Introduction to Machine Learning

Linear Regression

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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

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

Linear Regression

- 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

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

$$y = \mathbf{w}^\top \mathbf{x} = w_1 x_1 + w_2 x_2 + \ldots + w_d x_d$$

- Will pass through origin
- Add intercept

$$y = w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_d x_d$$

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

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.

Learning Parameters - Least Squares Approach

- Minimize *squared loss*

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

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

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

Machine Learning as Optimization Problem[1]

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

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

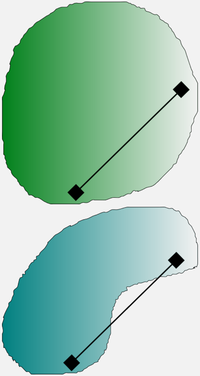
[1] Adapted from http://ttic.uchicago.edu/~gregory/courses/ml2012/lectures/tutorial_optimization.pdf. Also see, http://www.stanford.edu/~boyd/cvxbook/ and http://scipy-lectures.github.io/advanced/mathematical_optimization/.

Solving Optimization Problems

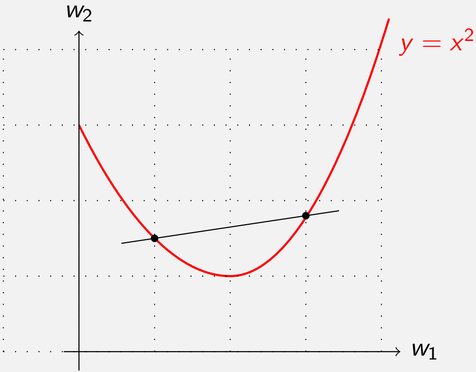
- Methods for **general optimization problems**
  - Simulated annealing, genetic algorithms
- Exploiting *structure* in the optimization problem
  - **Convexity**, Lipschitz continuity, smoothness

Convexity

Convex Sets



Convex Functions



Convex Optimization

- Optimality Criterion

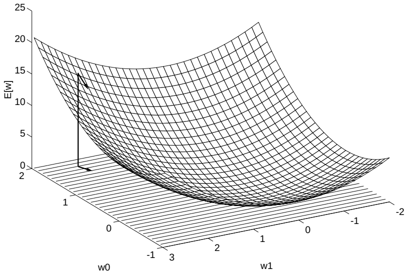
$$\begin{aligned} \underset{w}{\text{minimize}} \quad & f_0(w) \\ \text{subject to} \quad & f_i(w) \leq 0, \ i = 1, \ldots, m. \end{aligned}$$

  where all $f_i(w)$ are **convex functions**.
- w_0 is feasible if $w_0 \in Dom\ f_0$ and all constraints are satisfied
- A feasible w^* is optimal if $f_0(w^*) \leq f_0(w)$ for all w satisfying the constraints

Gradient of a Function

- Denotes the direction of steepest ascent

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



Finding Extremes of a Single Variable Function

- Set derivative to 0
- Second derivative for minima or maxima

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 E at $\mathbf{w}$

Training Rule for Gradient Descent

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

For each weight component:

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

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

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