EE2211 Pre-Tutorial 8

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Agenda

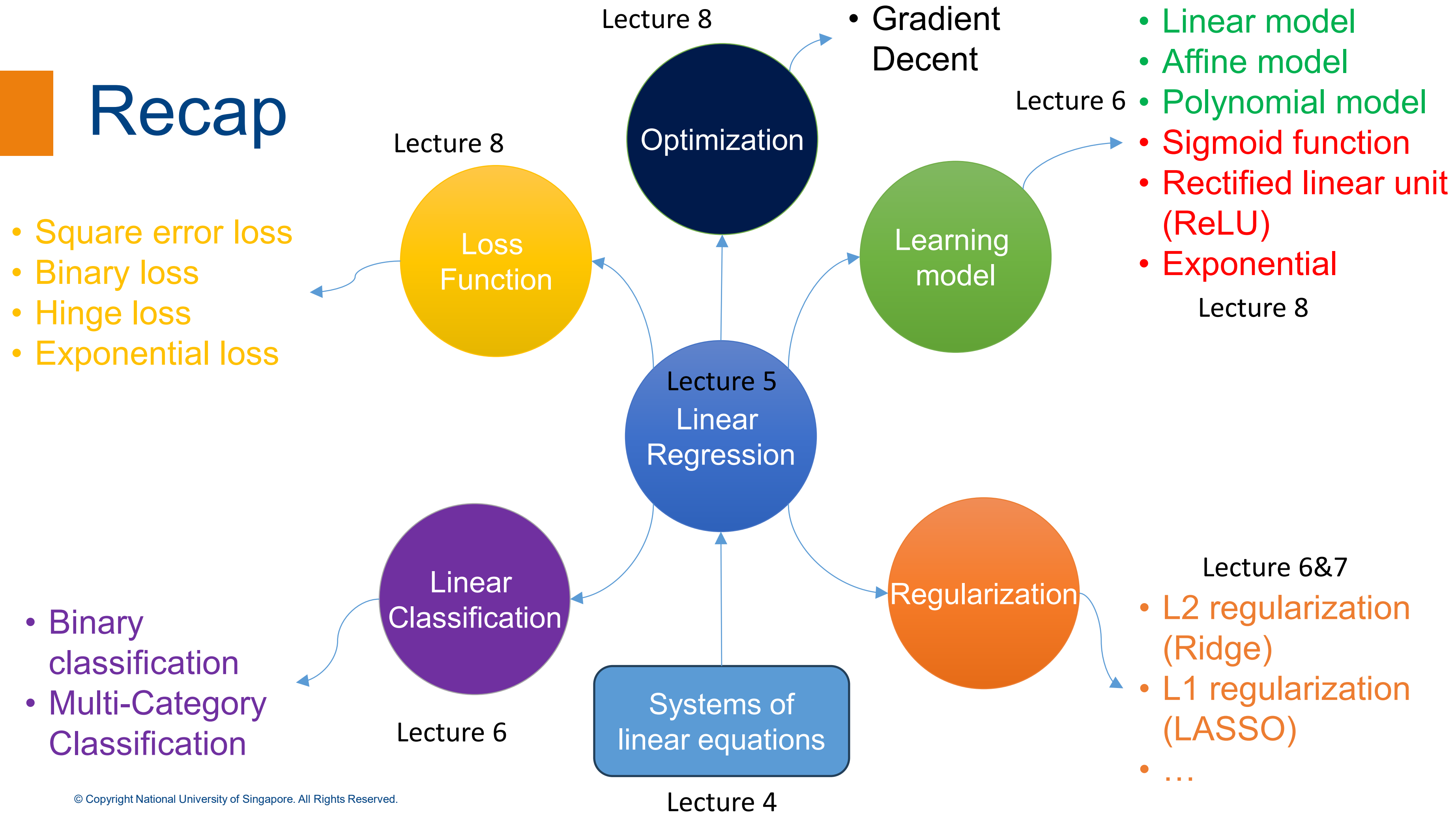
- Recap
- Self-learning
- Tutorial 8

Today’s Attendance

Recap

- Fundamental Machine Learning Algorithms I
  - Systems of linear equations
  - Least squares, Linear regression
  - Ridge regression, Polynomial regression
- Fundamental Machine Learning Algorithms II
  - Over-fitting, bias/variance trade-off
  - Optimization, Gradient descent
  - Decision Trees, Random Forest

Recap



Lecture 8
Optimization
• Gradient Decent
Lecture 8
Loss Function
• Square error loss
• Binary loss
• Hinge loss
• Exponential loss
Lecture 6
• Linear model
• Affine model
• Polynomial model
• Sigmoid function
• Rectified linear unit (ReLU)
• Exponential
Lecture 8
Learning model
Lecture 5
Linear Regression
Linear Classification
• Binary classification
• Multi-Category Classification
Lecture 6
Systems of linear equations
Lecture 4
Regularization
Lecture 6&7
• L2 regularization (Ridge)
• L1 regularization (LASSO)
• …

Loss Function & Learning Model

- For polynomial regression (previous lectures)

$$\operatorname*{argmin}_{\mathbf{w}} C(\mathbf{w}) = \operatorname*{argmin}_{\mathbf{w}} (\mathbf{P}\mathbf{w} - \mathbf{y})^T(\mathbf{P}\mathbf{w} - \mathbf{y}) + \lambda \mathbf{w}^T\mathbf{w}$$

$$= \operatorname*{argmin}_{\mathbf{w}} \sum_{i=1}^{m} (\mathbf{p}_i^T\mathbf{w} - y_i)^2 + \lambda \mathbf{w}^T\mathbf{w}$$

- Let $f(\mathbf{x}_i, \mathbf{w})$ be the prediction of target y_i from features $\mathbf{x}_i$ for i-th training sample. For example, suppose $f(\mathbf{x}_i, \mathbf{w}) = \mathbf{p}_i^T\mathbf{w}$, then above becomes

$$\operatorname*{argmin}_{\mathbf{w}} C(\mathbf{w}) = \operatorname*{argmin}_{\mathbf{w}} \sum_{i=1}^{m} (f(\mathbf{x}_i, \mathbf{w}) - y_i)^2 + \lambda \mathbf{w}^T\mathbf{w}$$

- Let $L(f(\mathbf{x}_i, \mathbf{w}), y_i)$ be the penalty for predicting $f(\mathbf{x}_i, \mathbf{w})$ when true value is y_i. For example, suppose $L(f(\mathbf{x}_i, \mathbf{w}), y_i) = (f(\mathbf{x}_i, \mathbf{w}) - y_i)^2$, then above becomes

$$\operatorname*{argmin}_{\mathbf{w}} C(\mathbf{w}) = \operatorname*{argmin}_{\mathbf{w}} \sum_{i=1}^{m} L(f(\mathbf{x}_i, \mathbf{w}), y_i) + \lambda \mathbf{w}^T\mathbf{w}$$

Building Blocks of ML Algorithms

- From previous slide

$$\underset{\mathbf{w}}{\operatorname{argmin}}\, C(\mathbf{w}) = \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{i=1}^{m} L(f(\mathbf{x}_i, \mathbf{w}), y_i) + \lambda \mathbf{w}^T \mathbf{w}$$

- To make it even more general, we can write

Cost function

Loss function L

Regrularization R

$$\underset{\mathbf{w}}{\operatorname{argmin}}\, C(\mathbf{w}) = \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{i=1}^{m} L(f(\mathbf{x}_i, \mathbf{w}), y_i) + \lambda R(\mathbf{w})$$

Learning mode f

Mapping input features to output predictions

- Learning model f reflects our belief about the relationship between the features $\mathbf{x}_i$ & target y_i
- Loss function L is the penalty for predicting $f(\mathbf{x}_i, \mathbf{w})$ when the true value is y_i
- Regularization R encourages less complex models
- Cost function C is the final optimization criterion we want to minimize
- Optimization routine to find solution to cost function

Measure the error between the model's predictions and the actual target values

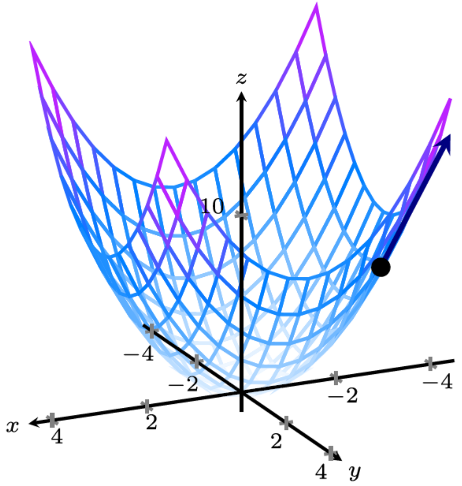
Motivations for Gradient Descent

- Different learning function f, loss function L & regularization R give rise to different learning algorithms
- In polynomial regression (previous lectures), optimal $\mathbf{w}$ can be written with the following "closed-form" formula (primal solution):

$$\hat{\mathbf{w}} = (\mathbf{P}_{train}^T \mathbf{P}_{train} + \lambda \mathbf{I})^{-1} \mathbf{P}_{train}^T \mathbf{y}_{train}$$

- For other learning function f, loss function L & regularization R, optimizing $C(\mathbf{w})$ might not be so easy
- Usually have to estimate $\mathbf{w}$ iteratively with some algorithm
- Optimization workhorse for modern machine learning is gradient descent

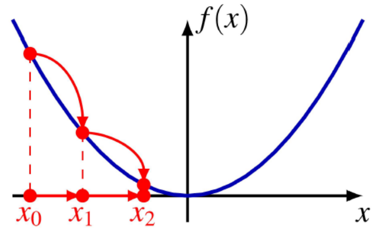
Gradient Descent Algorithm

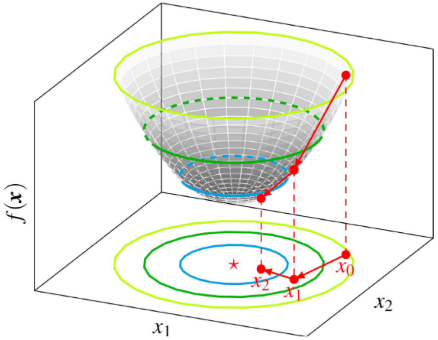


- Suppose we want to minimize $C(\mathbf{w})$ with respect to $\mathbf{w} = [w_1, \cdots, w_d]^T$
- Gradient $\nabla_{\mathbf{w}} C(\mathbf{w}) = \begin{pmatrix} \frac{\partial C}{\partial w_1} \\ \frac{\partial C}{\partial w_2} \\ \vdots \\ \frac{\partial C}{\partial w_d} \end{pmatrix}$
  - $\nabla_{\mathbf{w}} C(\mathbf{w})$ is vector & function of $\mathbf{w}$
  - $\nabla_{\mathbf{w}} C(\mathbf{w})$ is direction at $\mathbf{w}$ where C is increasing most rapidly, so $-\nabla_{\mathbf{w}} C(\mathbf{w})$ is direction at $\mathbf{w}$ where C is decreasing most rapidly
- Gradient Descent:

Initialize $\mathbf{w}_0$ and learning rate η;
while *true* **do**
  Compute $\mathbf{w}_{k+1} \leftarrow \mathbf{w}_k - \eta \nabla_{\mathbf{w}} C(\mathbf{w}_k)$
  if *converge* **then**
    return $\mathbf{w}_{k+1}$
  end
end

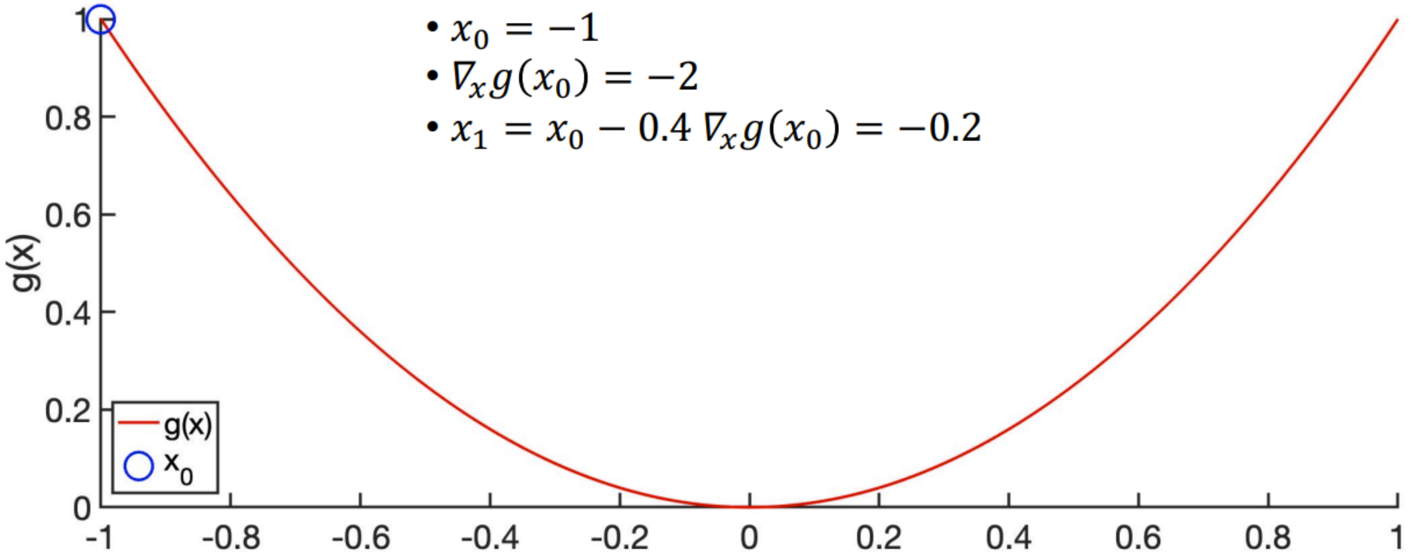
Iteration: $x^{k+1} = x^k - \tau \nabla f(x^k)$





Gradient Descent

– Gradient $\nabla_x g(x) = 2x$
– Initialize $x_0 = -1$, learning rate $\eta = 0.4$
– At each iteration, $x_{k+1} = x_k - \eta \nabla_x g(x_k)$

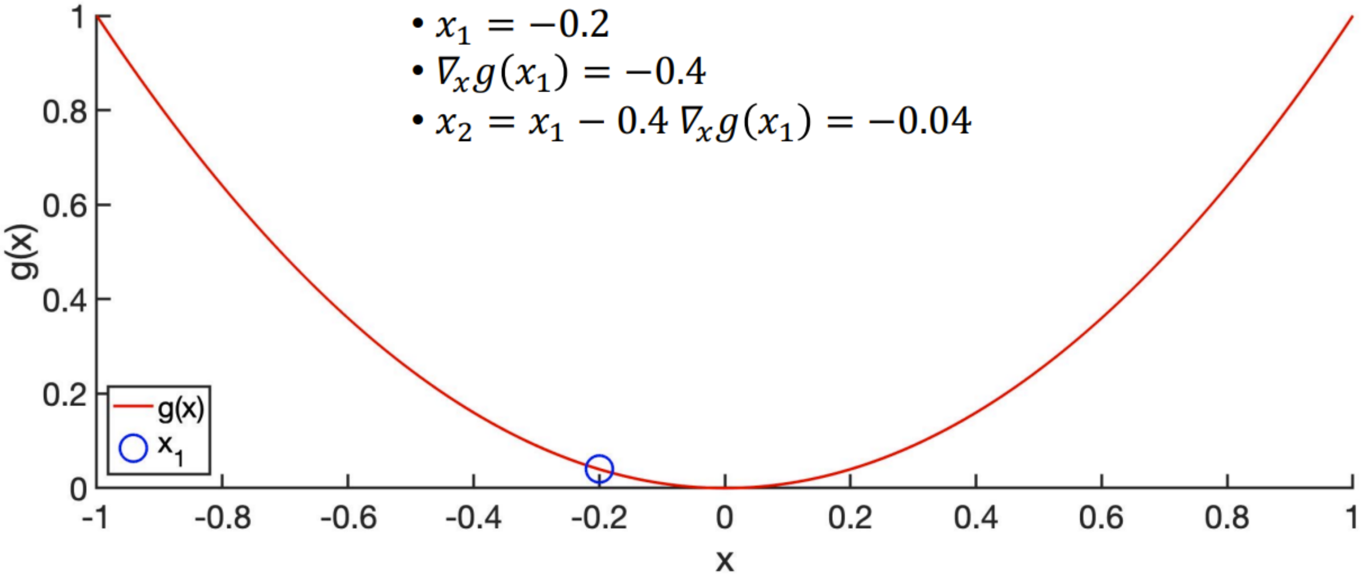


- $x_0 = -1$
- $\nabla_x g(x_0) = -2$
- $x_1 = x_0 - 0.4\, \nabla_x g(x_0) = -0.2$

Gradient Descent

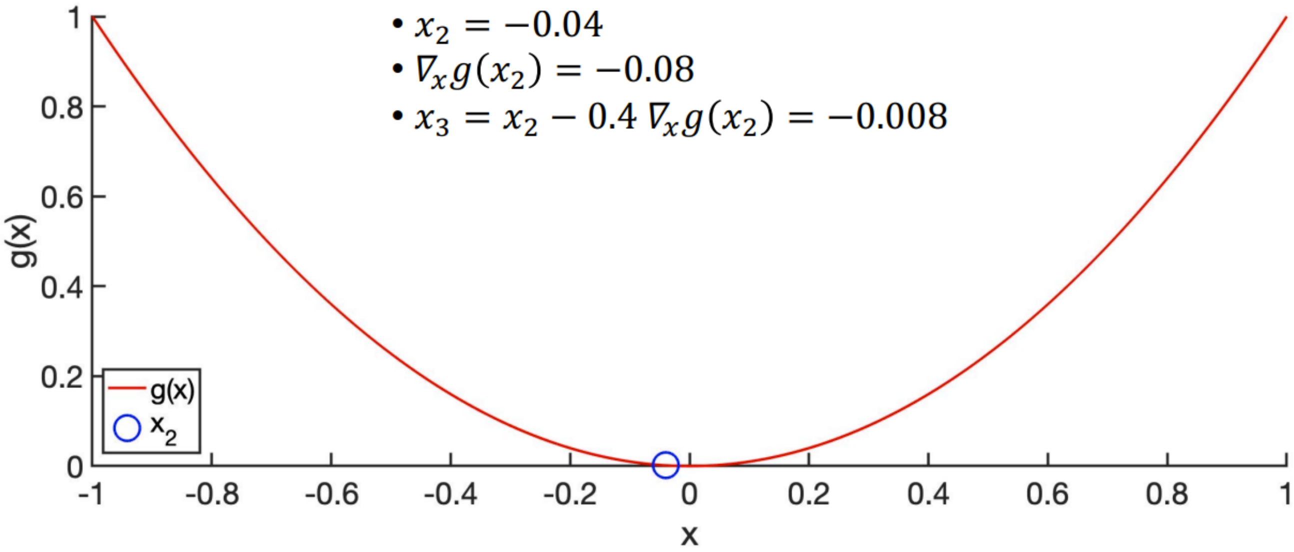
– Gradient $\nabla_x g(x) = 2x$
– Initialize $x_0 = -1$, learning rate $\eta = 0.4$
– At each iteration, $x_{k+1} = x_k - \eta \nabla_x g(x_k)$

- $x_1 = -0.2$
- $\nabla_x g(x_1) = -0.4$
- $x_2 = x_1 - 0.4\, \nabla_x g(x_1) = -0.04$



Gradient Descent

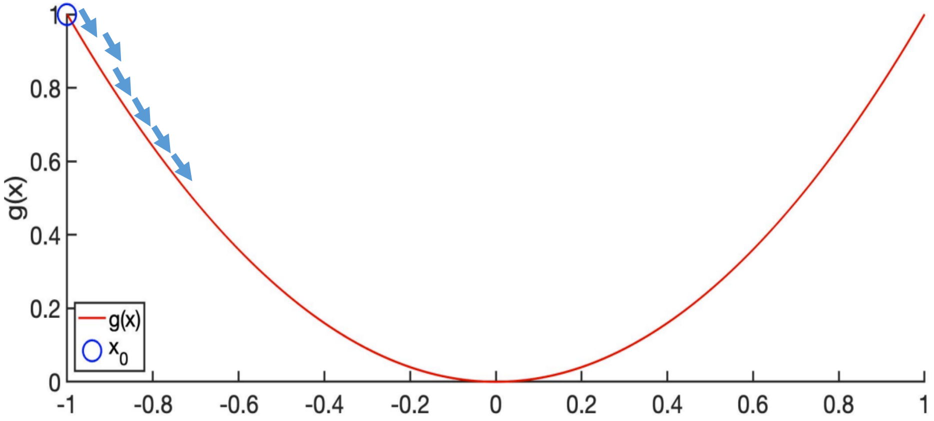
- Gradient $\nabla_x g(x) = 2x$
- Initialize $x_0 = -1$, learning rate $\eta = 0.4$
- At each iteration, $x_{k+1} = x_k - \eta \nabla_x g(x_k)$



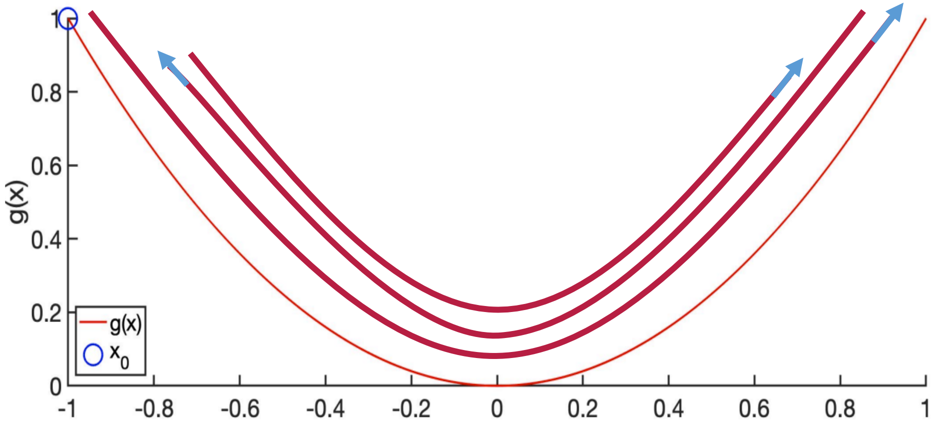
- $x_2 = -0.04$
- $\nabla_x g(x_2) = -0.08$
- $x_3 = x_2 - 0.4\, \nabla_x g(x_2) = -0.008$

Learning Rate

If learning rate is too small, may take too long to converge



If learning rate is too big, may jump between local minima and never converge



Different Learning Models

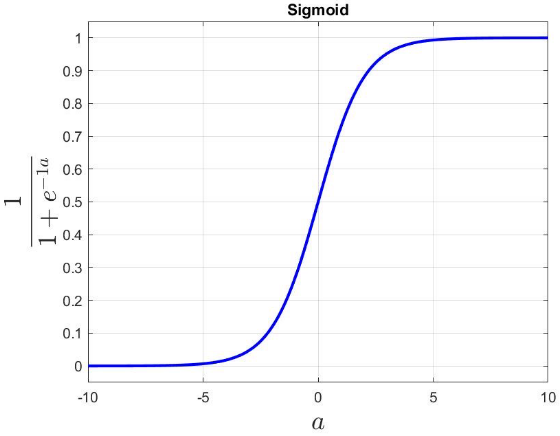
- Different learning models $f(\mathbf{x}_i, \mathbf{w})$ reflect our beliefs about the relationship between the features $\mathbf{x}_i$ and target y_i
  - For example, $f(\mathbf{x}_i, \mathbf{w}) = \mathbf{p}_i^T \mathbf{w}$ assumes polynomial relationship between features and target

- Suppose we are performing classification (rather than regression), so y_i is class -1 or class 1
  - $\mathbf{p}_i^T \mathbf{w}$ is number between $-\infty$ to ∞.
  - Can use sigmoid function to map $\mathbf{p}_i^T \mathbf{w}$ to between 0 and 1:

$$f(\mathbf{x}_i, \mathbf{w}) = \sigma(\mathbf{p}_i^T \mathbf{w})$$
$$\sigma(a) = \frac{1}{1 + e^{-a}}$$

Binary classification, logistic regression, neural networks (activation function).

Tut8_Q4



  - If $f(\mathbf{x}_i, \mathbf{w})$ is closer to 0 (or 1), we predict class -1 (or class 1)

- More generally, in one layer neural network: $f(\mathbf{x}_i, \mathbf{w}) = \sigma(\mathbf{p}_i^T \mathbf{w})$, where activation function σ can be sigmoid or some other functions & $\mathbf{p}$ is linear

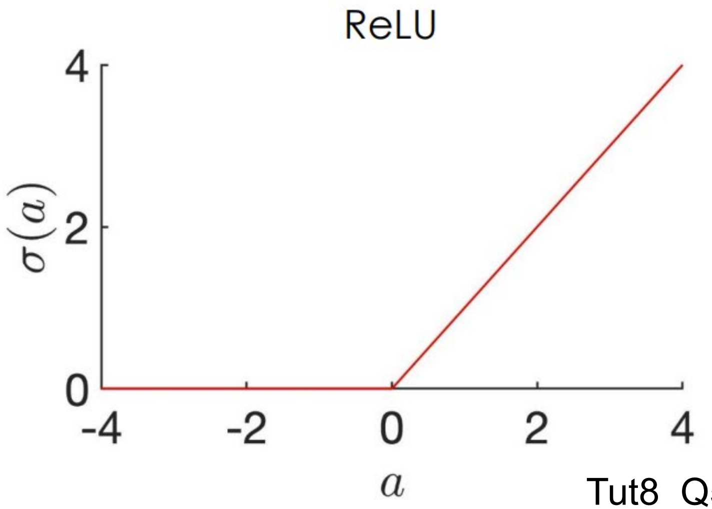
Different Learning Models

- $f(\mathbf{x}_i, \mathbf{w}) = \sigma(\mathbf{p}_i^T \mathbf{w})$, where σ can be different functions:
- Rectified linear unit (ReLU): $\sigma(a) = \max(0, a)$

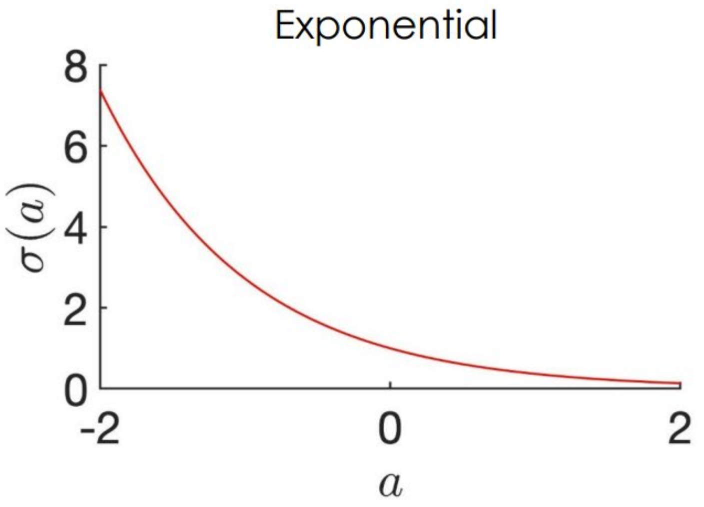
Deep learning, especially in neural networks.

- Exponential: $\sigma(a) = \exp(-a)$

Growth/decay models, probability distributions, some neural network activations.



Tut8_Q5



Tut8_Q2

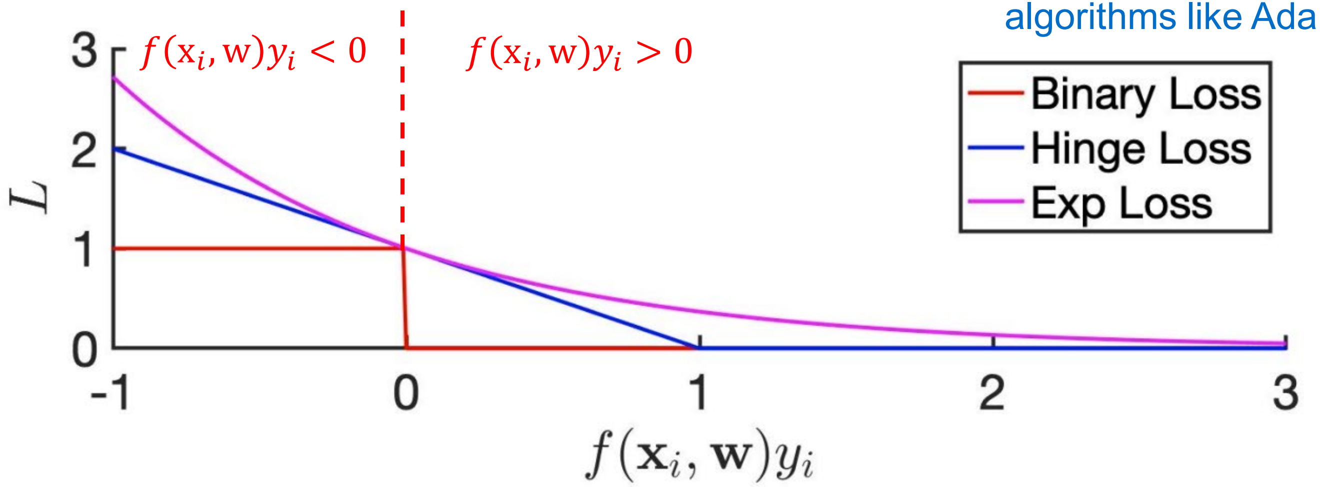
Different Loss Functions

- Binary loss, where y_i is class -1 or class 1 & $f(\mathbf{x}_i, \mathbf{w})$ is a number between $-\infty$ and ∞: $L(f(\mathbf{x}_i, \mathbf{w}), y_i) = \begin{cases} 0 & \text{if } f(\mathbf{x}_i, \mathbf{w})y_i > 0 \\ 1 & \text{if } f(\mathbf{x}_i, \mathbf{w})y_i < 0 \end{cases}$

- Binary loss not differentiable, so two other possibilities
  - Hinge loss: $L(f(\mathbf{x}_i, \mathbf{w}), y_i) = \max(0, 1 - f(\mathbf{x}_i, \mathbf{w})y_i)$
  - Exponential loss: $L(f(\mathbf{x}_i, \mathbf{w}), y_i) = \exp(-f(\mathbf{x}_i, \mathbf{w})y_i)$

Hinge Loss: Used primarily for support vector machines (SVMs).

Exp Loss: Often used in boosting algorithms like AdaBoost.



Regression

Collect Data → Model and Loss Function → Learning/Training: compute w → Prediction /Testing: Compute y_{new}

$$Xw = y$$

- X: Samples
- y: Target values

"closed-form" formula

$$\frac{1}{m}\sum_{i=1}^{m}(f_{\mathbf{w},b}(\mathbf{x}_i) - y_i)^2$$

- Linear or Affine function
- Squared error loss function

$$\widehat{\mathbf{w}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

- Check the invertibility
- Least square approximation (left-inverse)

$$\hat{f}_{\mathbf{w}}(\mathbf{X}_{new}) = \mathbf{X}_{new}\widehat{\mathbf{w}}$$

- Prediction for new inputs
- Testing: Mean Squared Error (MSE)

$$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

Iterative estimation using gradient descent

- Different learning models and loss functions

- Compute gradient: $\nabla_{\mathrm{w}} C(\mathrm{w})$
- Gradient descent (update w): $\mathrm{w}_{\mathrm{k}+1} \leftarrow \mathrm{w}_{\mathrm{k}} - \eta\nabla_{\mathrm{w}} C(\mathrm{w})$

Recap

- Building blocks of machine learning algorithms
  - Learning model: reflects our belief about relationship between features & target we want to predict
  - Loss function: penalty for wrong prediction
  - Regularization: penalizes complex models
  - Optimization routine: find minimum of overall cost function
- Gradient descent algorithm
  - At each iteration, compute gradient & update model parameters in direction opposite to gradient
  - If learning rate η is too big => may not converge
  - If learning rate η is too small => converge very slowly
- Different learning models, e.g., linear, polynomial, sigmoid, ReLU, exponential, etc
- Different loss functions, e.g., square error, binary, exponential, logistic, etc

THANK YOU