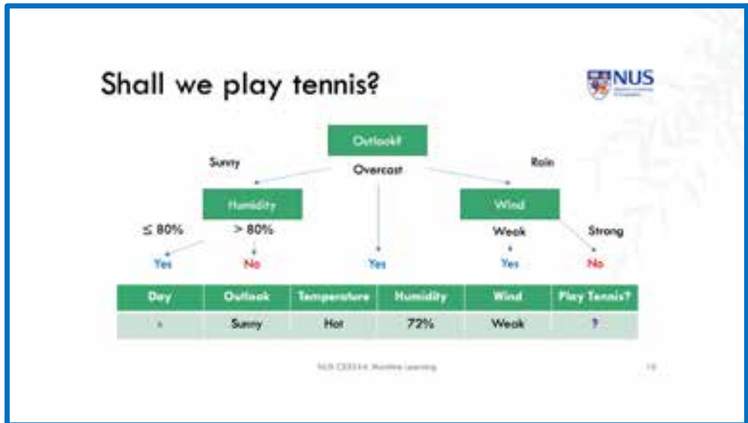
Linear Classifiers and Logistic Regression

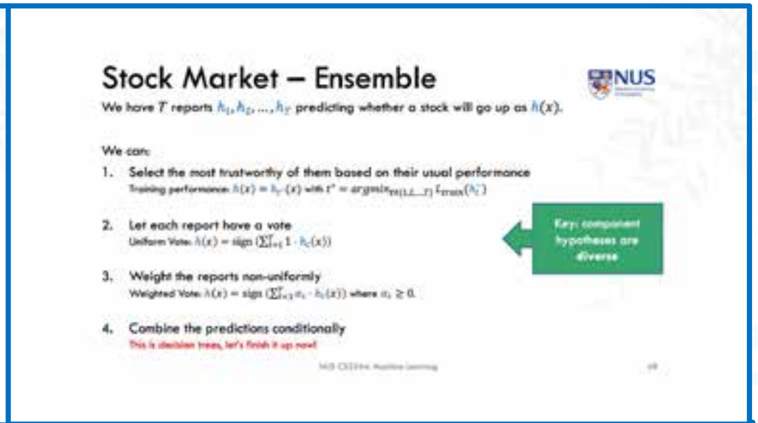
4A

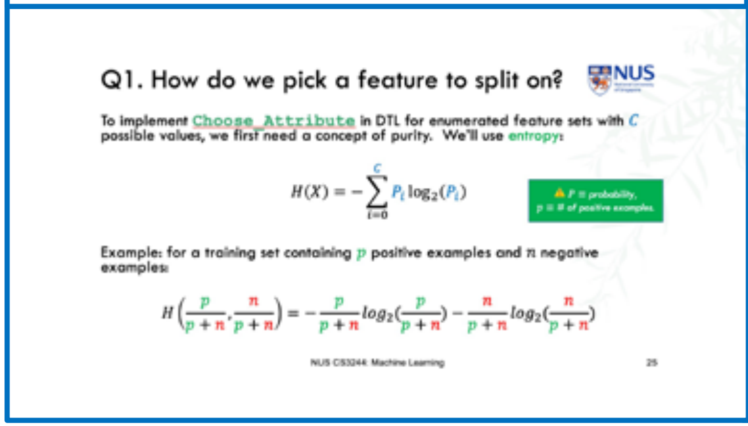
CS 3244
Machine Learning

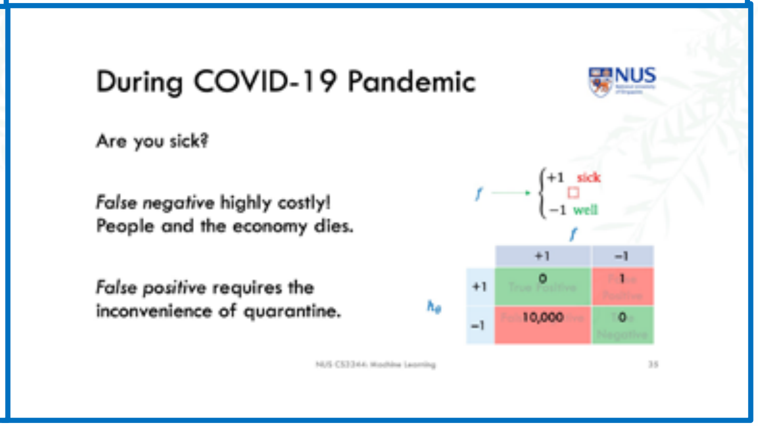
NUS | Computing

Recap from Week 03









Forecast for Week 04A

Learning Outcomes for this week

- Describe the basic idea of linear classification;
- Understand how both linear and logistic regression works;

Other important concepts:

- Curse of Dimensionality
- Gradient Descent
- Non-linear Mappings

Curse of Dimensionality

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The Curse of Dimensionality

k NN is one classifier that suffers from the curse of dimensionality.

What is this “curse”?

Photo by silvana amicone on Unsplash

In high dimensions:

The number of points needed to keep the same density grows exponentially.

The distance between arbitrary points is similar, making it hard to distinguish.

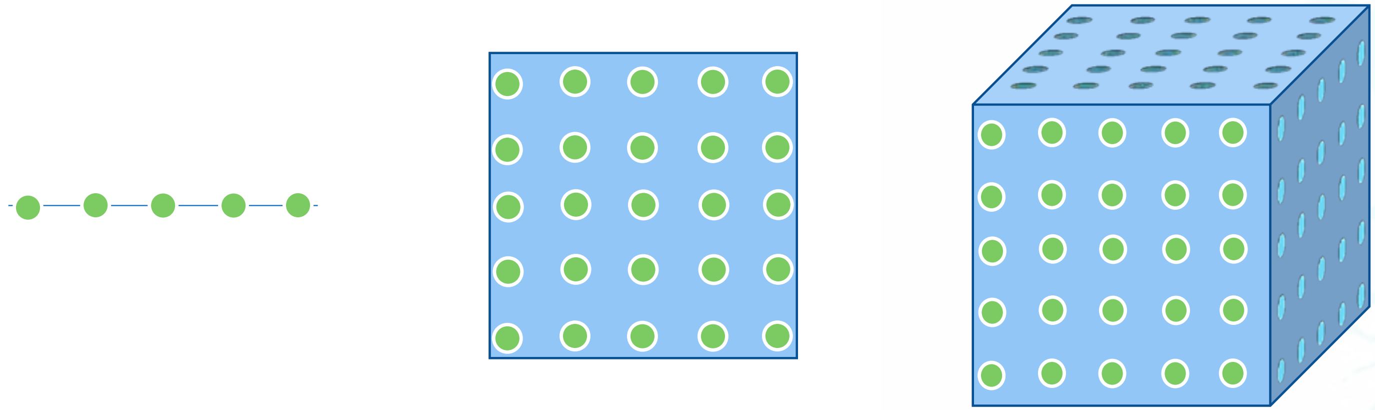
Sparsity with high dimensions

$m = 5$
$n = 1$

Chart illustration idea: Stanford CS229N

Sparsity with high dimensions

$m = 5$, $n = 1$ | $m = 25$, $n = 2$ | $m = 125$, $n = 3$



Sparsity problem: maintaining density of samples depends on exponential growth of the data

Chart illustration idea: Stanford CS229N

Unit Hypercube w/ Colab

Let's Go! (5 minutes)

http://www.comp.nus.edu.sg/~cs3244/AY2122S1/04.colab.html

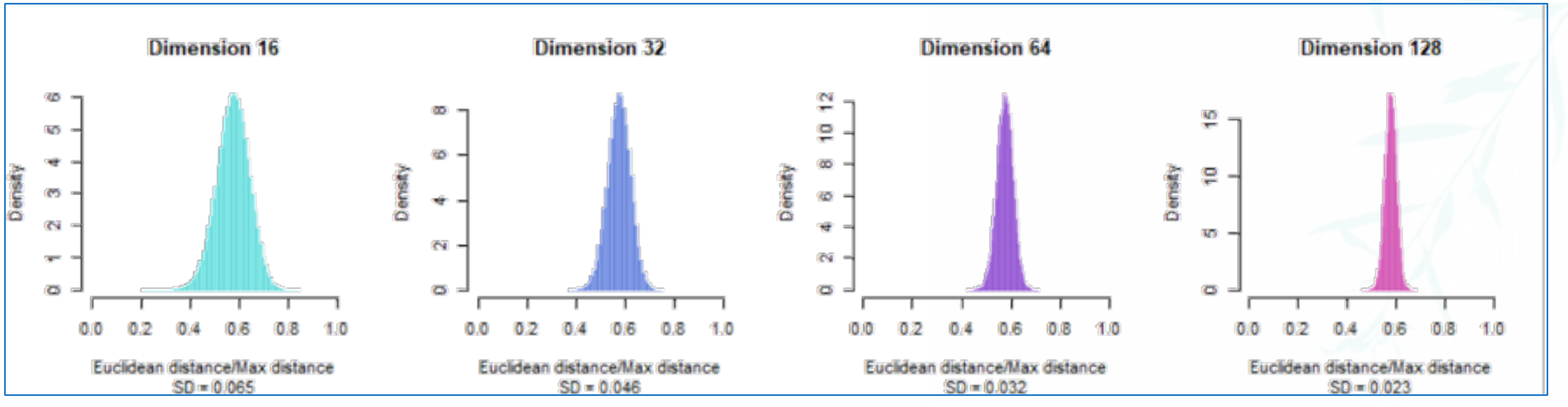
Standard Deviation σ grows slowly

```
1 dimensions:
#   Generated 200 points
Average distance (STD) of test point to 200 samples: 0.908554 (0.627194)
2 dimensions:
#   Generated 200 points
Average distance (STD) of test point to 200 samples: 1.357414 (0.672876)
3 dimensions:
#   Generated 200 points
Average distance (STD) of test point to 200 samples: 2.104206 (0.862900)
4 dimensions:
#   Generated 200 points
Average distance (STD) of test point to 200 samples: 2.857518 (0.851753)
8 dimensions:
#   Generated 200 points
Average distance (STD) of test point to 200 samples: 4.298752 (0.915833)
10 dimensions:
#   Generated 200 points
Average distance (STD) of test point to 200 samples: 4.240121 (0.873999)
100 dimensions:
#   Generated 200 points
Average distance (STD) of test point to 200 samples: 14.180229 (0.844941)
200 dimensions:
#   Generated 200 points
Average distance (STD) of test point to 200 samples: 19.588471 (0.845534)
```

Curse of Dimensionality

In high dimensional space, most points are nearly the same distance away.

The result: learners that depend on distance break down in high dimensions.



https://stats.stackexchange.com/questions/451027/mathematical-demonstration-of-the-distance-concentration-in-high-dimensions

Summary – in high dimensions

Hard to visualize, but 3B1B does a great job: *Thinking outside the 10-dimensional box* https://www.youtube.com/watch?v=zwAD6dRSVyI

Difficult to get sufficient samples

Most points end up far away; Euclidean distance becomes less meaningful

- High dimensional hypercube is most all “edge” space, far from the center of the hypercube

Choose or design an appropriate distance metric

Linear Models

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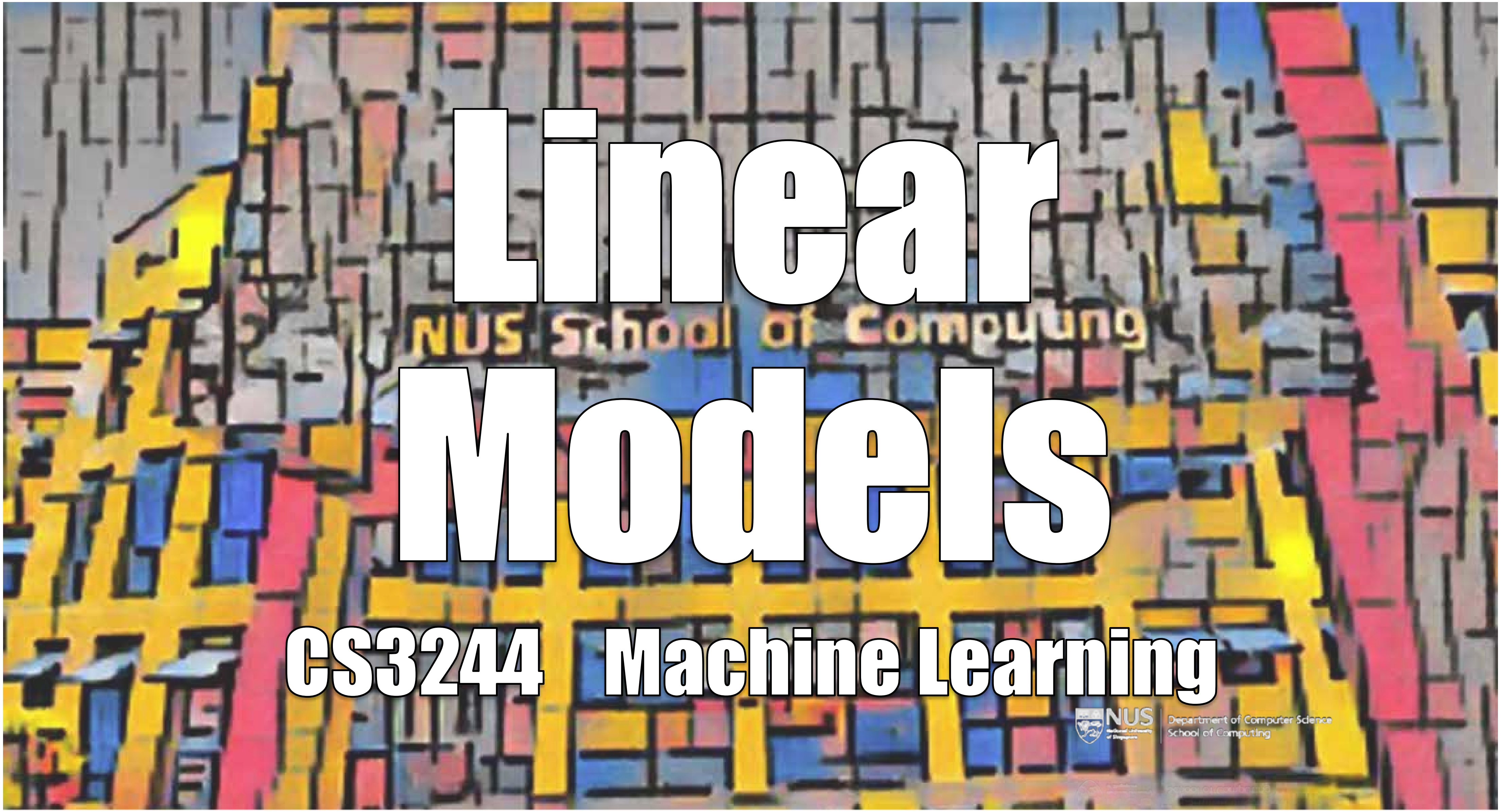
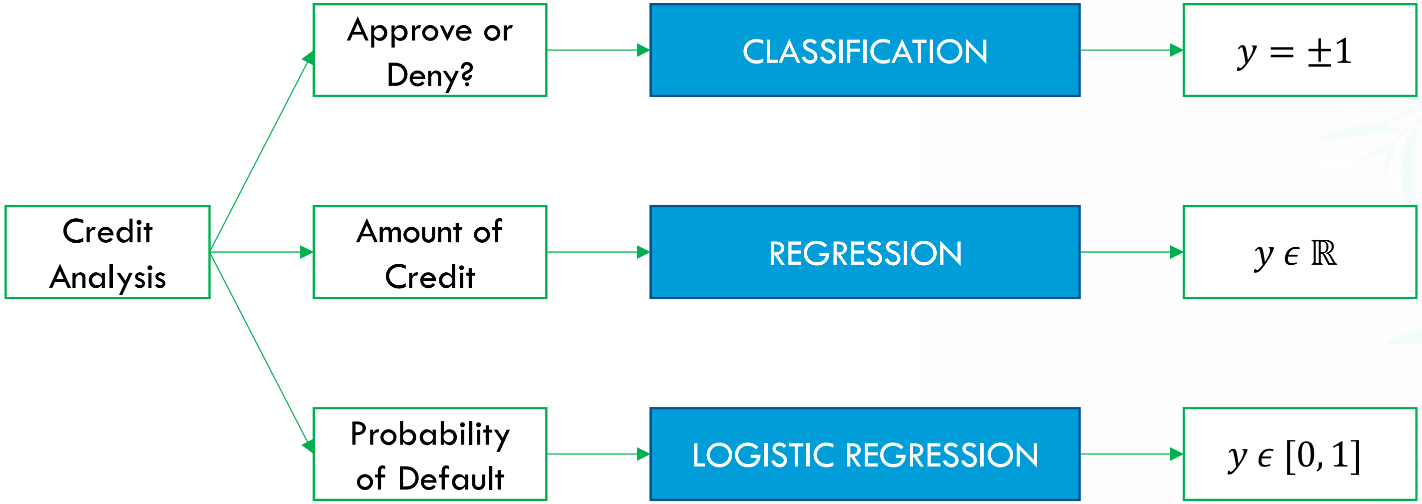


Three learning problems

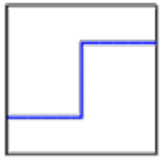


Linear models are the fundamental models.

The linear model is the first model to try.

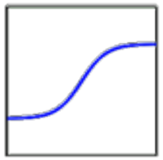
The linear signal

$$s = \boldsymbol{\theta}^{\top}\mathbf{x}$$



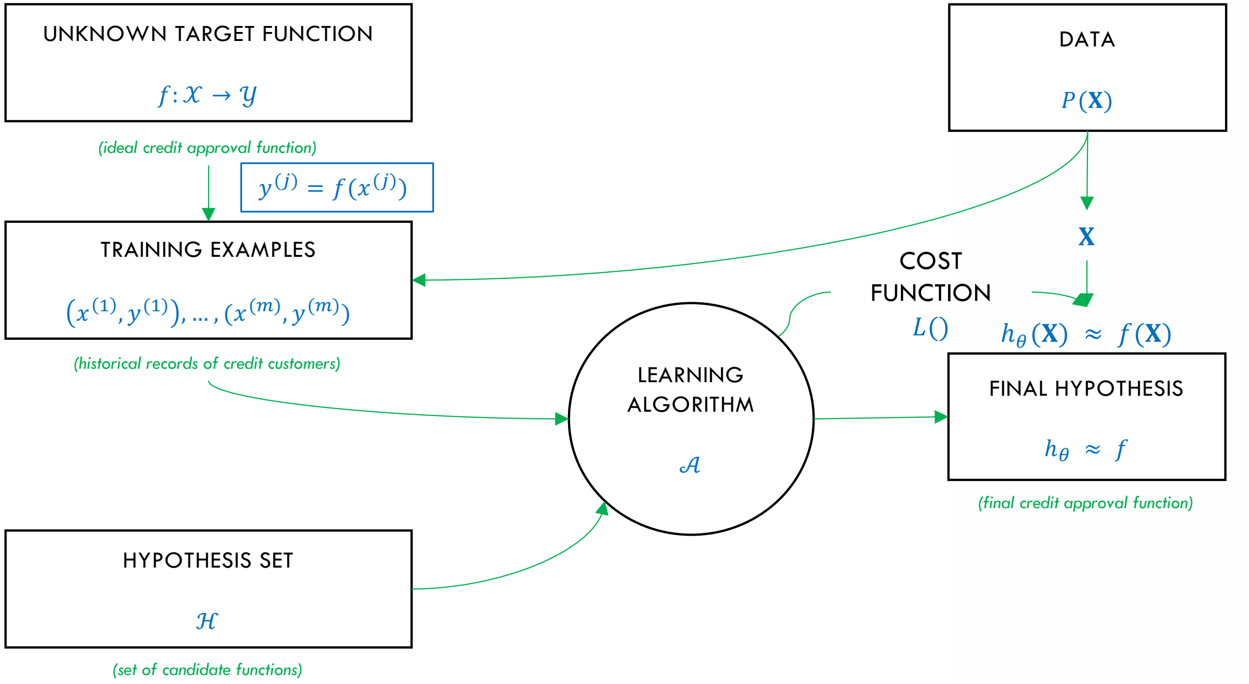
$\text{sign}\,(\boldsymbol{\theta}^{\top}\mathbf{x})$ $\quad y = \pm 1$

$\boldsymbol{\theta}^{\top}\mathbf{x}$ $\quad y \in \mathbb{R}$



$g(\boldsymbol{\theta}^{\top}\mathbf{x})$ $\quad y \in [0, 1]$

Recap: The Learning Diagram

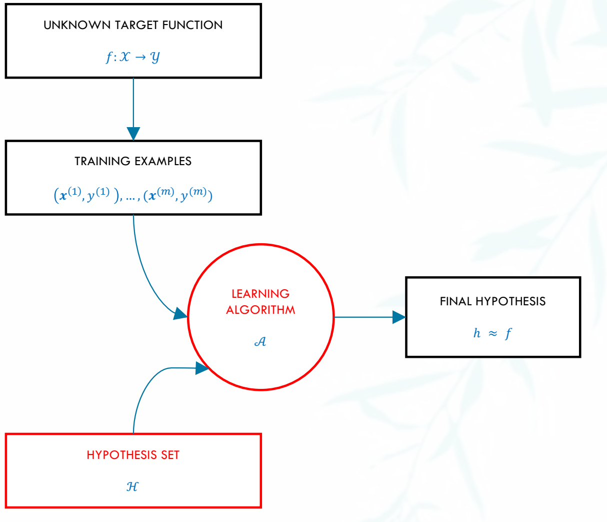


Choosing a model

We choose a Learning Algorithm $\mathcal{A}$ (equivalent to choosing $\mathcal{H}$), and any associated hyperparameters.

We employ $\mathcal{A}$ to then choose an h parameterized by its θ.

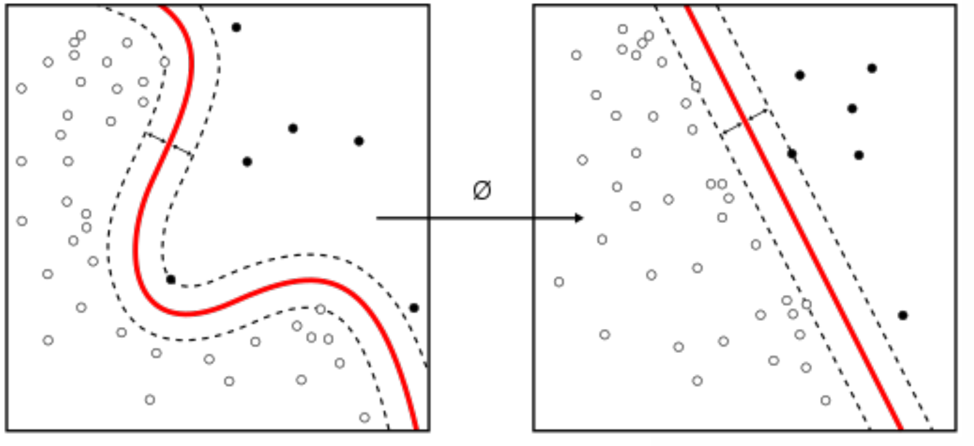
i.e., the learning algorithm $\mathcal{A}$ selects $h_\theta \in \mathcal{H}$.



$\mathcal{H}$ for linear models

$\mathcal{H}$ represents the universe of possible hypotheses that a certain learning algorithm A can generate.

That is, given the choices of θ, what types of decision boundaries can it generate?



What do you think? 👍 or 👎

Do we extend credit to this person, if this is all the information we know?

Criterion	Value
Age	32 years

Artwork credits: Project DebtRelief

Credit Approval

Do we extend credit to this person?

Criterion	Value
Age	32 years

$$h(x): [[x > 25]]$$

$[\![test]\!]$ here means return 1 if $test$ is true, 0 otherwise.

Normalize x:

$$h(x): \left[\!\left[\left(\frac{x}{100}\right) > 0.25\right]\!\right]$$

The 'bias weight' θ_0 corresponds to the threshold. θ_1 and θ_0 are parameters!.

Offset (Bias)

$$h(\mathbf{x}): \left(\frac{1}{100}\right) x_1 - (0.25)x_0 > 0$$

Introduce artificial x_0 as always equal to 1.

Credit Approval

Do we extend credit to this person?

Criterion	Value
Age	32 years
~~Gender~~	~~Male~~
Salary	40 K

Credit Approval

Do we extend credit to this person?

Criterion	Value
Age	32 years
~~Gender~~	~~Male~~
Salary	40 K
Debt	26 K
…	…
Years in Job	1 year
Years at Current Residence	3 years

$$h(\mathbf{x}): \theta_2 x_2 + \left(\frac{1}{100}\right) x_1 + (-0.25) x_0 > 0$$

$$h(\mathbf{x}): \theta_3 x_3 + \theta_2 x_2 + \theta_1 x_1 + \theta_0 x_0 > 0$$

$$h(\mathbf{x}): \sum_{i=1}^{n} \theta_i x_i > 0$$

Artwork credits: Project DebtRelief

Simplifying with vector notation

$$h(\boldsymbol{x}): \theta_n x_n + \cdots + \theta_0 x_0 > 0$$

Two vectors: $\boldsymbol{\theta} = \theta_n, \ldots, \theta_0$ and $\mathbf{x} = x_n, \ldots, x_0$.

🧐 by default vectors are ______ vectors

How to multiply?

Simplifying with vector notation

How to multiply? ____________

Which to transpose? $\boldsymbol{\theta}$ or $\mathbf{x}$?

🥇 🥈

$$\begin{bmatrix} \theta_0 \\ \cdots \\ \theta_n \end{bmatrix} \times \begin{bmatrix} x_0 & \cdots & x_n \end{bmatrix} =$$

$$\begin{bmatrix} \theta_0 & \cdots & \theta_n \end{bmatrix} \times \begin{bmatrix} x_0 \\ \cdots \\ x_n \end{bmatrix} =$$

Simplifying with vector notation

How about with an entire matrix $\mathbf{X}$ of instances?

(Recall $\mathbf{X}$ is the data matrix, $\mathbf{x}$s stacked on top of each other)

(Recall

Which to transpose? $\boldsymbol{\theta}^\top \mathbf{X}$ or $\mathbf{X}\boldsymbol{\theta}$?

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

e.g., $\mathbf{X}$ consisting of $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$

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

e.g., $\mathbf{X}$ consisting of $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$

$$= \begin{bmatrix} x_1^{(1)} & x_2^{(1)} & x_3^{(1)} \\ x_1^{(2)} & x_2^{(2)} & x_3^{(2)} \end{bmatrix} \times \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix} = \begin{bmatrix} \theta_1 x_1^{(1)} + \theta_2 x_2^{(1)} + \theta_3 x_3^{(1)} \\ \theta_1 x_1^{(1)} + \theta_2 x_2^{(2)} + \theta_3 x_3^{(3)} \end{bmatrix}$$

$$= \begin{bmatrix} \boldsymbol{\theta}^\top \mathbf{x}^{(1)} \\ \boldsymbol{\theta}^\top \mathbf{x}^{(2)} \end{bmatrix}$$

$$= \begin{bmatrix} \hat{y}^{(1)} \\ \hat{y}^{(2)} \end{bmatrix}$$

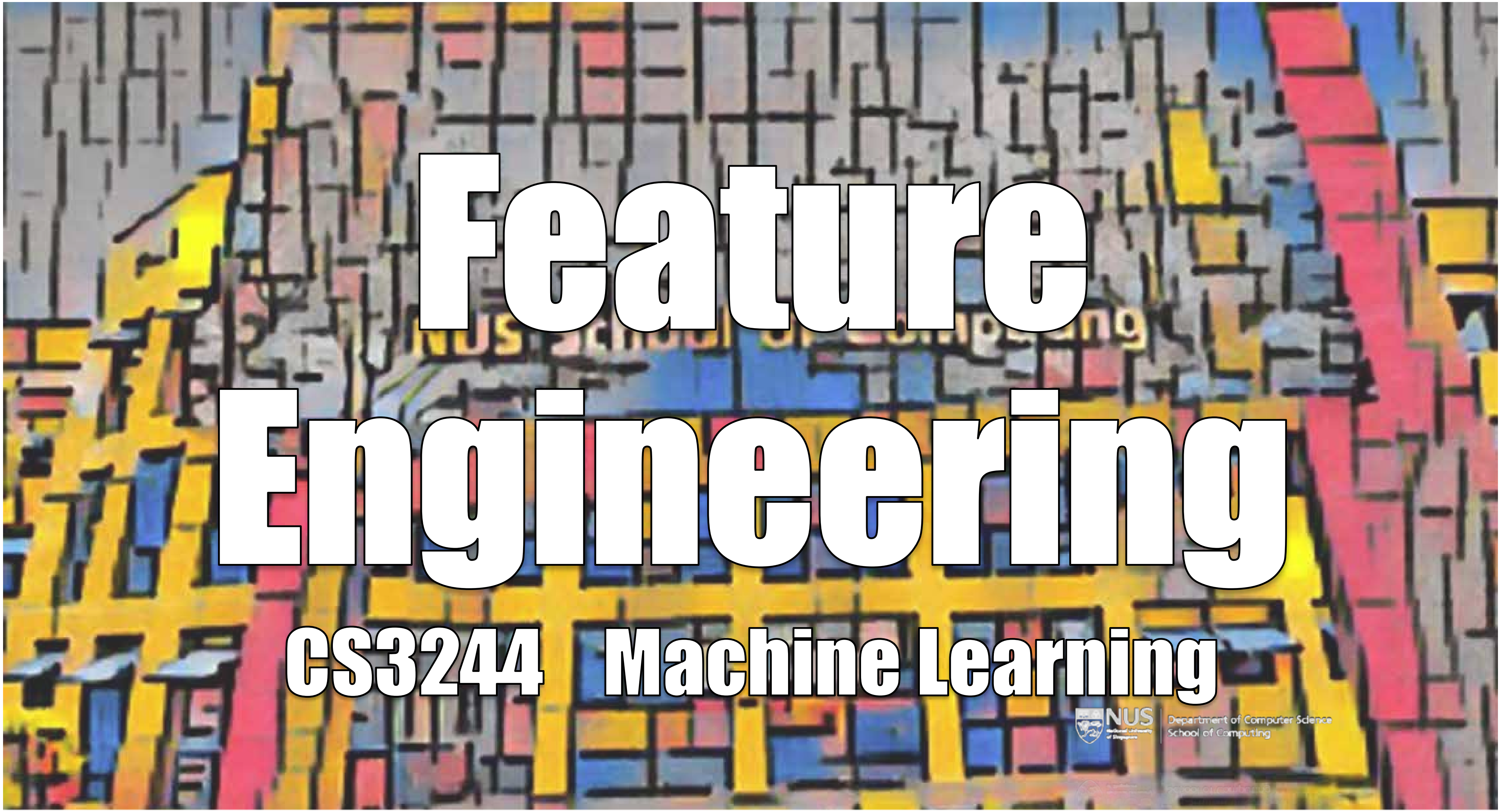
A simple $\mathcal{H}$: hyperplane with a threshold (bias)

For an input $\mathbf{x} = (x_1, x_2, \dots, x_n)$ *'attributes of a customer'*

- Approve credit if: $\sum_{i=1}^{n} \theta_i x_i > 0$
- Deny credit otherwise: $\sum_{i=1}^{n} \theta_i x_i < 0$

This linear formula $h \epsilon \mathcal{H}$ can be written as:

$$h_\theta(x) = \text{sign}\,(\sum_{i=1}^{n} \theta_i x_i)$$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MNIST (recap)

Each digit is a 16x16 pixel gray-intensity image.

[-1 -1 -1 -1 -1 -1 -1 -0.63 0.86 -0.17 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -0.99 0.3 1 0.31 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -0.41 1 0.99 -0.57 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -0.68 0.83 1 0.56 -1 -1 -1 -1
-1 -1 -1 -1 -1 -1 -1 -0.94 0.54 1 0.78 -0.72 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 0.1 1 0.92 -0.44 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -0.26 0.95 1 -0.16 -1 -1 -1 -0.99 -0.71 -0.83 -1 -1 -1 -1 -1 -0.8 0.91 1 0.3 -
0.96 -1 -1 -0.55 0.49 1 0.88 0.09 -1 -1 -1 -1 0.28 1 0.88 -0.8 -1 -0.9 0.14 0.97 1 1 1 0.99 -0.74 -1 -1 -0.95 0.84 1 0.32 -1 -1 0.35 1 0.65 -0.10 -0.18 1 0.98 -0.72 -1 -1 -0.63 1 1 0.07 -0.92 0.11
0.96 0.30 -0.88 -1 -0.07 1 0.64 -0.99 -1 -1 -0.67 1 1 0.75 0.34 1 0.70 -0.94 -1 -1 0.54 1 0.02 -1 -1 -1 -0.90 0.79 1 1 1 1 0.53 0.18 0.81 0.83 0.97 0.86 -0.63 -1 -1 -1 -1 -0.45 0.82 1 1 1 1 1 1 1 1
0.13 -1 -1 -1 -1 -1 -1 -0.48 0.81 1 1 1 1 1 1 0.21 -0.94 -1 -1 -1 -1 -1 -1 -1 -0.97 -0.42 0.30 0.82 1 0.48 -0.47 -0.99 -1 -1 -1 -1]

Input representation

Raw input $\mathbf{x} = (x_0, x_1, x_2, x_3, x_4, \dots, x_{256})$

Too many (257) parameters!

Linear model: $(\theta_0, \theta_1, \theta_2, \dots, \theta_{256})$

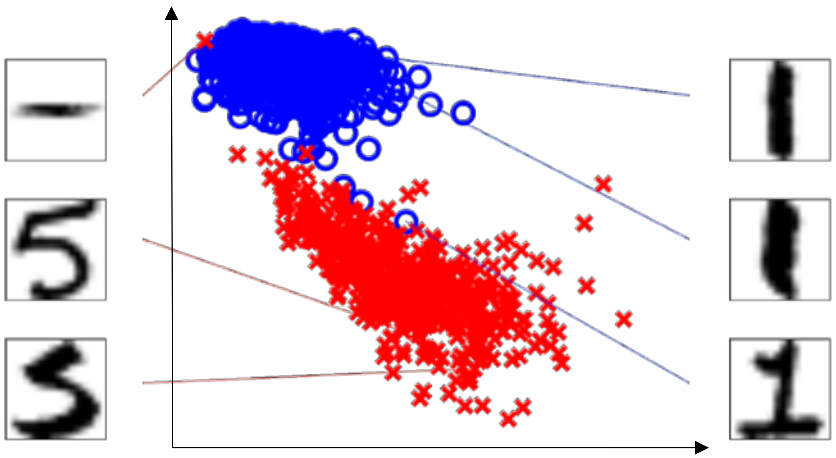
Features: extract useful information, e.g.,

Intensity and symmetry: $\mathbf{x} = (x_0, x_1, x_2)$

Linear model: $(\theta_0, \theta_1, \theta_2)$

Illustration of features

$\mathbf{x} = (x_0, x_1, x_2)$ x_1= intensity x_2= symmetry



Your Turn: which axes is which?

Linear Regression

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Credit Approval

How much credit do we extend this person?

Criterion	Value
Age	32 years
Gender	Male
Salary	40 K
Debt	26 K
…	…
Years in Job	1 year
Years at Current Residence	3 years

~~Classification: Approve/Deny~~

- Regression: Credit line (real-valued dollar amount)
- Input: <*table on the left*>
- Linear regression output: $h_\theta(\mathbf{x}) = \sum_{i=0}^{n} \theta_i x_i = \theta^\top \mathbf{x}$
  $= \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$
- Officers decide on credit lines based on historical data $\mathbf{X}$: $(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(m)}, y^{(m)})$

$y^{(j)} \in \mathbb{R}$ is the credit line for customer $x^{(j)}$; regression tries to replicate this.

Artwork credits: Project DebtRelief

Linear Regression

$$\mathbf{X}\boldsymbol{\theta}$$

$\mathbb{R}$-valued cost function

How well does $h_\theta(\mathbf{x}) = \theta^\top \mathbf{x}$ approximate $f(\mathbf{x})$?

In linear regression, we use *squared error*: $(h_\theta(\mathbf{x}) - f(\mathbf{x}))^2$

Training error:

$\mathbb{R}$-valued cost function

How well does $h_\theta(\mathbf{x}) = \theta^\top \mathbf{x}$ approximate $f(\mathbf{x})$?

In linear regression, we use *squared error*: $(h_\theta(\mathbf{x}) - f(\mathbf{x}))^2$

Training error:

The sweet spot: Plausible AND Convenient

$$L_{train}(h) = \underbrace{\frac{1}{m}\sum_{j=1}^{m}}_{\text{Pointwise Average}} \underbrace{(h_\theta(x^{(j)}) - y^{(j)})^2}_{\text{How bad is our prediction?}}$$

Illustration of linear regression

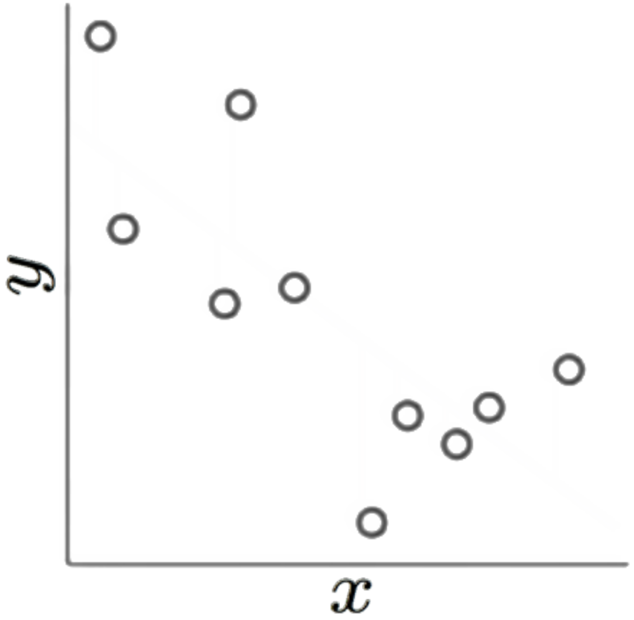
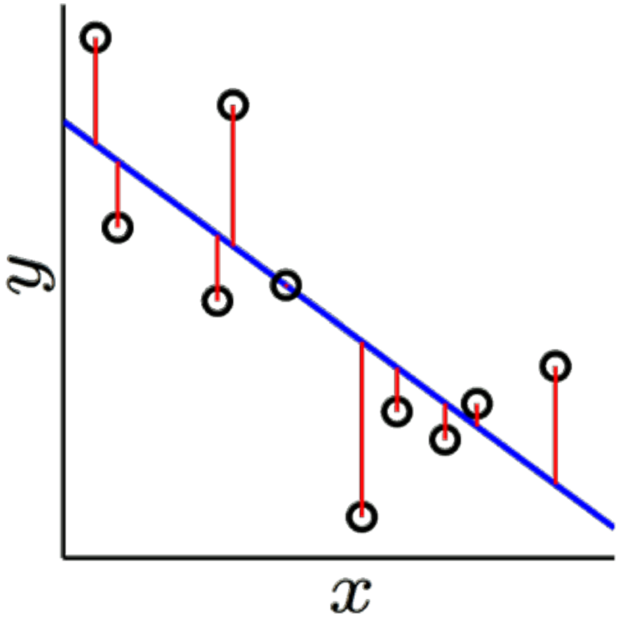
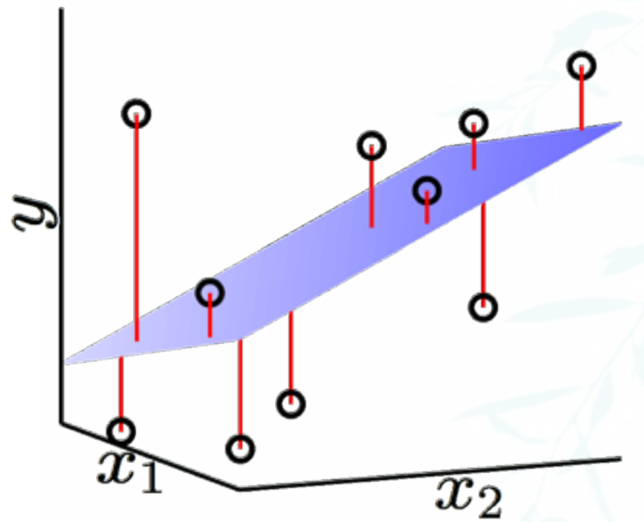


Illustration of linear regression





Hypothesis: $h_\theta(\mathbf{x}) = \theta_0 + \theta_1 x_1$


Logistic
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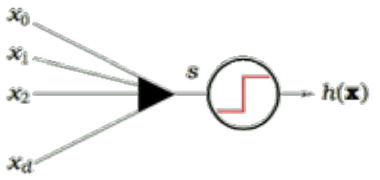
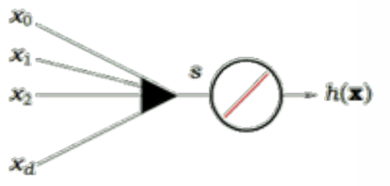
A third linear model

$$s = \sum_{i=0}^{n} \theta_i x_i$$

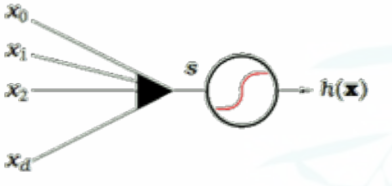
Linear classification



Linear regression



Logistic regression



The logistic function g

We choose a form for $g(\cdot)$ out of convenience.
We use the logistic function, which has the form:

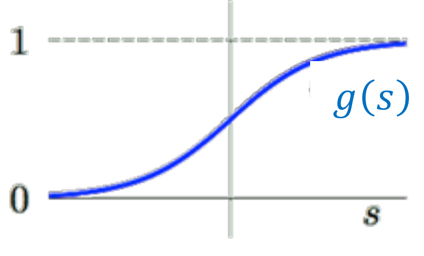
$$g(s) = \frac{exp^s}{1 + exp^s}$$

The logistic function g

We choose a form for $g(\cdot)$ out of convenience.
We use the logistic function, which has the form:

$$g(s) = \frac{exp^s}{1 + exp^s}$$

$g(s)$: needs to map any x: $\mathbb{R}$ to y: $[0,1]$



Soft threshold: uncertainty

Sigmoid: flattened out 's' shape

Probability Interpretation

$h_\theta(\mathbf{x}) = g(s)$ is interpreted as a probability

Logistic regression $\equiv y \in [0,1]$

Example:	*Prediction of heart attacks*
Input $\mathbf{x}$:	cholesterol level, age, weight, diabetic, etc.
output $g(s)$:	Likelihood of a heart attack
The signal:	$s = \theta^\top \mathbf{x}$ “risk score”

Photo credits: Wikipedia - Chinese Buffet

Labels are binary, yet our outputs are probabilities

$$\mathbf{X} = \left(\mathbf{x}^{(1)}, y^{(1)} = \pm 1\right), \dots \left(\mathbf{x}^{(m)}, y^{(m)} = \pm 1\right)$$

$\mathbf{x}^{(j)}$ – a person's health information

$y^{(j)} = \pm 1$ – did they have a heart attack?

Why?

We cannot measure a probability.

We can only see the occurrence of an event and try to infer a probability.

Genuine Probability

Data $(\mathbf{x}, y)$ with binary y, generated by a noisy target:

$$P(y|x) = \begin{cases} f(\mathbf{x}) & \text{for } y = +1; \\ 1 - f(\mathbf{x}) & \text{for } y = -1. \end{cases}$$

The target $f: \mathbb{R}^n \to [0,1]$ is the probability

Learn $h_\theta(\mathbf{x}) = g(\boldsymbol{\theta}^\top \mathbf{x}) \approx f(\mathbf{x})$

Cost Function for Logistic Regression

For logistic regression,

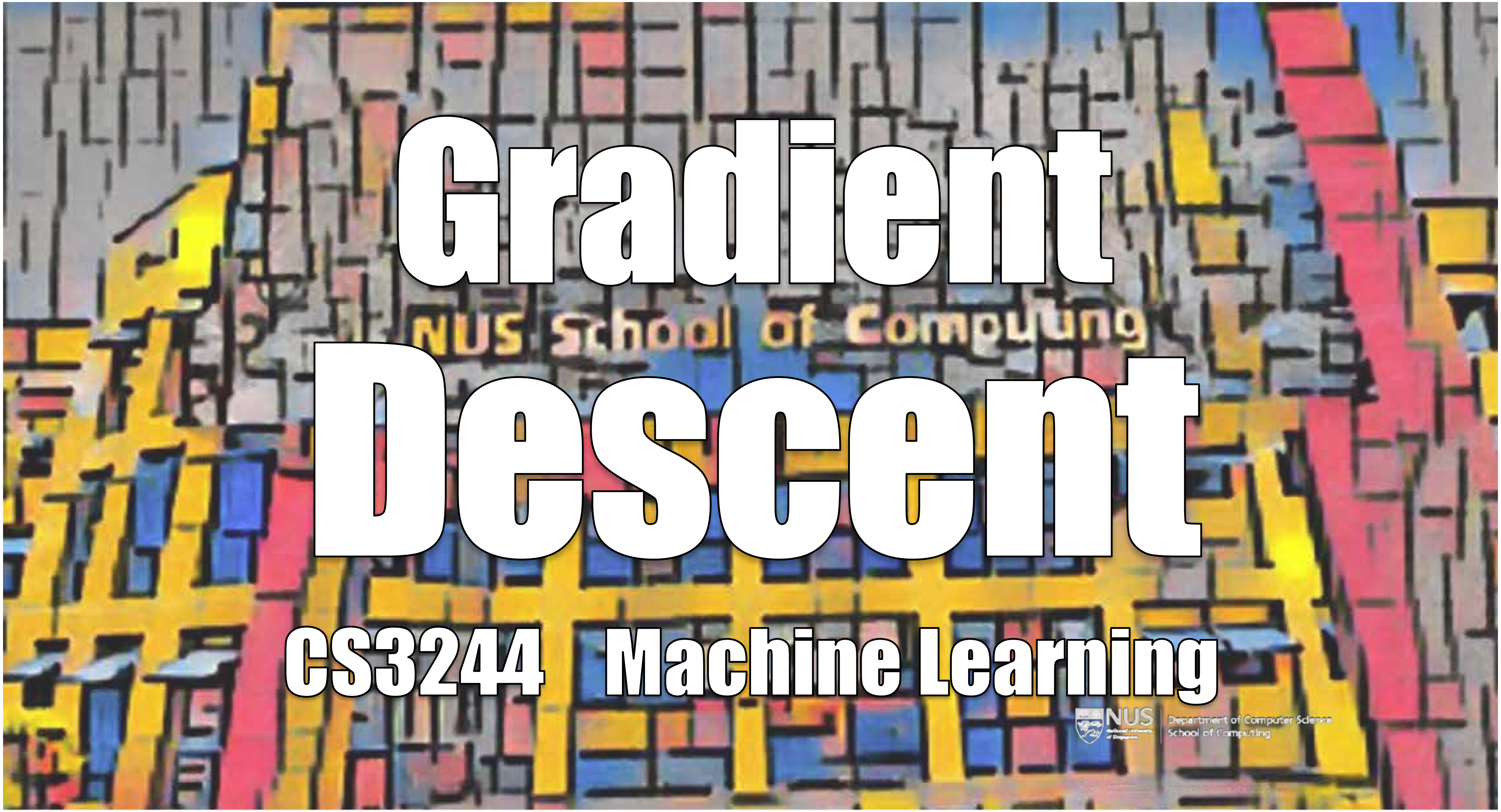
$$L_{train}(\boldsymbol{\theta}) = \frac{1}{m}\sum_{j=1}^{m} ln(1 + exp^{-y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}})$$

Iterative Solution

Compare to linear regression:

$$L_{train}(\boldsymbol{\theta}) = \frac{1}{m}\sum_{j=1}^{m}\left(\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)} - y^{(j)}\right)^2$$

Closed-form solution; but iteration also possible


Gradient
Descent
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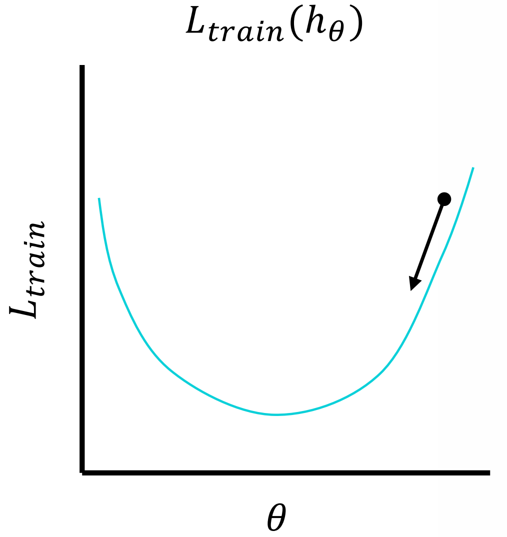
Climbing up (down) one step at a time

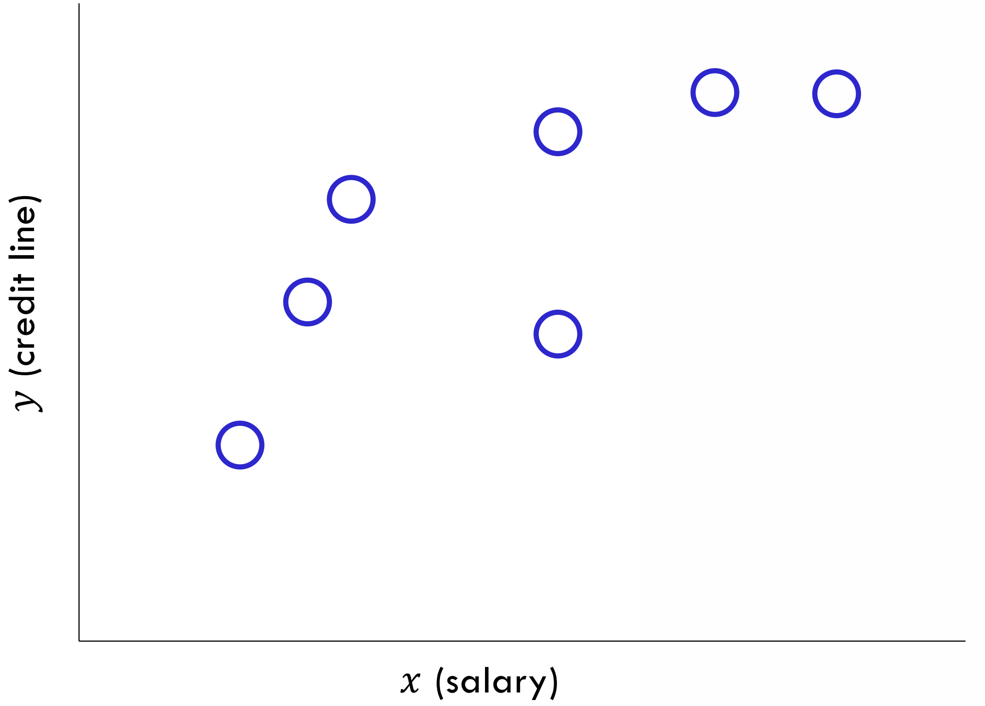
Photo credits: Wikimedia

Our L_{train} only has one valley

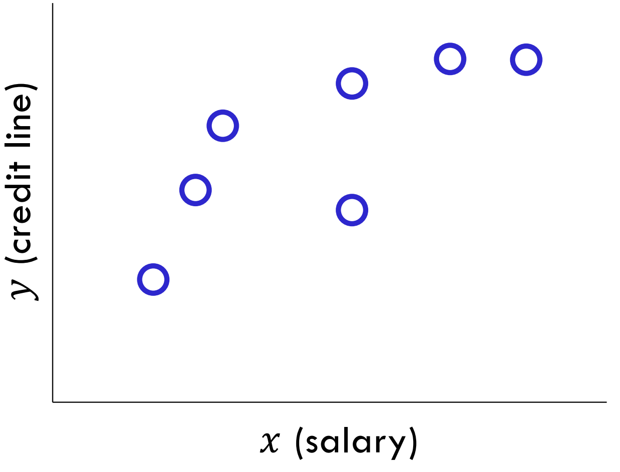


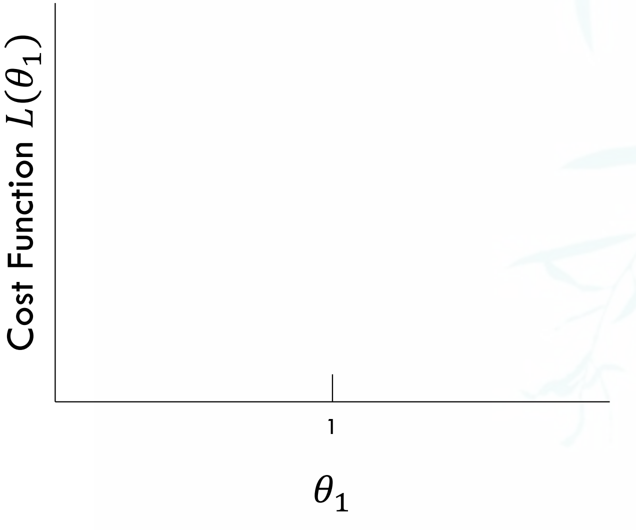
… Because L_{train} is a convex function of $\boldsymbol{\theta}$.

Univariate Linear Regression: Salary to predict Credit Line

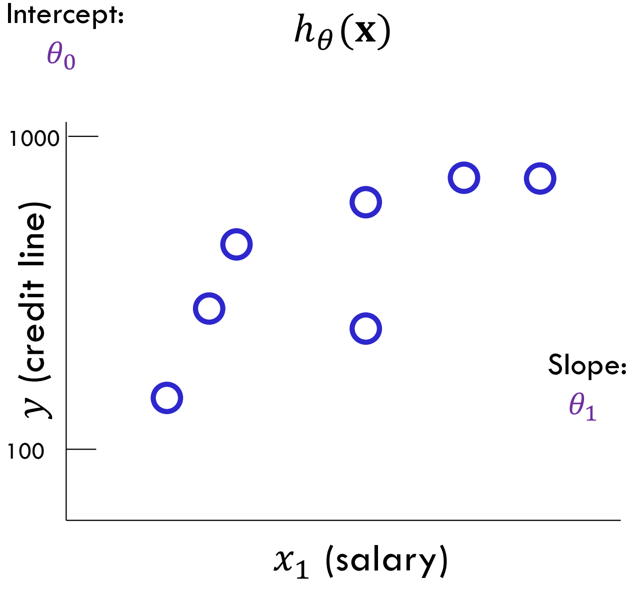


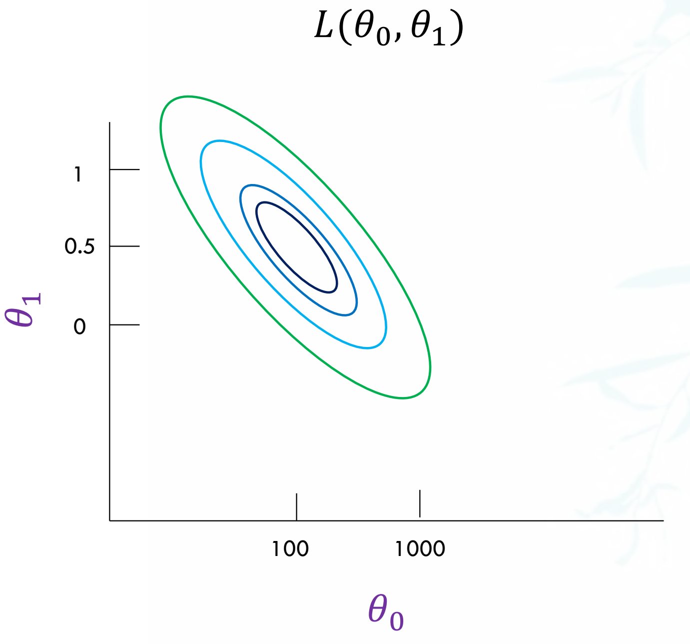
Ignoring the bias term





Cost Function $L(\theta_0, \theta_1)$





Iterative method: gradient descent

General method for nonlinear optimization

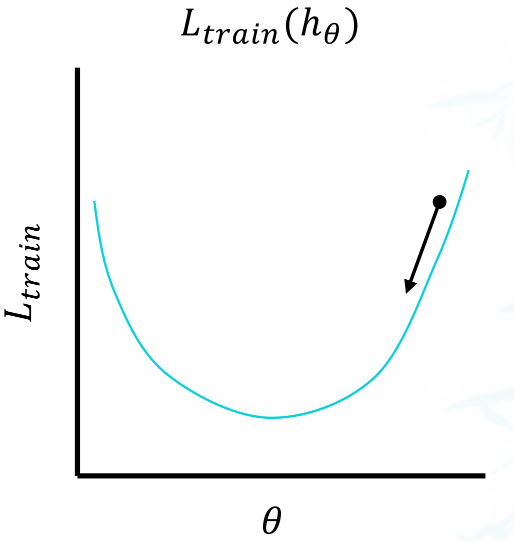
Start at $\theta(0)$; take a step along steepest slope

Notation: $\boldsymbol{\theta}(t) \equiv$ set of parameters at iteration t

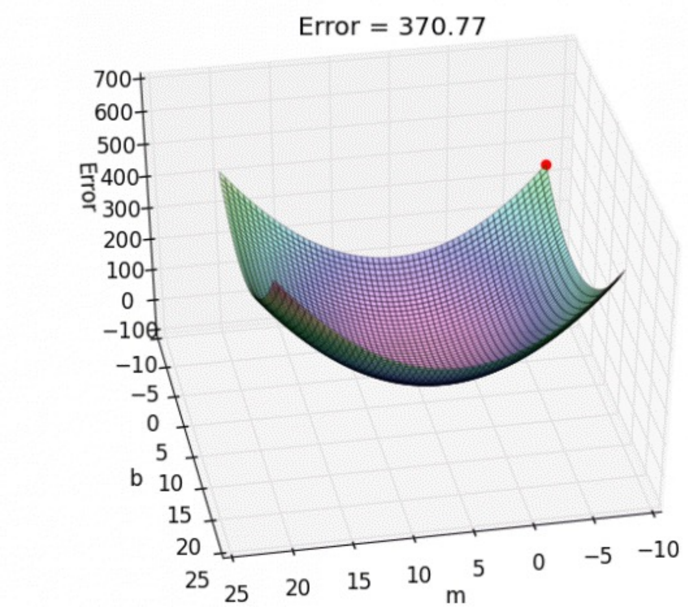
Fixed step size η : $\theta(1) = \theta(0) + \eta v$

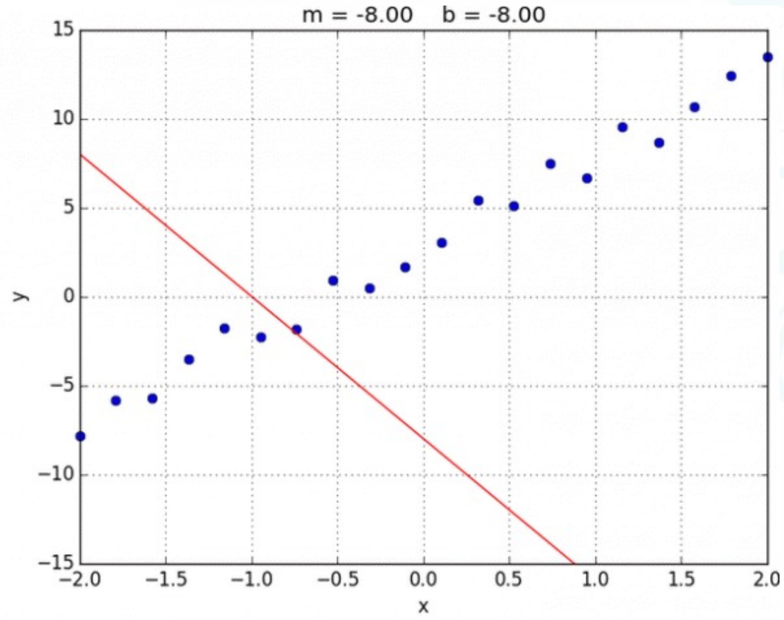
We get to pick the direction of v. What is the best direction to pick?

The one to minimize L_{train}.



Gradient descent can minimize any smooth function. Oh yeah!





Credits: Alykhan Tejani's Medium Post

Formula for the direction v

$$\Delta L_{train} = L_{train}(\theta(t+1)) - L_{train}(\theta(t))$$

$$= L_{train}(\theta(t) + \eta v) - L_{train}(\theta(t))$$

$$= \eta \nabla L_{train}(\theta(t)^{\top}) v + O(\eta^2)$$

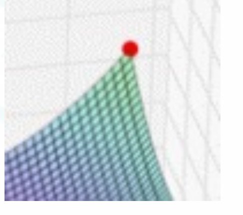
$$\geq -\eta \left\| \nabla L_{train}(\theta(t)) \right\|$$

Taylor approximation
$f(x_1) =$
$f(x_0) + \nabla f(x_0) \cdot (x_1 - x_0)$
$+ O(\|x_1 - x_0\|^2)$

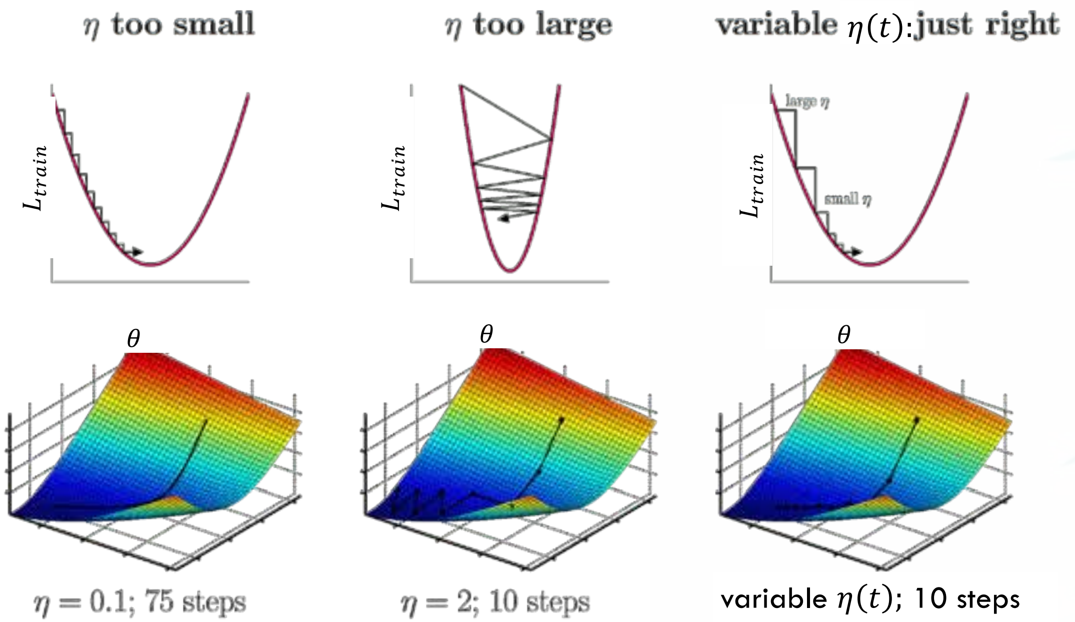
Notation: ∇ ("nabla") ≡ Gradient. Generalization of slope for higher dimensions

Create v to be a unit vector:

$$v = -\frac{\nabla L_{train}(\theta(\mathrm{t}))}{\|\nabla L_{train}(\theta(t))\|}$$



Goldilocks step size



η should increase with the slope

Varying step size, for free

Instead of

$$\Delta\theta = \eta v$$

$$= -\eta \frac{L_{train}(\theta(t))}{\|L_{train}(\theta(t))\|}$$

Have

$$\Delta\theta = -\alpha L_{train}(\theta(t))$$

Fixed learning <u>rate</u> α instead of fixed learning <u>step</u> η

Logistic regression algorithm

1. Initialize the weights at $t = 0$ to $\theta(0)$
2. Do
3. Compute the gradient

$$\nabla(t) = \nabla L_{train}(\theta(t)) = -\frac{1}{m}\sum_{j=1}^{m} \frac{y^{(j)}x^{(j)}}{1 + e^{y^{(j)}\theta(t)^{\top}x^{(j)}}}$$

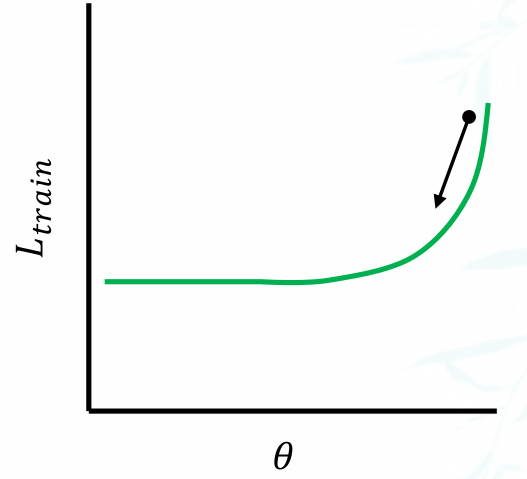
4. // Move in the direction $v(t) = -\nabla(t)$
   Update the weights $\theta(t+1) = \theta(t) - \alpha \nabla L_{train}$
5. Continue to next iteration, until it is time to stop
6. Return the final weights θ^*

Termination Condition

When to stop?

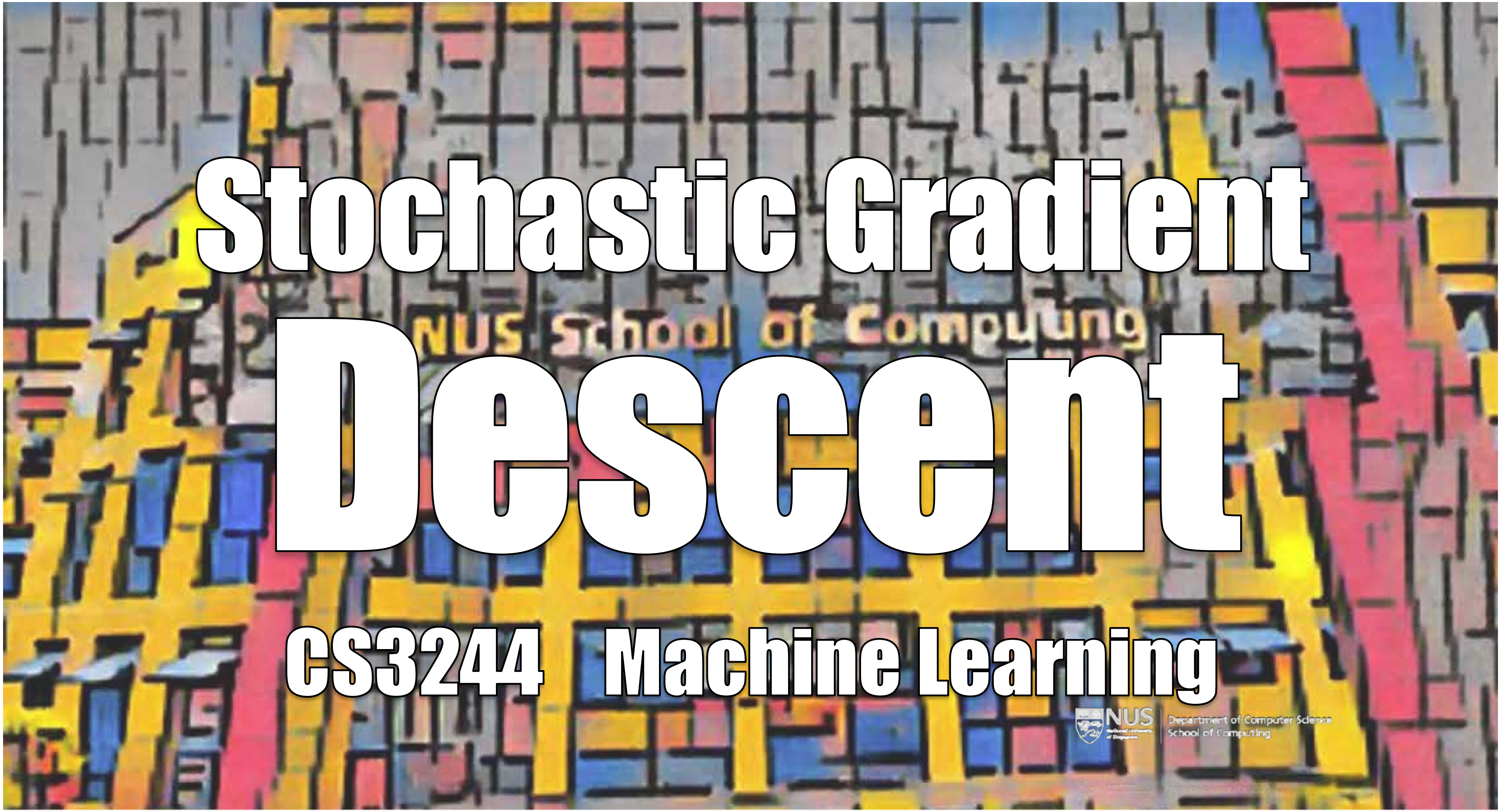
Natural choice: *gradient* < *threshold*

But lots of flat regions in most spaces:



Instead, use criteria:

1. error change is small and/or;
2. error is small;
3. maximum number of iterations is reached.


Stochastic Gradient
Descent
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(Batch) Gradient Descent

Gradient Descent minimizes:

$$L_{train}(\theta) = \frac{1}{m}\sum_{j=1}^{m} \underbrace{l\left(h_\theta\left(\mathbf{x}^{(j)}\right), y^{(j)}\right)}_{\ln(1+e^{y^{(j)}\theta^\top \mathbf{x}^{(j)}})}$$

By iterative steps along $-\nabla L$:

$$\Delta\theta = -\alpha \nabla L_{train}(\theta(t))$$

$-\alpha\nabla L_{train}$ is based on **all** examples $(\mathbf{X}, y)$

This is **"batch"** Gradient Descent

Overly conservative?

In Zoom breakout or physical subgroups:

(5 mins): Suggest a way to speed up Gradient Descent

Hint: $-\alpha \nabla L_{train}$ is based on **all** examples $(\mathbf{X}, y)$

Ask one member to write it to the #general thread. Upvote others that you like.

Stochastic Gradient Descent

A variation of GD that considers only the error on one data point.

Pick <u>one</u> $(\mathbf{x}^{(*)}, y^{(*)})$ at a time.

Apply GD to $l(h_\theta(\mathbf{x}^{(*)}), y^{(*)})$

"Average" Direction: $\mathbb{E}_*\left[-\nabla l(h_\theta(\mathbf{x}^{(*)}), y^{(*)})\right]$

$$= \frac{1}{m}\sum_{k=1}^{m} -\nabla l(h_\theta(\mathbf{x}^{(*)}), y^{(*)})$$
$$= -\nabla L_{train}$$

Stochastic Gradient Descent (SGD)

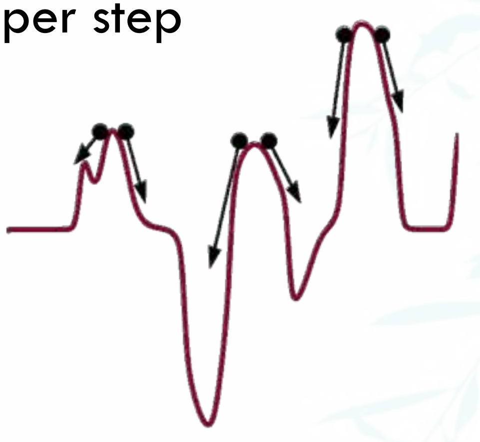
Photo credits: Wikipedia - Singapore Dollar

Benefits of SGD

1. Cheaper computation: Fraction $1/m$ cheaper per step

2. Stochastic: Helps escape local minima

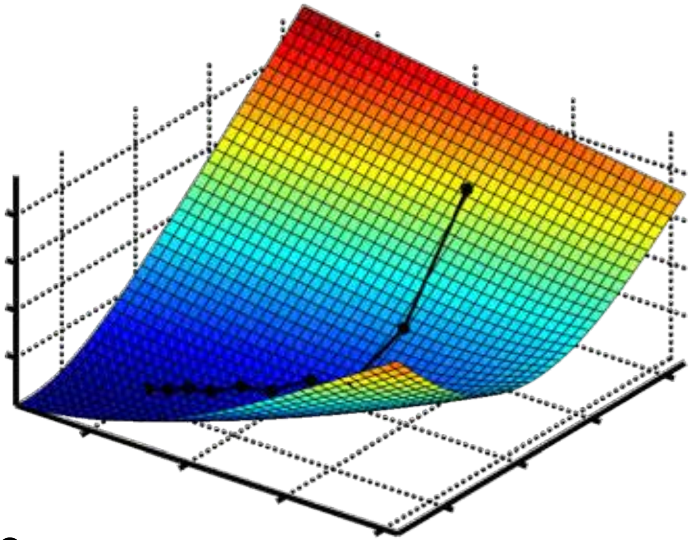
3. Simple



Rule of Thumb:
$\alpha = 0.1$ usually works!

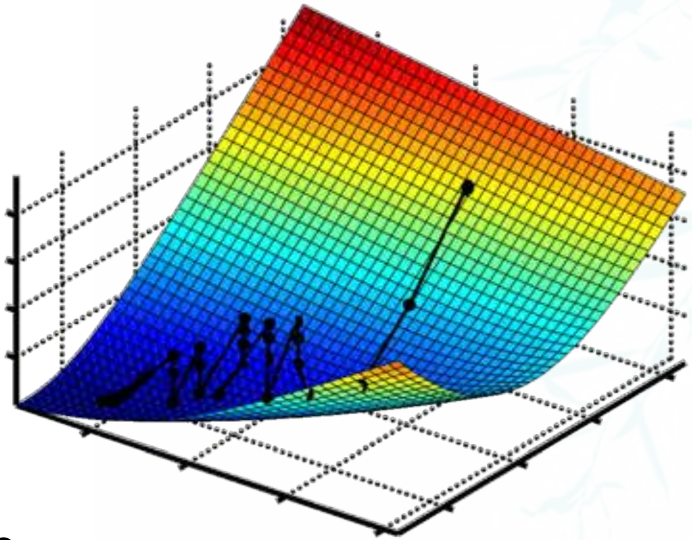
GD vs. SGD on $m = 10$

GD



10 steps

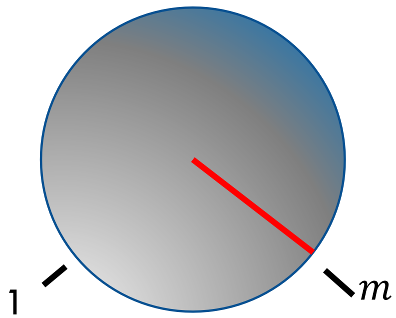
SGD



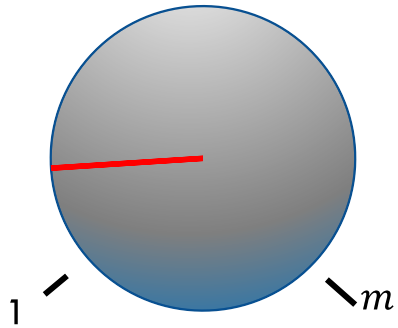
30 steps

Mini Batch Gradient Descent

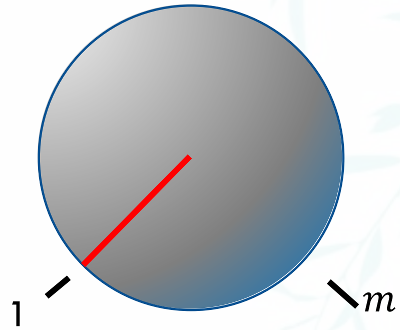
Gradient Descent



Mini Batch



Stochastic Gradient Descent



Batch size determined

Normal Equation for Linear Regression

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⚠️ Math Ahead

This part of lecture has heavy math.

You may need to pay close attention and perhaps review the recording later.

The expression for L_{train}

$$L_{train} = \frac{1}{m}\sum_{j=1}^{m}(\boldsymbol{\theta}^\top \mathbf{x}^{(j)} - y^{(j)})^2$$

$$= \frac{1}{m}\|\mathbf{X}\boldsymbol{\theta} - \mathbf{y}\|^2$$

where $\mathbf{X} = \begin{bmatrix} -{\mathbf{x}^{(1)}}^\top - \\ -{\mathbf{x}^{(2)}}^\top - \\ -{\mathbf{x}^{(3)}}^\top - \\ \vdots \\ -{\mathbf{x}^{(m)}}^\top - \end{bmatrix}$, $\mathbf{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ y^{(3)} \\ \vdots \\ y^{(m)} \end{bmatrix}$

Minimizing L_{train}

Let's re-write L_{train} first.

$$L_{train} = \frac{1}{m} \|\mathbf{X}\boldsymbol{\theta} - \mathbf{y}\|^2$$

Minimizing L_{train}

Let's re-write L_{train} first.

$$L_{train} = \frac{1}{m}\|\mathbf{X\theta} - \mathbf{y}\|^2$$

$$= (\mathbf{X\theta} - \mathbf{y})^\top(\mathbf{X\theta} - \mathbf{y})$$

$$= (\mathbf{X\theta})^\top\mathbf{X\theta} - (\mathbf{X\theta})^\top\mathbf{y}$$

$$-\mathbf{y}^\top\mathbf{X\theta} \quad + \mathbf{y}^\top\mathbf{y}$$

$$= \mathbf{\theta}^\top\mathbf{X}^\top\mathbf{X\theta} - 2(\mathbf{X\theta})^\top\mathbf{y} + \mathbf{y}^\top\mathbf{y}$$

$\mathbf{y}$ and $\mathbf{X\theta}$ both vectors, ordering in multiplication doesn't matter

Then solve for $\mathbf{\theta}$:

$$\frac{\partial L_{train}}{\partial \mathbf{\theta}} \equiv$$

$\nabla L \equiv$ A vector with all n component partial derivatives of L.

$$\frac{\partial L_{train}}{\partial \mathbf{\theta}} = \begin{bmatrix} \frac{\partial L}{\partial \theta_0}(\theta_0, \dots, \theta_n) \\ \dots \\ \frac{\partial L}{\partial \theta_n}(\theta_0, \dots, \theta_n) \end{bmatrix}$$

Jacobian: stack of gradients as partial derivatives.

Minimizing L_{train}

Let's re-write L_{train} first.

$$L_{train} = \frac{1}{m}\|\mathbf{X\theta} - \mathbf{y}\|^2$$
$$= (\mathbf{X\theta} - \mathbf{y})^\top(\mathbf{X\theta} - \mathbf{y})$$
$$= (\mathbf{X\theta})^\top\mathbf{X\theta} - (\mathbf{X\theta})^\top\mathbf{y}$$
$$-\mathbf{y}^\top\mathbf{X\theta} \quad + \mathbf{y}^\top\mathbf{y}$$
$$= \boldsymbol{\theta}^\top\mathbf{X}^\top\mathbf{X\theta} - 2(\mathbf{X\theta})^\top\mathbf{y} + \mathbf{y}^\top\mathbf{y}$$

Then solve for $\boldsymbol{\theta}$:

$$\frac{\partial L_{train}}{\partial \boldsymbol{\theta}} \equiv \mathbf{X}^\top\mathbf{X\theta} - \mathbf{X}^\top\mathbf{y} = \overleftarrow{\mathbf{0}}$$
$$\mathbf{X}^\top\mathbf{X\theta} = \mathbf{X}^\top\mathbf{y}$$
$$\boldsymbol{\theta} = \left((\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\right)\mathbf{y}$$

Column of zeroes

$(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top$ is called the **pseudo inverse** of $\mathbf{X}$

The pseudo inverse $\mathbf{X}^{\dagger}$

$$\mathbf{X}^{\dagger} = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}$$

$$\underbrace{\begin{bmatrix} \quad & \quad & \quad \end{bmatrix}}_{n+1 \times m} \quad \underbrace{\begin{bmatrix} \quad \\ \quad \\ \quad \end{bmatrix}}_{m \times n+1}$$

The pseudo inverse $\mathbf{X}^{\dagger}$

$$\mathbf{X}^{\dagger} = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}$$

$$\underbrace{\begin{bmatrix} \underbrace{\left[\qquad\right]}_{(n+1)\times(n+1)} \end{bmatrix}^{-1} \underbrace{\left[\qquad\qquad\right]}_{(n+1)\times m}}_{(n+1)\times m}$$

Linear regression by Normal Equation

1. Construct the matrix $\mathbf{X}$ and the vector y from the data set as follows:

$$\mathbf{X} = \underbrace{\begin{bmatrix} -\mathbf{x}^{(1)^\top} - \\ -\mathbf{x}^{(2)^\top} - \\ -\mathbf{x}^{(3)^\top} - \\ \vdots \\ -\mathbf{x}^{(m)^\top} - \end{bmatrix}}_{\text{input data matrix}}, \quad y = \underbrace{\begin{bmatrix} y^{(1)} \\ y^{(2)} \\ y^{(3)} \\ \vdots \\ y^{(m)} \end{bmatrix}}_{\text{target vector}}$$

1. Compute the pseudo inverse $\mathbf{X}^{\dagger} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top$
2. Return $\theta = \mathbf{X}^{\dagger} y$

The normal equation for LR. One-step learning!

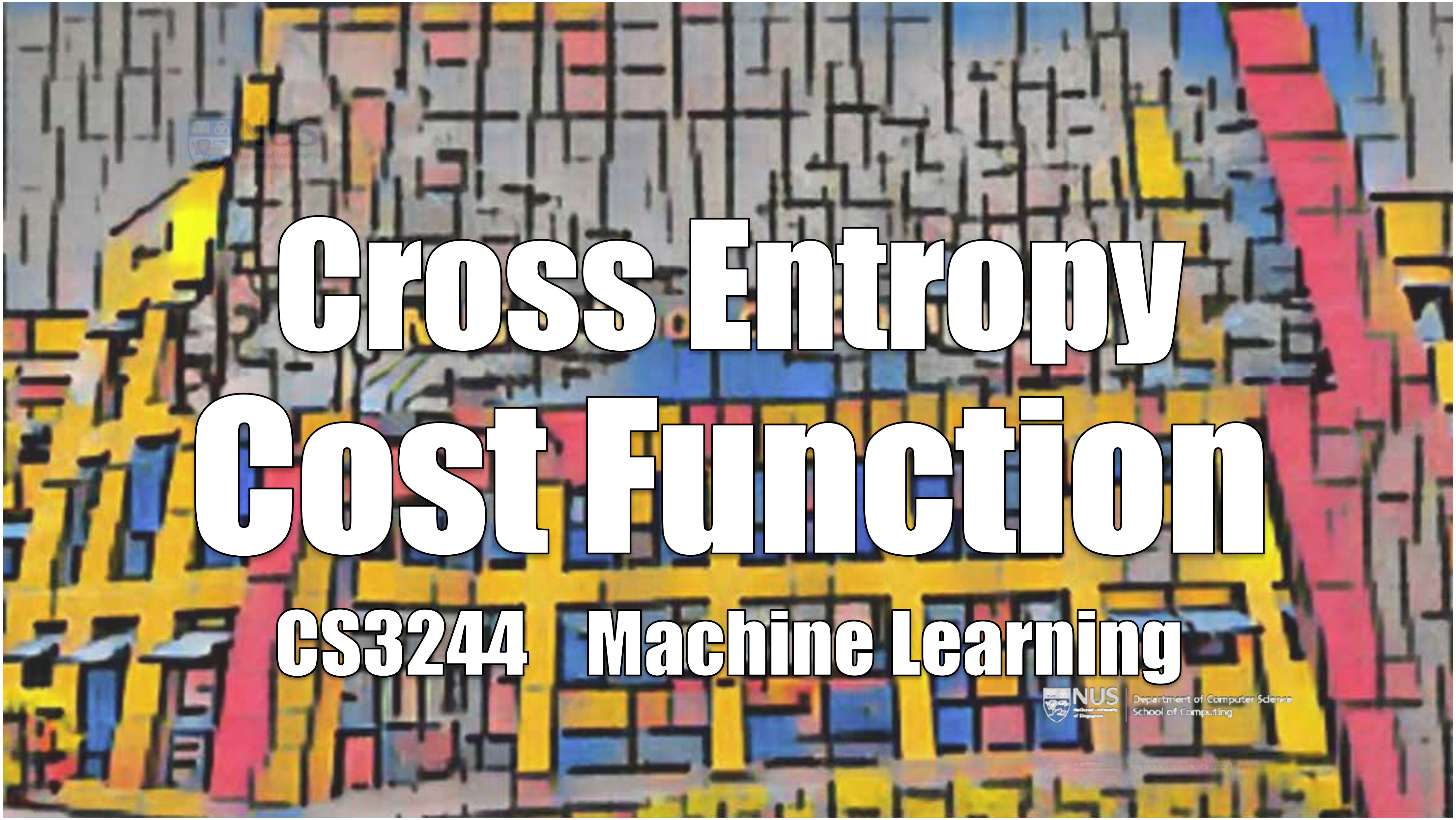
Linear Regression – Summary

Two methods for training

1. Gradient Descent
   - Works well, even when n is large
   - Works even if $\mathbf{X}^\top\mathbf{X}$ is non-invertible

Your Turn: What are some reasons that $\mathbf{X}^\top\mathbf{X}$ might not be invertible?

2. Normal Equation
   - Don't need to choose α
   - Don't need to iterate
   - Need to compute $(\mathbf{X}^\top\mathbf{X})^{-1}$, an $O(n^3)$ operation



Cross Entropy Cost Function

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Logistic Regression Cost Function

For each $(\mathbf{x}, y)$, y is generated by probability $f(\mathbf{x})$

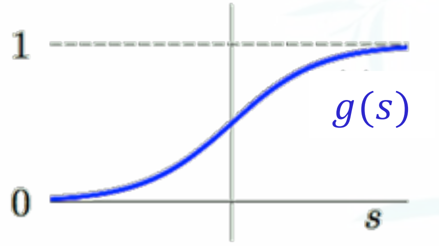
Plausible cost function based on likelihood:

If $h_\theta = f$, how "likely" is it to obtain output y from input $\mathbf{x}$?

$$P(y|\mathbf{x}) = \begin{cases} h_\theta(\mathbf{x}) & \text{for } y = +1; \\ 1 - h_\theta(\mathbf{x}) & \text{for } y = -1. \end{cases}$$

Formula for likelihood

$$P(y|\mathbf{x}) = \begin{cases} h_\theta(\mathbf{x}) & \text{for } y = +1; \\ 1 - h_\theta(\mathbf{x}) & \text{for } y = -1. \end{cases}$$



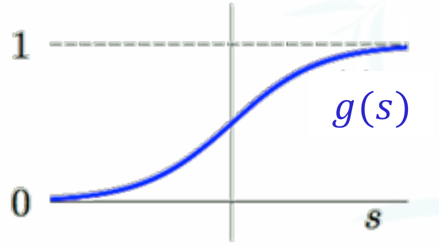
Substitute $h_\theta(\mathbf{x}) = g(\boldsymbol{\theta}^\top \mathbf{x})$,

noting $g(-s) = 1 - g(s)$

$P(y|\mathbf{x}) = g(y \cdot \boldsymbol{\theta}^\top \mathbf{x})$

Formula for likelihood

$$P(y|\mathbf{x}) = \begin{cases} h_\theta(\mathbf{x}) & \text{for } y = +1; \\ 1 - h_\theta(\mathbf{x}) & \text{for } y = -1. \end{cases}$$



Substitute $h_\theta(\mathbf{x}) = g(\boldsymbol{\theta}^\top \mathbf{x})$,

noting $g(-s) = 1 - g(s)$

$$P(y|\mathbf{x}) = g(y \cdot \boldsymbol{\theta}^\top \mathbf{x})$$

Likelihood of $\mathbf{X} = \left(\mathbf{x}^{(1)}, y^{(1)}\right), \dots, \left(\mathbf{x}^{(m)}, y^{(m)}\right)$
where samples are i.i.d. is:

$$P(y^{(1)}, \dots, y^{(m)} | \mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}) = \prod_{j=1}^{m} P\left(y^{(j)} | \mathbf{x}^{(j)}\right) \quad = \prod_{j=1}^{m} g\left(y^{(j)} \boldsymbol{\theta}^\top \mathbf{x}^{(j)}\right)$$

Maximizing the likelihood ≡ Minimizing cross entropy

$$= max \qquad \prod_{j=1}^{m} g\left(y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}\right)$$

Maximizing the likelihood ≡ Minimizing cross entropy

$$= max \qquad \prod_{j=1}^{m} g\left(y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}\right)$$

$$\Leftrightarrow max \qquad \frac{1}{\mathrm{m}}\ln\left(\prod_{j=1}^{m} g\left(y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}\right)\right)$$

$$= max \qquad \frac{1}{m}\sum_{j=1}^{m} \ln g\left(y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}\right)$$

$$\Leftrightarrow min \qquad -\frac{1}{m}\sum_{j=1}^{m} \ln g\left(y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}\right)$$

Maximizing the likelihood ≡ Minimizing cross entropy

$$= max \quad \prod_{j=1}^{m} g\left(y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}\right)$$

$$\Leftrightarrow max \quad \frac{1}{\mathrm{m}}\ln\left(\prod_{j=1}^{m} g\left(y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}\right)\right)$$

$$= max \quad \frac{1}{m}\sum_{j=1}^{m}\ln g\left(y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}\right)$$

$$\Leftrightarrow min \quad -\frac{1}{m}\sum_{j=1}^{m}\ln g\left(y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}\right)$$

$$= min \quad \frac{1}{m}\sum_{j=1}^{m}\ln\left(\frac{1}{g\left(y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}\right)}\right)$$

$$g(s) = \frac{e^{s}}{1+e^{s}} = \left[g(s) = \frac{1}{1+e^{-s}}\right]$$

$$\boxed{L_{train}(\theta) = \frac{1}{m}\sum_{j=1}^{m}\underbrace{\ln\left(1+e^{-y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}}\right)}}$$

"cross entropy" error

Maximizing the likelihood ≡ Minimizing cross entropy

$$= max \quad \prod_{j=1}^{m} g\left(y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}\right)$$

$$\Leftrightarrow max \quad \frac{1}{\mathrm{m}} \ln\left(\prod_{j=1}^{m} g\left(y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}\right)\right)$$

$$= max \quad \frac{1}{m}\sum_{j=1}^{m} \ln g\left(y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}\right)$$

$$\Leftrightarrow min \quad -\frac{1}{m}\sum_{j=1}^{m} \ln g\left(y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}\right)$$

$$= min \quad \frac{1}{m}\sum_{j=1}^{m} \ln\left(\frac{1}{g\left(y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}\right)}\right)$$

$$g(s) = \frac{e^s}{1+e^s} = \left[g(s) = \frac{1}{1+e^{-s}}\right]$$

Plug in

$$= min \quad \frac{1}{m}\sum_{j=1}^{m} \ln\left(1 + e^{-y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}}\right)$$

$$\boxed{L_{train}(\theta) = \frac{1}{m}\sum_{j=1}^{m} \underbrace{\ln\left(1 + e^{-y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}}\right)}}$$

"cross entropy" error

Summary: Minimizing L_{train}

For logistic regression,

$$L_{train}(\boldsymbol{\theta}) = \frac{1}{m}\sum_{j=1}^{m} ln(1 + e^{-y^{(j)}\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)}})$$

Iterative Solution

Compare to linear regression:

$$L_{train}(\boldsymbol{\theta}) = \frac{1}{m}\sum_{j=1}^{m} \left(\boldsymbol{\theta}^{\top}\mathbf{x}^{(j)} - y^{(j)}\right)^2$$

Closed-form Solution; Iteration also possible