning Test of Time Award for NIPS 2007 paper:*

"The Trade Offs of Large Scale Learning" by Leon Bottou and Olivier Bousquet.

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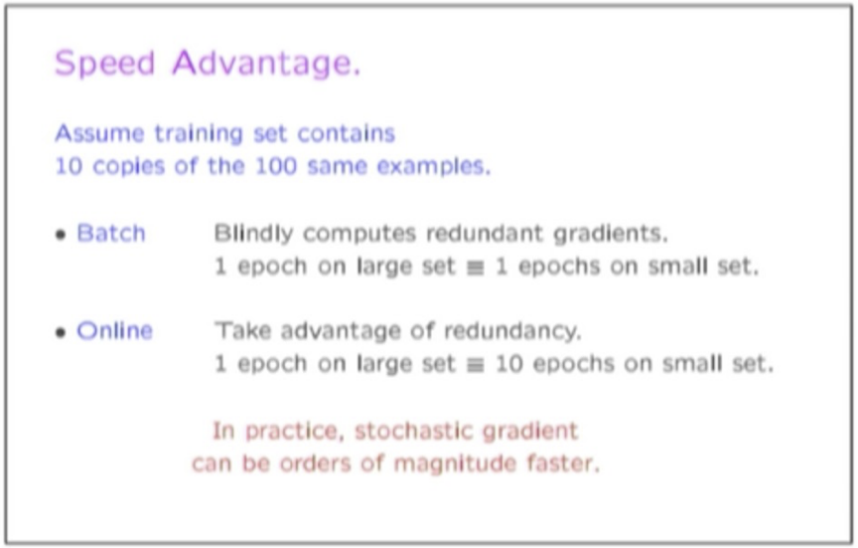

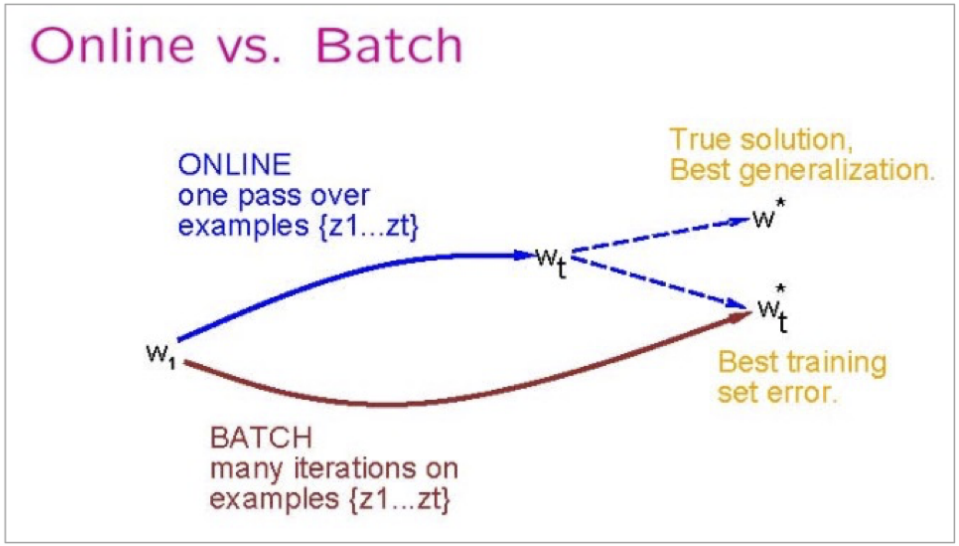

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- Optimization algorithms that use the entire training set to compute the gradient are called batch or deterministic gradient methods. Ones that use a single training example for that task are called stochastic or online gradient methods
- Most of the algorithms we use for machine learning fall somewhere in between!
- These are called minibatch or minibatch stochastic methods.

Batch, Stochastic and Mini-batch Stochastic Gradient Descent

Algorithm 1 Batch Gradient Descent at Iteration k

Require: Learning rate ϵ_k

Require: Initial Parameter θ

while stopping criteria not met **do**

  Compute gradient estimate over N examples:

  $\hat{\mathbf{g}} \leftarrow +\frac{1}{N}\nabla_\theta \sum_i L(f(\mathbf{x}^{(i)};\theta), \mathbf{y}^{(i)})$

  Apply Update: $\theta \leftarrow \theta - \epsilon\hat{\mathbf{g}}$

end while

Algorithm 2 Stochastic Gradient Descent at Iteration k

Require: Learning rate ϵ_k

Require: Initial Parameter θ

while stopping criteria not met **do**

  Sample example $(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})$ from training set

  Compute gradient estimate:

  $\hat{\mathbf{g}} \leftarrow +\nabla_\theta L(f(\mathbf{x}^{(i)};\theta), \mathbf{y}^{(i)})$

  Apply Update: $\theta \leftarrow \theta - \epsilon\hat{\mathbf{g}}$

end while

Mini-batch

Algorithm 8.1 Stochastic gradient descent (SGD) update at training iteration k

Require: Learning rate ϵ_k.

Require: Initial parameter $\boldsymbol{\theta}$

while stopping criterion not met **do**

  Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.

  Compute gradient estimate: $\hat{\boldsymbol{g}} \leftarrow +\frac{1}{m}\nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)};\boldsymbol{\theta}), \boldsymbol{y}^{(i)})$

  Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \epsilon\hat{\boldsymbol{g}}$

end while

Figure credit: *Shubhendu Trivedi et al., Goodfellow et al.*

Coming Back to Univariate Linear Regression

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- Cost Function: Sum of squared errors.

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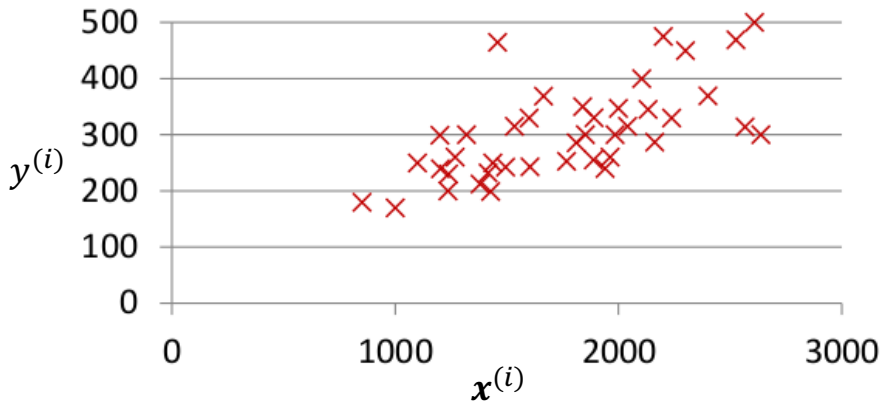

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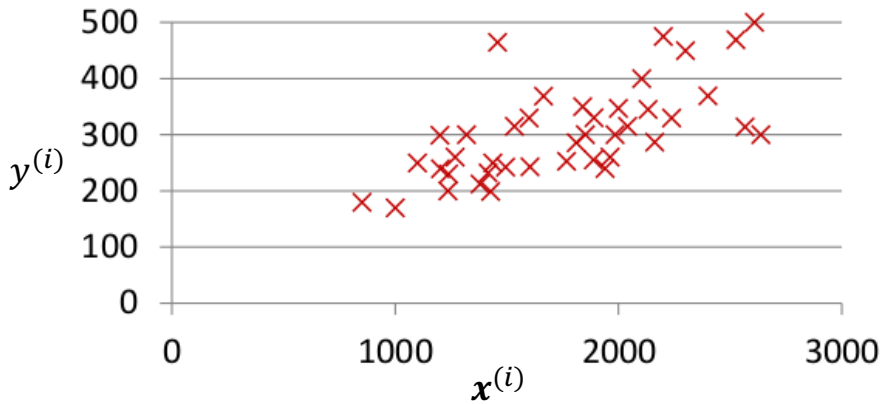

- Optimization objective: find model parameters (θ_0, θ_1) that will minimize the sum of squared errors.
- Gradient of the cost function w.r.t. θ_0:

$$\frac{J(\theta_0, \theta_1)}{\theta_0} = \frac{1}{N} \sum_{i=1}^{N} \left(h_{\boldsymbol{\theta}}(x^{(i)}) - y^{(i)} \right)$$

- Gradient of the cost function w.r.t. θ_1:

$$\frac{J(\theta_0, \theta_1)}{\theta_1} = \frac{1}{N} \sum_{i=1}^{N} \left(h_{\boldsymbol{\theta}}(x^{(i)}) - y^{(i)} \right) x^{(i)}$$

- Apply your favorite gradient based optimization algorithm.

Univariate Linear Regression

§ These being linear equations of $\boldsymbol{\theta}$, have a unique closed form solution too.

$$\theta_1 = \frac{N\sum_{i=1}^{N} y^{(i)}x^{(i)} - \left(\sum_{i=1}^{N} x^{(i)}\right)\left(\sum_{i=1}^{N} y^{(i)}\right)}{N\sum_{i=1}^{N}\left(x^{(i)}\right)^2 - \left(\sum_{i=1}^{N} x^{(i)}\right)^2}$$

$$\theta_0 = \frac{1}{N}\left\{\sum_{i=1}^{N} y^{(i)} - \theta_1 \sum_{i=1}^{N} x^{(i)}\right\}$$

Multivariate Linear Regression

- We can easily extend to multivariate linear regression problems, where $\mathbf{x} \in \mathbb{R}^d$
- hypothesis: $h_{\boldsymbol{\theta}}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_d x_d$. For convenience of notation, define $x_0 = 1$.
- Thus h is simply the dot product of the parameters and the input vector.

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta}^T \mathbf{x}$$

- Cost Function: Sum of squared errors.

$$J(\boldsymbol{\theta}) = J(\theta_0, \theta_1, \cdots, \theta_d) = \frac{1}{2N} \sum_{i=1}^{N} \left(\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)} \right)^2 \tag{1}$$

- We will use the following to write the cost function in a compact matrix vector notation

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta}^T \mathbf{x} = \mathbf{x}^T \boldsymbol{\theta}$$

Multivariate Linear Regression

$$\begin{bmatrix} \widehat{y}^{(1)} \\ \widehat{y}^{(2)} \\ \vdots \\ \widehat{y}^{(N)} \end{bmatrix} = \begin{bmatrix} h_\theta(\mathbf{x^{(1)}}) \\ h_\theta(\mathbf{x^{(2)}}) \\ \vdots \\ h_\theta(\mathbf{x^{(N)}}) \end{bmatrix} = \begin{bmatrix} \mathbf{x}_0^{(1)} & \mathbf{x}_1^{(1)} & \mathbf{x}_2^{(1)} & \cdots & \mathbf{x}_d^{(1)} \\ \mathbf{x}_0^{(2)} & \mathbf{x}_1^{(2)} & \mathbf{x}_2^{(2)} & \cdots & \mathbf{x}_d^{(2)} \\ \vdots & \vdots & \ddots & \vdots & \\ \mathbf{x}_0^{(N)} & \mathbf{x}_1^{(N)} & \mathbf{x}_2^{(N)} & \cdots & \mathbf{x}_d^{(N)} \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_d \end{bmatrix} \tag{2}$$

$$\widehat{\mathbf{y}} = \mathbf{X}\boldsymbol{\theta}$$

Here, $\mathbf{X}$ is a $N \times (d+1)$ matrix with each row an input vector. $\widehat{\mathbf{y}}$ is a N length vector of the outputs in the training set.

Multivariate Linear Regression

§ Eqn. (1), gives,

$$J(\boldsymbol{\theta}) = \frac{1}{2N}\sum_{i=1}^{N}\left(\boldsymbol{\theta}^T\mathbf{x}^{(i)} - y^{(i)}\right)^2 = \frac{1}{2N}\sum_{i=1}^{N}\left(\widehat{y}^{(i)} - y^{(i)}\right)^2 \tag{3}$$

$$= \frac{1}{2N}||\widehat{\mathbf{y}} - \mathbf{y}||_2^2 = \frac{1}{2N}\left(\widehat{\mathbf{y}} - \mathbf{y}\right)^T\left(\widehat{\mathbf{y}} - \mathbf{y}\right)$$

$$= \frac{1}{2N}\left(\mathbf{X}\boldsymbol{\theta} - \mathbf{y}\right)^T\left(\mathbf{X}\boldsymbol{\theta} - \mathbf{y}\right) = \frac{1}{2N}\left\{\boldsymbol{\theta}^T\left(\mathbf{X}^T\mathbf{X}\right)\boldsymbol{\theta} - \boldsymbol{\theta}^T\mathbf{X}^T\mathbf{y} - \mathbf{y}^T\mathbf{X}\boldsymbol{\theta} + \mathbf{y}^T\mathbf{y}\right\}$$

$$= \frac{1}{2N}\left\{\boldsymbol{\theta}^T\left(\mathbf{X}^T\mathbf{X}\right)\boldsymbol{\theta} - \left(\mathbf{X}^T\mathbf{y}\right)^T\boldsymbol{\theta} - \left(\mathbf{X}^T\mathbf{y}\right)^T\boldsymbol{\theta} + \mathbf{y}^T\mathbf{y}\right\}$$

$$= \frac{1}{2N}\left\{\boldsymbol{\theta}^T\left(\mathbf{X}^T\mathbf{X}\right)\boldsymbol{\theta} - 2\left(\mathbf{X}^T\mathbf{y}\right)^T\boldsymbol{\theta} + \mathbf{y}^T\mathbf{y}\right\}$$

Multivariate Linear Regression

§ Equating the gradient of the cost function to 0,

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \frac{1}{2N}\left\{2\mathbf{X}^T\mathbf{X}\boldsymbol{\theta} - 2\mathbf{X}^T\mathbf{y} + 0\right\} = 0$$

$$\mathbf{X}^T\mathbf{X}\boldsymbol{\theta} - \mathbf{X}^T\mathbf{y} = 0$$

$$\boldsymbol{\theta} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y} \tag{4}$$

Multivariate Linear Regression

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$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \frac{1}{2N}\left\{2\mathbf{X}^T\mathbf{X}\boldsymbol{\theta} - 2\mathbf{X}^T\mathbf{y} + 0\right\} = 0$$
$$\mathbf{X}^T\mathbf{X}\boldsymbol{\theta} - \mathbf{X}^T\mathbf{y} = 0$$
$$\boldsymbol{\theta} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y} \tag{4}$$

§ This gives a closed form solution, but another option is to use iterative solution (just like the univariate case).

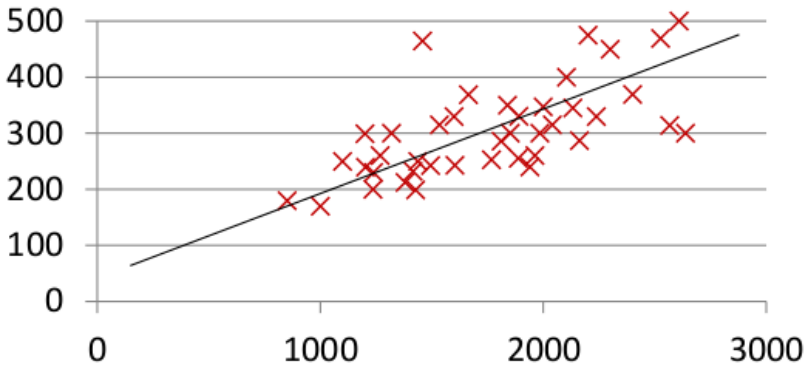
$$\frac{\partial J(\boldsymbol{\theta})}{\partial \theta_j} = \frac{1}{N}\sum_{i=1}^{N}\left(h_{\boldsymbol{\theta}}(x^{(i)}) - y^{(i)}\right)x_j^{(i)}$$

Multivariate Linear Regression

- Iterative Gradient Descent needs to perform many iterations and need to choose a stepsize parameter judiciously. But it works equally well even if the number of features (d) is large.
- For the least square solution, there is no need to choose the step size parameter or no need to iterate. But, evaluating $\left(\mathbf{X}^T\mathbf{X}\right)^{-1}$ can be slow if d is large.

Linear Regression as Maximum Likelihood Estimation

- So far we tried to fit a "straightline" ("hyperplane" to be more precise) for linear regression problem.
- This is, in a sense, a "constrained" way of looking at the problem. Datapoints may not be perfectly fit to the hyperplane, but "how uncertain" they are from the hyperplane is never considered.



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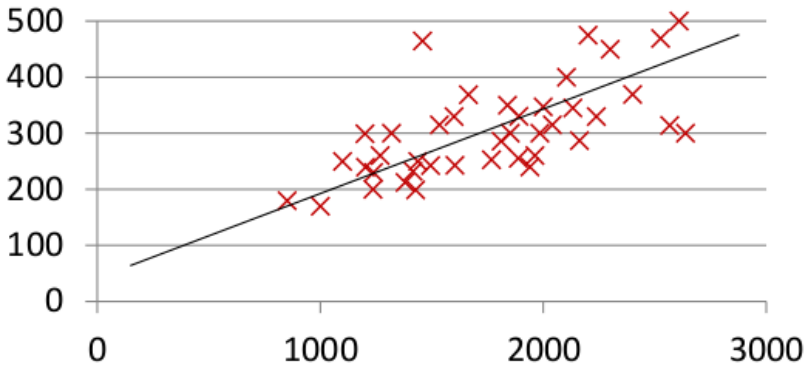


- An alternate view considers the following.
  - $y^{(i)}$ are generated from the $\mathbf{x}^{(i)}$ following a underlying hyperplane.
  - But we don't get to "see" the generated data. Instead we "see" a noisy version of the $y^{(i)}$'s.
  - Maximum likelihood (or in general, probabilistic estimation) models this uncertainty in determining the data generating function.

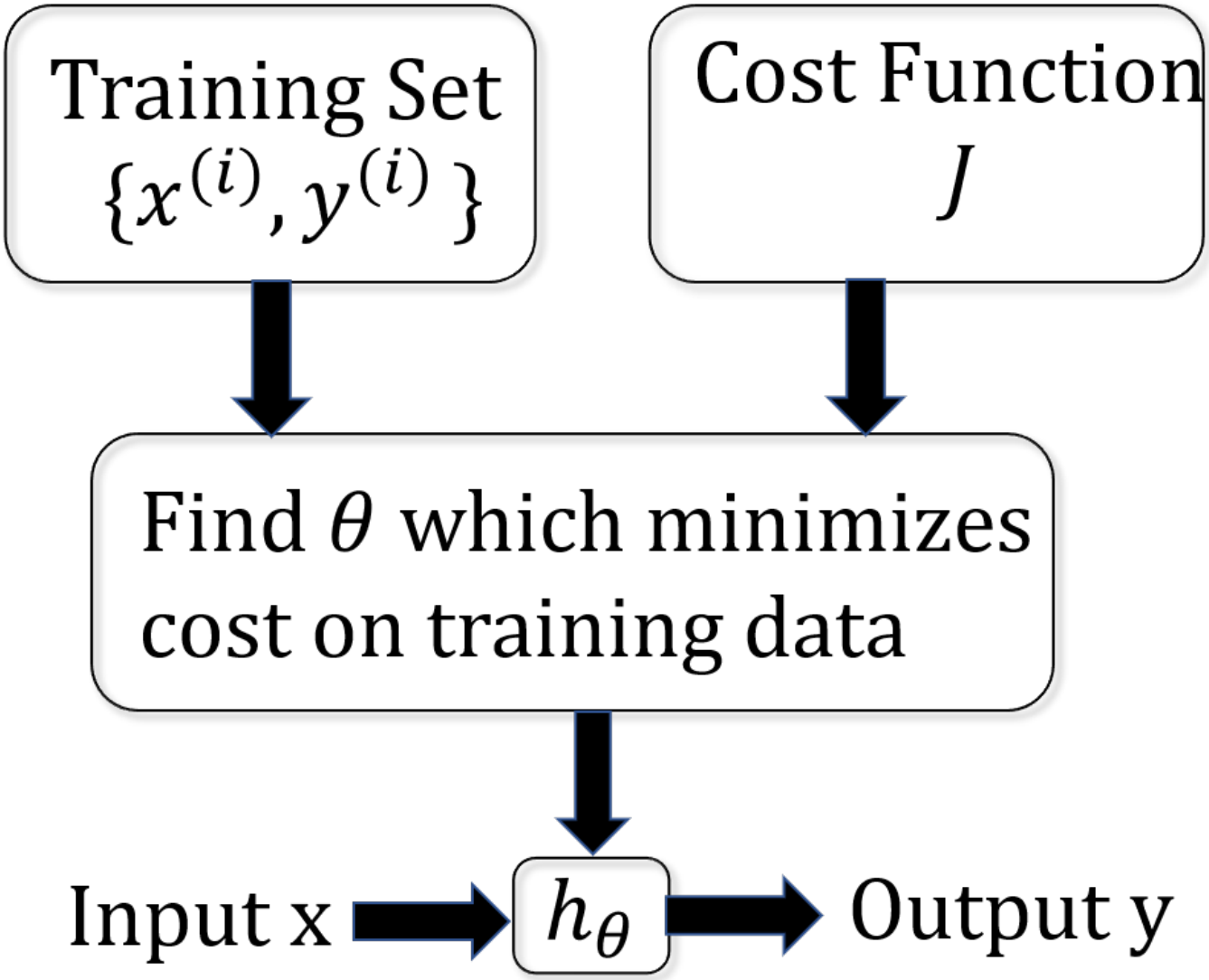
Linear Regression as Maximum Likelihood Estimation

- Thus data are assumed to be generated as follows.

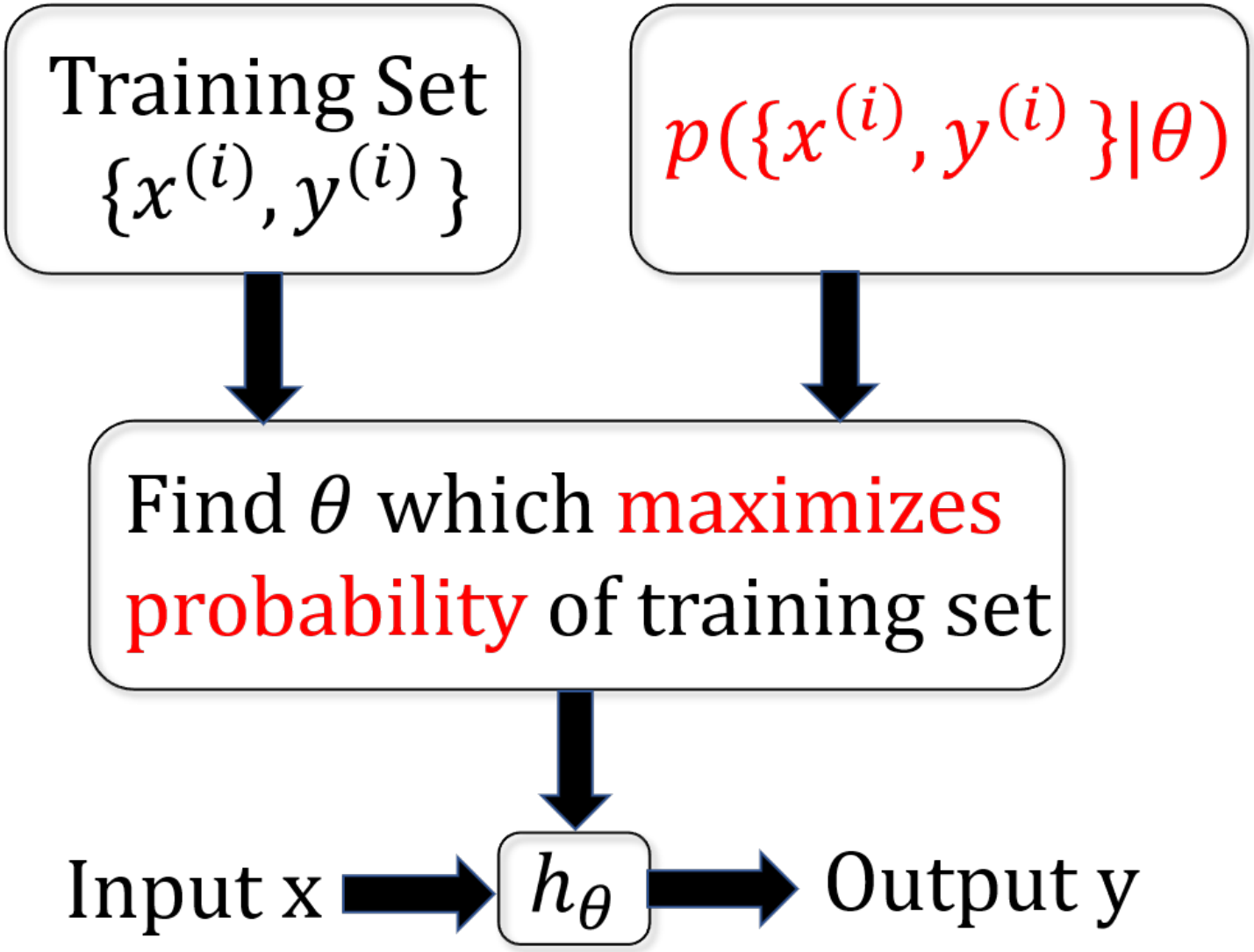
$$y^{(i)} = h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) + \epsilon^{(i)}$$

  where $\epsilon^{(i)}$ is an additive noise following some probability distribution.
- So, $\left(\mathbf{x}^{(i)}, y^{(i)}\right)$'s form a joint distribution.
- The idea is to assume a probability distribution on the noise and the probability distribution is parameterised by some additional parameters (*e.g.*, Gaussian with 0 mean and covariance σ^2).
- Then find the parameters (both $\boldsymbol{\theta}$ and σ^2) that is "most likely" to generate the data.

Recall: Cost Function



Alternate View: "Maximum Likelihood"



Maximum Likelihood for Linear Regression

- Let us assume that the noise is Gaussian distributed with mean 0 and variance σ^2

$$y^{(i)} = h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) + \epsilon^{(i)} = \boldsymbol{\theta}^T \mathbf{x}^{(i)} + \epsilon^{(i)}$$

- Noise $\epsilon^{(i)} \sim \mathcal{N}(0, \sigma^2)$ and thus $y^{(i)} \sim \mathcal{N}(\boldsymbol{\theta}^T \mathbf{x}^{(i)}, \sigma^2)$.

Maximum Likelihood for Linear Regression

- Let us assume that the noise is Gaussian distributed with mean 0 and variance σ^2

$$y^{(i)} = h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) + \epsilon^{(i)} = \boldsymbol{\theta}^T \mathbf{x}^{(i)} + \epsilon^{(i)}$$

- Noise $\epsilon^{(i)} \sim \mathcal{N}(0, \sigma^2)$ and thus $y^{(i)} \sim \mathcal{N}(\boldsymbol{\theta}^T \mathbf{x}^{(i)}, \sigma^2)$.
- Let us compute the likelihood.

$$\begin{aligned} p(\mathbf{y}|\mathbf{X}; \boldsymbol{\theta}, \sigma^2) &= \prod_{i=1}^{N} p(y^{(i)}|\mathbf{x}^{(i)}; \boldsymbol{\theta}, \sigma^2) \\ &= \prod_{i=1}^{N} (2\pi\sigma^2)^{-\frac{1}{2}} \, e^{-\frac{1}{2\sigma^2}\left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)^2} \\ &= (2\pi\sigma^2)^{-\frac{N}{2}} \, e^{-\frac{1}{2\sigma^2}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)^2} \\ &= (2\pi\sigma^2)^{-\frac{N}{2}} \, e^{-\frac{1}{2\sigma^2}\left(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\right)^T\left(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\right)} \end{aligned} \tag{5}$$

Maximum Likelihood for Linear Regression

- So we have got the likelihood as,

$$p(\mathbf{y}|\mathbf{X};\boldsymbol{\theta},\sigma^2) = (2\pi\sigma^2)^{-\frac{N}{2}}\, e^{-\frac{1}{2\sigma^2}\left(\mathbf{y}-\mathbf{X}\boldsymbol{\theta}\right)^T\left(\mathbf{y}-\mathbf{X}\boldsymbol{\theta}\right)}$$

- The log likelihood is

$$l(\boldsymbol{\theta},\sigma^2) = -\frac{N}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\left(\mathbf{y}-\mathbf{X}\boldsymbol{\theta}\right)^T\left(\mathbf{y}-\mathbf{X}\boldsymbol{\theta}\right)$$

Maximum Likelihood for Linear Regression

- So we have got the likelihood as,

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- Maximizing the likelihood w.r.t. $\boldsymbol{\theta}$ means maximizing $-\left(\mathbf{y}-\mathbf{X}\boldsymbol{\theta}\right)^T\left(\mathbf{y}-\mathbf{X}\boldsymbol{\theta}\right)$ which in turn means minimizing $\left(\mathbf{y}-\mathbf{X}\boldsymbol{\theta}\right)^T\left(\mathbf{y}-\mathbf{X}\boldsymbol{\theta}\right)$.
- Note the similarity with what we did earlier.
- Thus linear regression can be equivalently viewed as minimizing error sum of squares as well as maximum likelihood estimation under zero mean Gaussian noise assumption.

Maximum Likelihood for Linear Regression

- In a similar manner, the maximum likelihood estimate of σ^2 can also be calculated.
- Remember, the log likelihood can be written as,

$$l(\boldsymbol{\theta}, \sigma^2) = -\frac{N}{2}\log(2\pi) - \frac{N}{2}\log(\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T x^{(i)}\right)^2$$

- Now, we take the partial derivative with respect to σ^2 (let's treat $v = \sigma^2$ as our variable for simplicity).

$$\frac{\partial l}{\partial v} = -\frac{N}{2}\frac{\partial}{\partial v}\log(v) - \frac{1}{2}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T x^{(i)}\right)^2 \frac{\partial}{\partial v}(v^{-1})$$

- Using standard derivatives $\frac{d}{dv}\ln(v) = \frac{1}{v}$ and $\frac{d}{dv}v^{-1} = -v^{-2}$:

$$\frac{\partial l}{\partial \sigma^2} = -\frac{N}{2\sigma^2} + \frac{1}{2(\sigma^2)^2}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T x^{(i)}\right)^2$$

Maximum Likelihood for Linear Regression

§ Now, we set the derivative to zero to find the optimum.

$$-\frac{N}{2\sigma^2} + \frac{1}{2(\sigma^2)^2}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T x^{(i)}\right)^2 = 0$$

$$-N\sigma^2 + \sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T x^{(i)}\right)^2 = 0$$

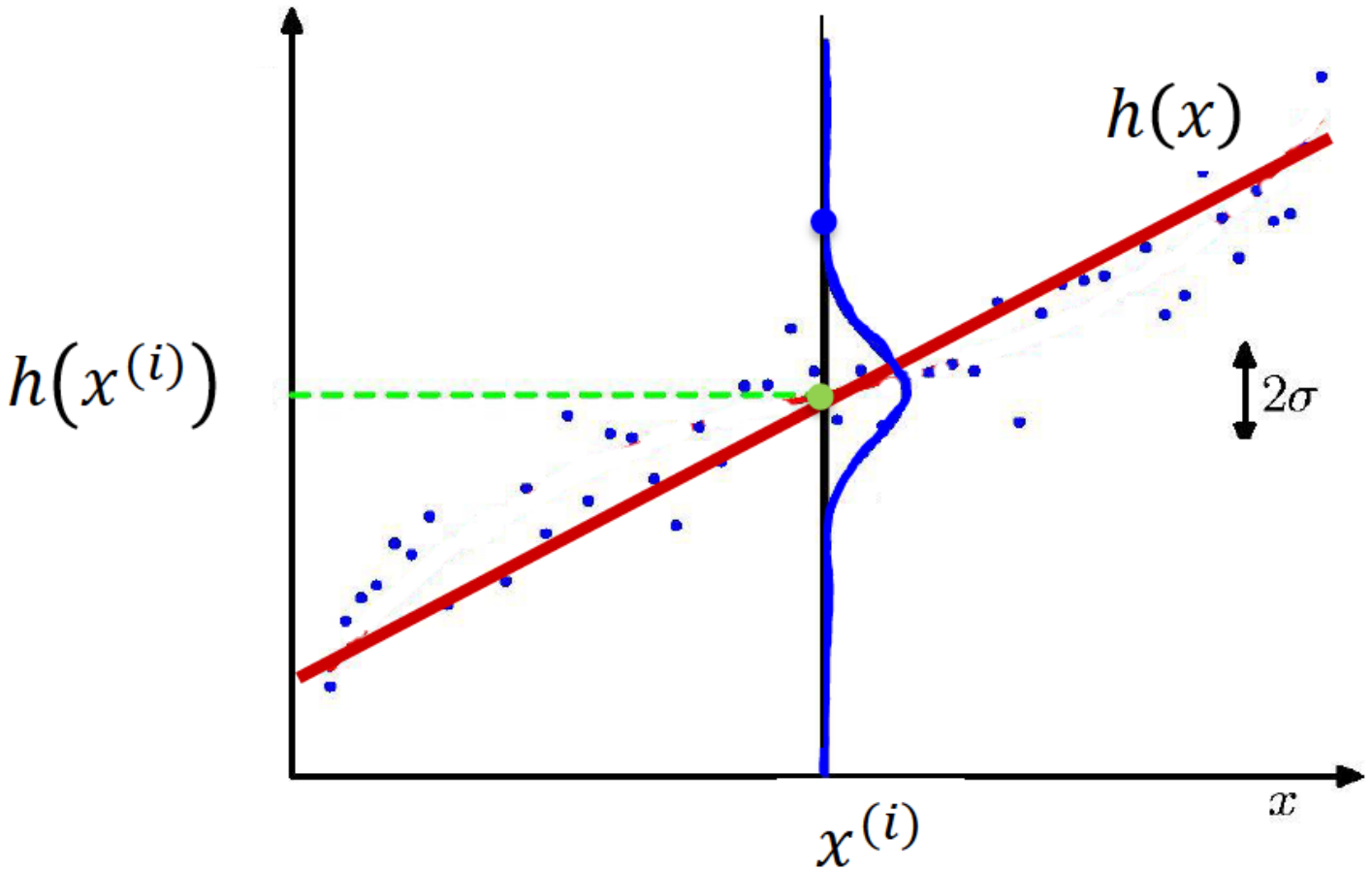
§ Rearranging terms gives us the MLE estimator:

$$\sigma^2_{MLE} = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T_{MLE} x^{(i)}\right)^2$$

Interpretation

The MLE estimate for the variance is simply the **average squared residual** (Mean Squared Error) of the model on the training data.

Maximum Likelihood for Linear Regression



Recall: Ordinary Least Squares (OLS)

In standard Linear Regression, we minimize the Sum of Squared Errors:

$$J(\boldsymbol{\theta}) = ||\mathbf{y} - \mathbf{X}\boldsymbol{\theta}||_2^2$$

The closed-form solution (MLE) is:

$$\widehat{\boldsymbol{\theta}}_{MLE} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Potential Problem

This requires inverting $\mathbf{X}^T\mathbf{X}$.

- What if $\mathbf{X}^T\mathbf{X}$ is ill-conditioned?
- What if features are highly correlated (multicollinearity)?
- inverting the matrix is numerically unstable

The Fix: Ridge Regression

Idea: Add a small positive element ($\delta^2 > 0$) to the diagonal of $\mathbf{X}^T\mathbf{X}$.

$$\mathbf{X}^T\mathbf{X} \quad \longrightarrow \quad (\mathbf{X}^T\mathbf{X} + \delta^2\mathbf{I})$$

This ensures the matrix is always Full Rank (invertible) and well-conditioned.

Ridge Regression Estimate

$$\hat{\boldsymbol{\theta}}_R = (\mathbf{X}^T\mathbf{X} + \delta^2\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$$

Implied Cost Function: It turns out (via calculus) that this is solution to the following **regularized quadratic cost function**.

$$J(\boldsymbol{\theta}) = \underbrace{||\mathbf{y} - \mathbf{X}\boldsymbol{\theta}||_2^2}_{\text{Error}} + \underbrace{\lambda||\boldsymbol{\theta}||_2^2}_{\text{Penalty/Regularizer}}$$

A Deeper Question

We fixed the numerical problem by adding $\delta^2\mathbf{I}$.

Is this just a mathematical hack?

- Does minimizing $||\boldsymbol{\theta}||^2$ have a statistical meaning?
- Why squared norm? Why not absolute value?

Let's look at this from a **Bayesian Probability** *perspective.*

Bayesian Linear Regression: The Setup

Let's incorporate a **Prior Belief** about our weights $\boldsymbol{\theta}$.

1. The Likelihood (Data)

Assume standard Gaussian noise (Like we did earlier). In Eqn. (5), we saw:

$$p(\mathbf{y}|\mathbf{X};\boldsymbol{\theta},\sigma^2) = (2\pi\sigma^2)^{-\frac{N}{2}} e^{-\frac{1}{2\sigma^2}\left(\mathbf{y}-\mathbf{X}\boldsymbol{\theta}\right)^T\left(\mathbf{y}-\mathbf{X}\boldsymbol{\theta}\right)}$$

2. The Prior (Belief)

We assume weights are likely small (centered at 0). Let's use a **Gaussian Prior**:

$$\boldsymbol{\theta} \sim \mathcal{N}(\mathbf{0}, \tau^2\mathbf{I})$$

The PDF is given by:

$$p(\boldsymbol{\theta}) = (2\pi\tau^2)^{-\frac{D}{2}} e^{-\frac{1}{2\tau^2}\boldsymbol{\theta}^T\boldsymbol{\theta}}$$

Deriving the MAP Estimate

The MAP estimate maximizes the log-posterior:

$$\hat{\boldsymbol{\theta}}_{MAP} = \arg\max_{\boldsymbol{\theta}} \left[\ln p(\mathbf{y}|\mathbf{X};\boldsymbol{\theta}) + \ln p(\boldsymbol{\theta})\right]$$

Expanding the terms:

$$\ln p(\mathbf{y}|\dots) = -\frac{N}{2}\ln(2\pi\sigma^2) - \frac{1}{2\sigma^2}(\mathbf{y}-\mathbf{X}\boldsymbol{\theta})^T(\mathbf{y}-\mathbf{X}\boldsymbol{\theta})$$

$$\ln p(\boldsymbol{\theta}) = -\frac{D}{2}\ln(2\pi\tau^2) - \frac{1}{2\tau^2}\boldsymbol{\theta}^T\boldsymbol{\theta}$$

Dropping terms that are constant *w.r.t.* $\boldsymbol{\theta}$:

$$\hat{\boldsymbol{\theta}}_{MAP} = \arg\max_{\boldsymbol{\theta}} \left[-\frac{1}{2\sigma^2}(\mathbf{y}-\mathbf{X}\boldsymbol{\theta})^T(\mathbf{y}-\mathbf{X}\boldsymbol{\theta}) - \frac{1}{2\tau^2}\boldsymbol{\theta}^T\boldsymbol{\theta}\right]$$

Deriving the MAP Estimate

From previous slide:

$$\hat{\boldsymbol{\theta}}_{MAP} = \arg\max_{\boldsymbol{\theta}} \left[-\frac{1}{2\sigma^2} ||\mathbf{y} - \mathbf{X}\boldsymbol{\theta}||_2^2 - \frac{1}{2\tau^2} ||\boldsymbol{\theta}||_2^2 \right]$$

Converting maximization to minimization, (multiply by $-2\sigma^2$):

$$\hat{\boldsymbol{\theta}}_{MAP} = \arg\min_{\boldsymbol{\theta}} \left[||\mathbf{y} - \mathbf{X}\boldsymbol{\theta}||_2^2 + \frac{2\sigma^2}{2\tau^2} ||\boldsymbol{\theta}||_2^2 \right]$$

$$\hat{\boldsymbol{\theta}}_{MAP} = \arg\min_{\boldsymbol{\theta}} \left[\underbrace{||\mathbf{y} - \mathbf{X}\boldsymbol{\theta}||_2^2}_{\text{SSE}} + \underbrace{\frac{\sigma^2}{\tau^2}}_{\lambda} \underbrace{||\boldsymbol{\theta}||_2^2}_{\text{Regularizer}} \right]$$

Conclusion

MAP with Gaussian Prior is identical to Ridge Regression with $\lambda = \frac{\sigma^2}{\tau^2}$.

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Conclusion

MAP with Gaussian Prior is identical to Ridge Regression with $\lambda = \frac{\sigma^2}{\tau^2}$.

Deriving the Ridge Estimator

We found the Objective Function:

$$J(\boldsymbol{\theta}) = (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \lambda\boldsymbol{\theta}^T\boldsymbol{\theta}$$

To find the optimal $\boldsymbol{\theta}$, we take the gradient $\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$ and set it to 0.

Step 1: Expand the terms

$$\begin{aligned} J(\boldsymbol{\theta}) &= (\mathbf{y}^T - \boldsymbol{\theta}^T\mathbf{X}^T) + (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \lambda\boldsymbol{\theta}^T\boldsymbol{\theta} \\ &= \mathbf{y}^T\mathbf{y} - \mathbf{y}^T\mathbf{X}\boldsymbol{\theta} - \boldsymbol{\theta}^T\mathbf{X}^T\mathbf{y} + \boldsymbol{\theta}^T\mathbf{X}^T\mathbf{X}\boldsymbol{\theta} + \lambda\boldsymbol{\theta}^T\boldsymbol{\theta} \end{aligned}$$

Note that $\mathbf{y}^T\mathbf{X}\boldsymbol{\theta}$ is a scalar, so it equals its transpose $\boldsymbol{\theta}^T\mathbf{X}^T\mathbf{y}$.

$$J(\boldsymbol{\theta}) = \mathbf{y}^T\mathbf{y} - 2\boldsymbol{\theta}^T\mathbf{X}^T\mathbf{y} + \boldsymbol{\theta}^T(\mathbf{X}^T\mathbf{X})\boldsymbol{\theta} + \lambda\boldsymbol{\theta}^T\boldsymbol{\theta}$$

Deriving the Ridge Estimator

Step 2: Take the Gradient

Using matrix calculus rules $\nabla_{\boldsymbol{\theta}}(\boldsymbol{\theta}^T \mathbf{A}\boldsymbol{\theta}) = 2\mathbf{A}\boldsymbol{\theta}$ (for symmetric $\mathbf{A}$) and $\nabla_{\boldsymbol{\theta}}(\mathbf{b}^T\boldsymbol{\theta}) = \mathbf{b}$,

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = 0 - 2\mathbf{X}^T\mathbf{y} + 2(\mathbf{X}^T\mathbf{X})\boldsymbol{\theta} + 2\lambda\boldsymbol{\theta}$$

Step 3: Set Gradient to Zero

$$-2\mathbf{X}^T\mathbf{y} + 2(\mathbf{X}^T\mathbf{X})\boldsymbol{\theta} + 2\lambda\mathbf{I}\boldsymbol{\theta} = 0$$

$$(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})\boldsymbol{\theta} = \mathbf{X}^T\mathbf{y}$$

Step 4: Solve for $\boldsymbol{\theta}$

$$\hat{\boldsymbol{\theta}}_{Ridge} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$$

This matches the "stabilized" inverse we saw earlier!

Changing the Prior: Ridge vs. Lasso

What if we used a **Laplacian Prior** ($P(\boldsymbol{\theta}) \propto e^{-|\boldsymbol{\theta}|}$) instead?

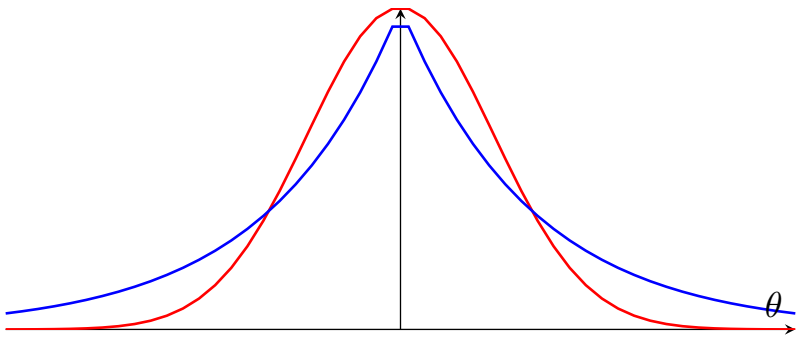
Ridge (L2)

- Prior: Gaussian
- Penalty: $\lambda||\boldsymbol{\theta}||_2^2$
- Solution: $\boldsymbol{\theta}$ is small, but non-zero.
- **Use case:** Handling multicollinearity (Matrix Conditioning).

Lasso (L1)

- Prior: Laplacian
- Penalty: $\lambda||\boldsymbol{\theta}||_1$
- Solution: Sparse (many $\theta_i = 0$).
- **Use case:** Feature Selection.

Gaussian (Red) vs Laplacian (Blue)

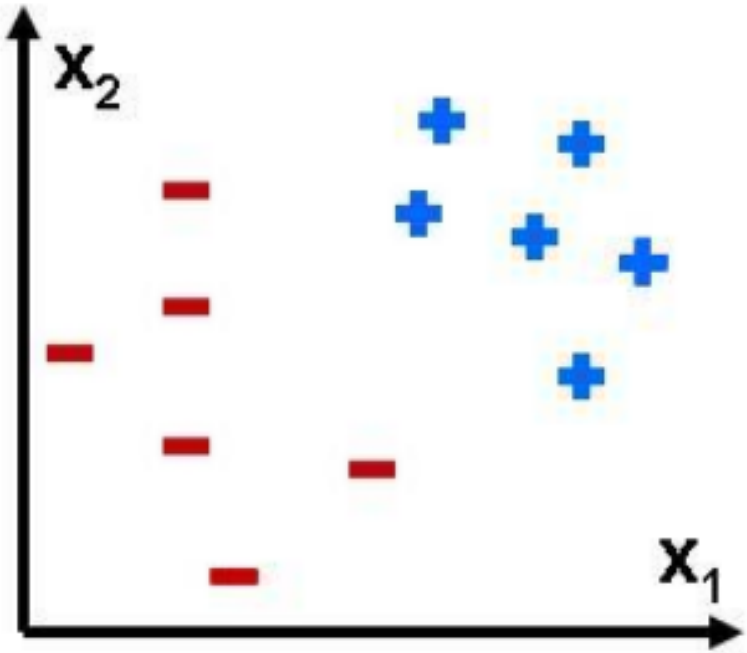


Summary: The Equivalence Table

Method	Algebraic View	Probabilistic View
OLS	Minimize SSE	MLE (Gaussian Noise)
Ridge	Stabilize Inverse $(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})$	MAP (Gaussian Prior)
Lasso	Constraint $\|\|\boldsymbol{\theta}\|\|_1 \leq t$	MAP (Laplacian Prior)

Classification

- $y \in \{0, 1\}$, where 0 : "Negative class" (*e.g.*, benign tumor), 1 : "Positive class" (*e.g.*, malignant tumor)
- Some more examples:
  - Email: Spam/ Not Spam?
  - Video: Viral/Not Viral?
  - Tremor: Earthquake/Nuclear explosion?



Linear classifiers with hard threshold

- Linear functions can be used to do classification as well as regression.
- For example,

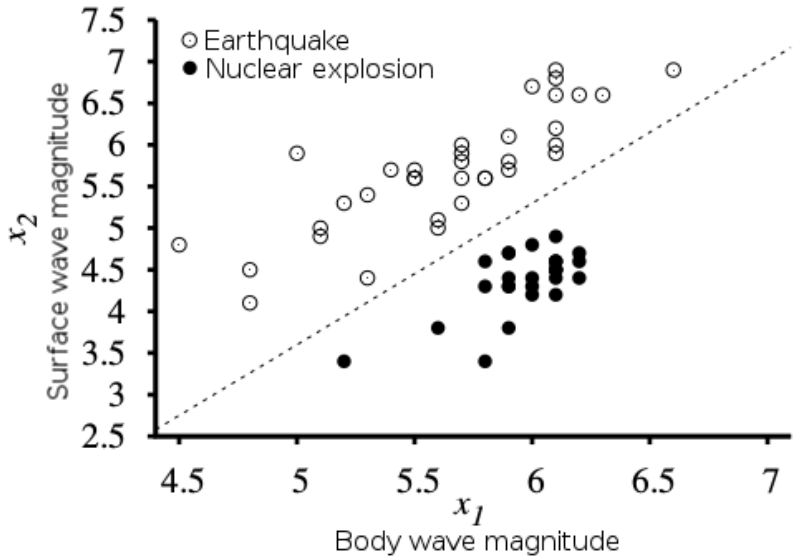


Figure credit: *AIMA: Russell, Norvig*

- A **decision boundary** is a line (or a surface, in higher dimensions) that separates the two classes.
- A linear function gives rise to a **linear separator** and the data that results in such a separator are called **linearly separable**.

Linear Classifier with Hard Threshold

§ The linear separator in the associated fig is given by,

$$x_2 = 1.7x_1 - 4.9$$

$$\implies -4.9 + 1.7x_1 - x_2 = 0$$

$$\implies [-4.9, 1.7, -1] \begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} = 0$$

$$\boldsymbol{\theta}^T \mathbf{x} = 0$$

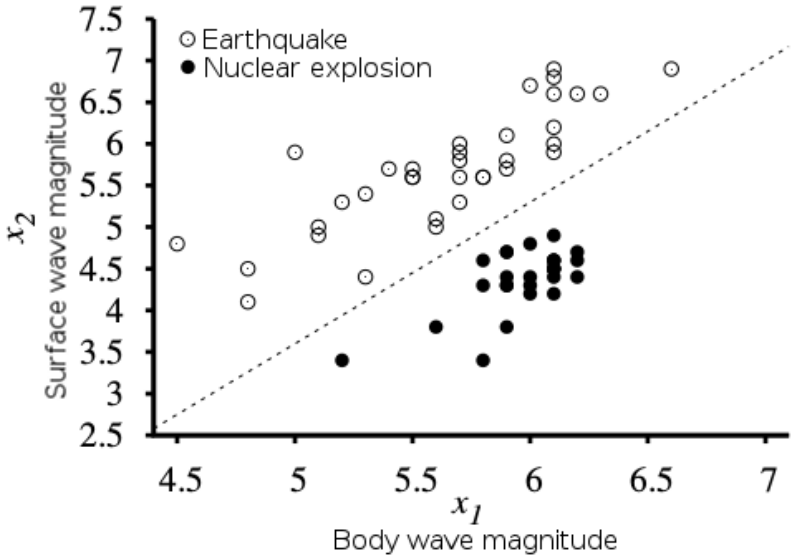
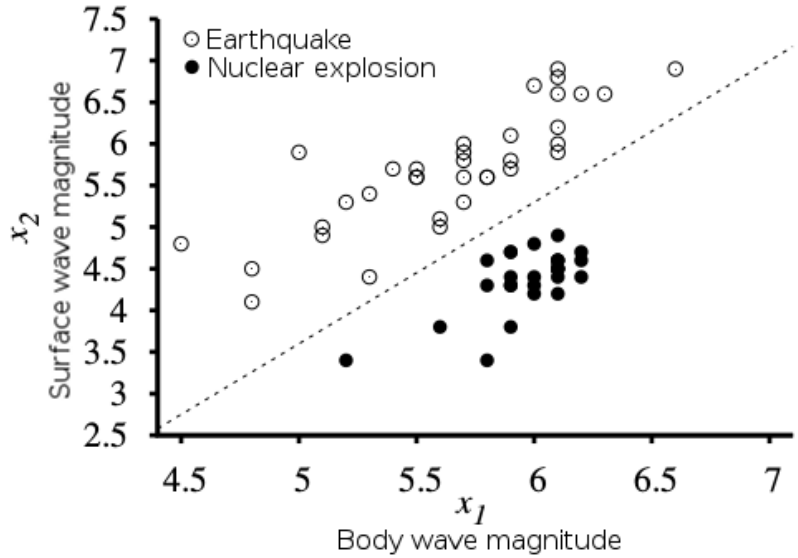


Figure credit: *AIMA: Russell, Norvig*

Linear Classifier with Hard Threshold



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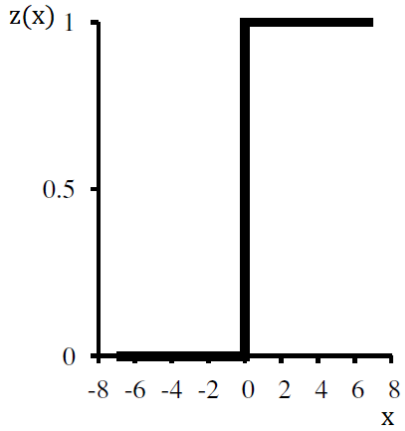
- The explosions $(y = 1)$ are to the right of this line with higher values of x_1 and lower values of x_2. So, they are points for which $\boldsymbol{\theta}^T \mathbf{x} \geq 0$
- Similarly earthquakes $(y = 0)$ are to the left of this line. So, they are points for which $\boldsymbol{\theta}^T \mathbf{x} < 0$
- The classification rule is then,

$$y(\mathbf{x}) = \begin{cases} 1 & \text{if } \boldsymbol{\theta}^T \mathbf{x} \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

Linear classifiers with hard threshold

§ Alternatively, we can think y as the result of passing the linear function $\boldsymbol{\theta}^T \mathbf{x}$ through a threshold function.



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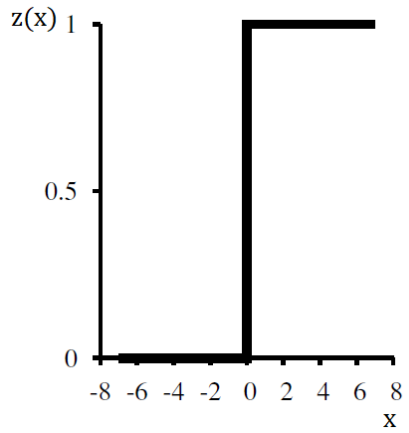

- To get the linear separator we have find the θ which minimizes classification error on the training set.
- For regression problems, we found θ in both closed form and by gradient descent. But both approaches required us to compute the gradient.
- This is not possible for the above threshold function as the gradient is undefined when the *value* at $x - axis = 0$ and 0 elsewhere.

Linear classifiers with hard threshold

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- Perceptron Rule - This algorithm does not compute the gradient to find θ.
- Perceptron Learning Rule can find a linear separator given the data is linearly separable.
- For data that are not linearly separable, the Perceptron algorithm fails.
- So, we need to go for a gradient based optimization approach
- Thus, we need to approximate the hard threshold function with something smooth.

$$\sigma(u) = \frac{1}{1 + e^{-u}}$$

$$y = \sigma(h_\theta(x)) = \sigma(\boldsymbol{\theta}^T \mathbf{x})$$

- Notice that the output is a number between 0 and 1, so it can be interpreted as a probability value belonging to Class 1.
- This is called a logistic regression classifier. The gradient computation is tedious but straight forward.

Maximum Likelihood Estimation of Logistic Regression

- Mathematically, the probability that an example belongs to class 1 is $P(y^{(i)} = 1|\mathbf{x}^{(i)}; \boldsymbol{\theta}) = \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)$
- Similarly, $P(y^{(i)} = 0|\mathbf{x}^{(i)}; \boldsymbol{\theta}) = 1 - \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)$
- Thus, $P(y^{(i)}|\mathbf{x}^{(i)}; \boldsymbol{\theta}) = \left(\sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)\right)^{y^{(i)}} \left(1 - \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)\right)^{(1-y^{(i)})}$

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- The joint probability of all the labels $\prod_{i=1}^{N} \left(\sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)\right)^{y^{(i)}} \left(1 - \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)\right)^{(1-y^{(i)})}$

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- So the log likelihood for logistic regression is given by,

$$l(\boldsymbol{\theta}) = \sum_{i=1}^{N} y^{(i)} \log \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right) + (1 - y^{(i)}) \log\left(1 - \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)\right)$$

Maximum Likelihood Estimation of Logistic Regression

§ Derivative of log likelihood w.r.t. one component of $\boldsymbol{\theta}$,

$$\begin{aligned}
\frac{\partial l(\boldsymbol{\theta})}{\partial \theta_j} &= \frac{\partial}{\partial \theta_j} \sum_{i=1}^{N} y^{(i)} \log \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)\right) \\
&= \sum_{i=1}^{N} \left[\frac{y^{(i)}}{\sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)} - \frac{1 - y^{(i)}}{1 - \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)}\right] \frac{\partial}{\partial \theta_j} \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right) \\
&= \sum_{i=1}^{N} \left[\frac{y^{(i)}}{\sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)} - \frac{1 - y^{(i)}}{1 - \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)}\right] \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)\left(1 - \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)\right) \mathbf{x}_j^{(i)} \\
&= \sum_{i=1}^{N} \left[\frac{y^{(i)} - \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)}{\sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)\left(1 - \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)\right)}\right] \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)\left(1 - \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)\right) \mathbf{x}_j^{(i)} \\
&= \sum_{i=1}^{N} \left[y^{(i)} - \sigma\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)\right] \mathbf{x}_j^{(i)} \qquad (6)
\end{aligned}$$

§ This is used in an iterative gradient ascent loop.