Introduction to Machine Learning

Linear Regression

Varun Chandola

Computer Science & Engineering
State University of New York at Buffalo
Buffalo, NY, USA
chandola@buffalo.edu

University at Buffalo
Department of Computer Science
and Engineering
School of Engeering and Applied Sciences

Outline

Basics

- Data - scalar (x), vector ($\mathbf{x}$), Matrix ($\mathbf{X}$)

Scalars

- Numeric ($x \in \mathbb{R}$)
- Categorical (e.g., $x \in \{0, 1\}$)
- Constants will be denoted as D, M, etc.

Vector

- Length of a vector $\mathbf{x} \in \mathbb{R}^D$
- Vector *dot* product ($\mathbf{x} \cdot \mathbf{y}$)
- Norm of a vector ($|\mathbf{x}|$, $\|\mathbf{x}\|, \|\mathbf{x}\|_p$)

Matrix

- Size of a matrix ($\mathbf{X} \in \mathbb{R}^{M \times N}$)
- Transpose of a matrix ($\mathbf{X}^\top$)
- Matrix product ($\mathbf{XY}$))

- A vector is a special matrix with only one column

$$\mathbf{x} \cdot \mathbf{y} \equiv \mathbf{x}^\top \mathbf{y}$$

- There is one scalar **target** variable y
- There is one vector **input** variable x
- Inductive bias:

$$y = \mathbf{w}^\top \mathbf{x}$$

Linear Regression Learning Task

Learn $\mathbf{w}$ given training examples, $\langle \mathbf{X}, \mathbf{y} \rangle$.

Geometric Interpretation

- Fitting a straight line to d dimensional data

$$y = \mathbf{w}^\top \mathbf{x}$$

$$y = \mathbf{w}^\top \mathbf{x} = w_1x_1 + w_2x_2 + \ldots + w_dx_d$$

- Will pass through origin
- Add intercept

$$y = w_0 + w_1x_1 + w_2x_2 + \ldots + w_dx_d$$

- Equivalent to adding another column in $\mathbf{X}$ of 1s.

Incorporating Bias/Intercept

Explicit Bias

$$\begin{aligned}\mathbf{x} &\equiv \{x_1, x_2, \ldots, x_d\} \\ \mathbf{w} &\equiv \{w_1, w_2, \ldots, w_d\} \\ y &= w_0 + \mathbf{w}^\top \mathbf{x}\end{aligned}$$

Implicit Bias

$$\begin{aligned}\mathbf{x} &\equiv \{1, x_1, x_2, \ldots, x_d\} \\ \mathbf{w} &\equiv \{w_0, w_1, w_2, \ldots, w_d\} \\ y &= \mathbf{w}^\top \mathbf{x}\end{aligned}$$

Learning Parameters - Least Squares Approach

- Minimize *squared loss*

$$J(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}(y_i - \mathbf{w}^\top \mathbf{x}_i)^2$$

- or,

$$J(\mathbf{w}) = \frac{1}{2}(\mathbf{y} - \mathbf{X}\mathbf{w})^\top(\mathbf{y} - \mathbf{X}\mathbf{w})$$

- Make prediction ($\mathbf{w}^\top \mathbf{x}_i$) as close to the target (y_i) as possible
- Least squares estimate

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

- *We will derive this expression in class.*

Machine Learning as Optimization Problem[1]

- Learning is optimization
- Faster optimization methods for faster learning
- Let $\mathbf{w} \in \mathbb{R}^d$ and $S \subset \mathbb{R}^d$ and $f_0(\mathbf{w}), f_1(\mathbf{w}), \ldots, f_m(\mathbf{w})$ be real-valued functions.
- Standard optimization formulation is:

$$\begin{array}{ll} \underset{\mathbf{w}}{\text{minimize}} & f_0(\mathbf{w}) \\ \text{subject to} & f_i(\mathbf{w}) \leq 0, \; i = 1, \ldots, m. \end{array}$$

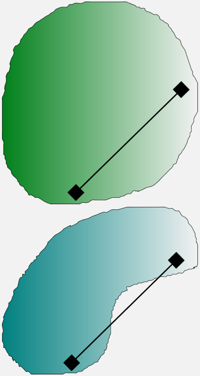
[1] Adapted from http://ttic.uchicago.edu/~gregory/courses/ml2012/lectures/tutorial_optimization.pdf. Also see, http://www.stanford.edu/~boyd/cvxbook/ and http://scipy-lectures.github.io/advanced/mathematical_optimization/.

Solving Optimization Problems

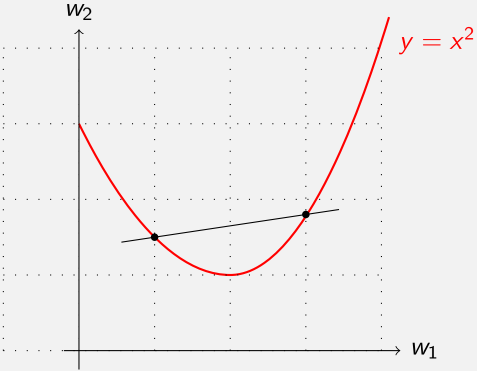
- Methods for **general optimization problems**
  - Simulated annealing, genetic algorithms
- Exploiting *structure* in the optimization problem
  - **Convexity**, Lipschitz continuity, smoothness

Convexity

Convex Sets



Convex Functions



Convex Optimization

- Optimality Criterion

$$\begin{aligned} \underset{\mathbf{w}}{\text{minimize}} \quad & f_0(\mathbf{w}) \\ \text{subject to} \quad & f_i(\mathbf{w}) \leq 0, \; i = 1, \ldots, m. \end{aligned}$$

  where all $f_i(\mathbf{w})$ are **convex functions**.
- $\mathbf{w}_0$ is feasible if $\mathbf{w}_0 \in Dom\ f_0$ and all constraints are satisfied
- A feasible $\mathbf{w}^*$ is optimal if $f_0(\mathbf{w}^*) \leq f_0(\mathbf{w})$ for all $\mathbf{w}$ satisfying the constraints

Matrix Calculus Basics

$$\frac{\partial \mathbf{a}^\top \mathbf{b}}{\partial \mathbf{a}} = \frac{\partial \mathbf{b}^\top \mathbf{a}}{\partial \mathbf{a}} = \mathbf{b}$$

$$\frac{\partial \mathbf{a}^\top \mathbf{M} \mathbf{a}}{\partial \mathbf{a}} = 2\mathbf{M}\mathbf{a}$$

where $\mathbf{M}$ is a symmetric matrix.

Evaluating Linear Regression Model

- How do we know that a model is good?
- What is a good evaluation/performance metric?

Root Mean Squared Error

$$RMSE = \sqrt{\sum_{i=1}^{N}(y^i - \hat{y}^i)^2}$$

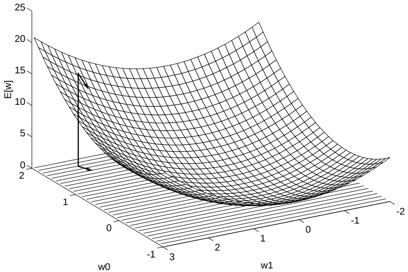
where $\hat{y}_i$ is the prediction for the i^{th} instance.

- What data to evaluate this on?
  - Training data?
  - Test data (**generalization error**)

Gradient of a Function

- Denotes the direction of steepest ascent

$$\nabla J(\mathbf{w}) = \begin{bmatrix} \frac{\partial J}{\partial w_0} \\ \frac{\partial J}{\partial w_1} \\ \vdots \\ \frac{\partial J}{\partial w_d} \end{bmatrix}$$



Finding Extremes of a Single Variable Function

1. Set derivative to 0

$$\nabla J(\mathbf{w}) = 0$$

2. Check second derivative for minima or maxima or saddle point

Finding Extremes of a Multiple Variable Function - Gradient Descent

1. Start from any point in variable space
2. Move along the direction of the steepest descent (or ascent)
   - By how much?
   - A learning rate (η)
   - What is the direction of steepest descent?
     - Gradient of J at $\mathbf{w}$

Training Rule for Gradient Descent

$$\mathbf{w} = \mathbf{w} - \eta \nabla J(\mathbf{w})$$

For each weight component:

$$w_j = w_j - \eta \frac{\partial J}{\partial w_j}$$

Convergence Guaranteed?

- Error surface contains only one global minimum
- Algorithm *will* converge
  - Examples need not be linearly separable
- η should be *small enough*
- Impact of too large η?
- Too small η?

Issues with Gradient Descent

- Slow convergence
- Stuck in local minima

Stochastic Gradient Descent [1]

- **Update weights after every training example.**
- For sufficiently small η, closely approximates Gradient Descent.

Gradient Descent	**Stochastic Gradient Descent**
Weights updated after summing error over all examples	Weights updated after examining each example
More computations per weight update step	Significantly lesser computations
Risk of local minima	Avoids local minima

Gradient Descent Based Method

- Minimize the squared loss using *Gradient Descent*

$$J(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}(y_i - \mathbf{w}^\top \mathbf{x}_i)^2$$

- Why?

References

Y. LeCun, B. Boser, J. S. Denker, D. Henderson, R. E. Howard, W. Hubbard, and L. D. Jackel.
Backpropagation applied to handwritten zip code recognition.
Neural Comput., 1(4):541–551, Dec. 1989.