Machine Learning

Contents

1 Regression

Important: Gradient descent and predictions are different. When finding optimal parameters, a dataset will be used, while a single data point will be used in prediction, outputting a single prediction value.

1.1 Linear regression

1.1.1 Squared error cost function

Measures how well line fits training data
m = num of training examples
$\vec{x}$ holds training example x values (length m)
$\vec{y}$ holds training example y values (length m)
$\hat{y}^{(i)} = w\vec{x}^{(i)} + b$

$$J(w,b) = \frac{1}{2m}\sum_{i=1}^{m}(\hat{y}^{(i)} - \vec{y}_i)^2$$

$\frac{1}{m}$ finds average error for larger data sets, $\frac{1}{2m}$ makes later calculations neater

1.1.2 Gradient descent

Find w, b for minimum of cost function $J(w,b)$

1. Start with some w, b (commonly $0, 0$)
2. Look around starting point and find direction that will move the point furthest downwards for a small step size

α = learning rate
Must simultaneously update w and b

$$w_1 = w_0 - \alpha\frac{\partial}{\partial w}J(w_0, b_0)$$
$$b_1 = b_0 - \alpha\frac{\partial}{\partial b}J(w_0, b_0)$$
$$\frac{\partial}{\partial w}J(w,b) = \frac{1}{m}\sum_{i=1}^{m}(\hat{y}^{(i)} - \vec{y}_i)\vec{x}^{(i)}$$
$$\frac{\partial}{\partial b}J(w,b) = \frac{1}{m}\sum_{i=1}^{m}(\hat{y}^{(i)} - \vec{y}_i)$$

1.2 Multiple linear regression

n_f = number of features
m = number of data points
$\vec{w}$ = vector of weights (length n_f)
X is a list of x vectors which hold n_f features (size $m \times n_f$)
Sum of predictions of all features is the prediction of multiple linear reg

$$f_{\vec{w},b}(\vec{x}) = \vec{w} \cdot \vec{x} + b$$

Gradient descent

$$\vec{w}_j = \vec{w}_j - \alpha\frac{\partial}{\partial \vec{w}_j}J(\vec{w}, b)$$
$$b = b - \alpha\frac{\partial}{\partial b}J(\vec{w}, b)$$

Cost function and its partial derivatives

$$J(\vec{w},b) = \frac{1}{2m}\sum_{i=1}^{m}(f_{\vec{w},b}(X^{(i)}) - \vec{y}_i)^2$$
$$\frac{\partial}{\partial \vec{w}_j}J(\vec{w},b) = \frac{1}{m}\sum_{i=1}^{m}(f_{\vec{w},b}(X^{(i)}) - \vec{y}_i)X_j^{(i)}$$
$$\frac{\partial}{\partial b}J(\vec{w},b) = \frac{1}{m}\sum_{i=1}^{m}(f_{\vec{w},b}(X^{(i)}) - \vec{y}_i)$$

1.3 Logistic regression

Sigmoid function

$$g(z) = \frac{1}{1+e^{-z}}$$
$$z = f_{\vec{w},b}(\vec{x})$$
$$\hat{y}^{(i)} = g(f_{\vec{w},b}(X^{(i)}))$$

$\hat{y}^{(i)}$ can be interpreted as the "probability" that class is 1, $0 \leq \hat{y}^{(i)} \leq 1$
ex. $\hat{y}^{(i)} = 0.7$ means there is a 70% chance y is 1
Logistic regression requires a new cost function because $f_{\vec{w},b}(\vec{x})$ for logistic regression is non-convex, trapping gradient descend in local minima.
Cost function

$$J(\vec{w},b) = \frac{1}{m}\sum_{i=1}^{m} L(\hat{y}^{(i)}, \vec{y}_i)$$

$$L(\hat{y}^{(i)}, \vec{y}_i) = \begin{cases} -\log(\hat{y}^{(i)}) & \text{if } \vec{y}_i = 1 \\ -\log(1-\hat{y}^{(i)}) & \text{if } \vec{y}_i = 0 \end{cases}$$

Simplified form

$$L(\hat{y}^{(i)}, \vec{y}_i) = -\vec{y}_i \log(\hat{y}^{(i)}) - (1-\vec{y}_i)\log(1-\hat{y}^{(i)})$$

The loss function will decrease as $\hat{y}^{(i)}$ approaches $\vec{y}_i$ on a graph of L vs f.
$\frac{\partial J(\vec{w},b)}{\partial \vec{w}_j}$ and $\frac{\partial J(\vec{w},b)}{\partial b}$ are the same as in linear regression, just the definition of f has changed.

1.4 Softmax regression

Generalization of logistic regression, y can have more than two possible values.
The most probable value of y is the value that when given to L yields the largest loss.
Calculate z_i with $\vec{x}$ only consisting of data points that have label i. In implementation, set all y values of data points with label equal to i to 1, and 0 for everything else.
n_f = num features
n_y = number of possible y outputs
W is a matrix of dimensions $n_y \times n_f$.
$\vec{b}$, $\vec{z}$, $\vec{a}$ are vectors of length n_y.

$$1 \leq i \leq n_y$$
$$\vec{z}_i = W^{(i)} \cdot \vec{x} + \vec{b}_i$$
$$\vec{a}_i = \frac{e^{\vec{z}_i}}{\sum_{k=1}^{n_y} e^{\vec{z}_k}}$$

$$L(\vec{a}, y) = \begin{cases} -\log \vec{a}_1 \text{ if } y = 1 \\ -\log \vec{a}_2 \text{ if } y = 2 \\ \vdots \\ -\log \vec{a}_n \text{ if } y = n \end{cases} \tag{1}$$

1.5 Feature scaling: z-score normalization

After z-score normalization, all features will have a mean of 0 and a standard deviation of 1
n_f = num features
$\vec{\mu}_j$ = mean of all values for feature j (length n_f)
$\vec{\sigma}_j$ = standard deviation of feature j (length n_f)

$$X_j^{(i)} = \frac{X_j^{(i)} - \vec{\mu}_j}{\vec{\sigma}_j}$$
$$\vec{\mu}_j = \frac{1}{m}\sum_{i=0}^{m-1} X_j^{(i)}$$
$$\vec{\sigma}_j^2 = \frac{1}{m}\sum_{i=0}^{m-1} (X_j^{(i)} - \vec{\mu}_j)^2$$

1.6 Over / underfitting

Underfit / high bias: does not fit training set well ($wx + b$ fit onto data points with $x + x^2$ shape)

Overfit / high variance: fits training set extremely well but does not generalize well ($w_1x + w_2x^2 + w_3x^3 + w_4x^4 + b$ fit onto training set of shape $x + x^2$ can have zero cost but predicts values outside the training set inaccurately)

Addressing overfitting

- Collect more data
- Select features ("Feature selection")
- Reduce size of parameters ("Regularization")

1.6.1 Regularization

Small values of $w_1, w_2, \cdots, w_n, b$ for simpler model, less likely to overfit

Given n_f features, there is no way to tell which features are important and which features should be penalized, so all features are penalized.

$$J_r(\vec{w}, b) = J(\vec{w}, b) + \frac{\lambda}{2m} \sum_{j=1}^{n_f} \vec{w}_j^2$$

Can include b by adding $\frac{\lambda}{2m} b^2$ to J_r but typically doesn't make a large difference.

The extra term in J_r is called the regularization term.

Effectively, $\lambda \propto \frac{1}{w}$. When trying to minimize cost, either the error term or the regularization term must decrease. The larger the lambda, the more the regularization term should decrease to minimize cost, decreasing w parameters.

Regularized linear regression

$$J_r(\vec{w}, b) = \frac{1}{2m} \sum_{i=1}^{m} \left[(f_{\vec{w},b}(X^{(i)}) - \vec{y}_i)^2 \right] + \frac{\lambda}{2m} \sum_{j=1}^{n_f} \vec{w}_j^2$$

For gradient descent, only $\frac{\partial J_r}{\partial \vec{w}_j}$ changes (b is not regularized):

$$\frac{\partial J_r}{\partial \vec{w}_j} = \frac{1}{m} \sum_{i=1}^{m} \left[(f_{\vec{w},b}(X^{(i)}) - \vec{y}_i) X_j^{(i)} \right] + \frac{\lambda}{m} \vec{w}_j$$

Regularized logistic regression

$$J_r(\vec{w}, b) = \frac{1}{m} \sum_{i=1}^{m} L(f_{\vec{w},b}(X^{(i)}), \vec{y}_i) + \frac{\lambda}{2m} \sum_{j=1}^{n_f} \vec{w}_j^2$$

For gradient descent, only $\frac{\partial J_r}{\partial w_j}$ changes (b is not regularized):

$$\frac{\partial J_r}{\partial \vec{w}_j} = \frac{1}{m} \sum_{i=1}^{m} \left[(f_{\vec{w},b}(X^{(i)}) - \vec{y}_i) X_j^{(i)} \right] + \frac{\lambda}{m} \vec{w}_j$$

2 Neural networks

n_ℓ = num layers excluding input
$n_n^{[\ell]}$ = n neurons in layer ℓ
n_f = num features
$\vec{W}$ is a vector (length n_ℓ) of matrices of size $n_n^{[\ell]} \times n_n^{[\ell-1]}$
$\vec{x}$ is a vector of outputs from each neuron in previous layer
$\vec{b}$ is a vector (length n_ℓ), holds a bias value for each layer
Z and A: vector (length n_ℓ) of vectors (length $n_n^{[\ell]}$)
g: activation function
$1 \leq i \leq n_\ell$
a (activation) = scalar output of a single neuron
Superscript $[i]$ is used to notate information relating to the ith layer in a neural network.

2.1 Choosing an activation function

sigmoid: $g(z) = \frac{1}{1+e^{-z}}$
tanh: $g(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$
linear: $g(z) = z$
ReLU: $g(z) = \max(0, z)$
Leaky ReLU: $g(z) = \max(\epsilon z, z)$ where ϵ is a small nonzero positive value < 1

For output layer

Binary classification, y = 0 or 1: use sigmoid
Regression, $-\infty \leq y \leq \infty$: use linear activation function
Regression, y ≥ 0: use ReLU

For hidden layer

ReLU is most common

2.2 Training a model

2.2.1 Forward propagation

Input $A^{[\ell-1]}$, output $A^{[\ell]}$, cache $Z^{[\ell]}$, $W^{[\ell]}$, $\vec{b}^{[\ell]}$

$$Z^{[\ell]} = W^{[\ell]} A^{[\ell-1]} + \vec{b}^{[\ell]}$$
$$A^{[\ell]} = g^{[\ell]}(Z^{[\ell]})$$

Up to $A^{[n_\ell]}$, in which case $\hat{y} = A_0^{[n_\ell]}$ assuming output layer has one unit

2.2.2 Back propagation

Input $\mathrm{d}a^{[\ell]}$, output $\mathrm{d}a^{[\ell-1]}$, $\mathrm{d}W^{[\ell-1]}$, $\mathrm{d}\vec{b}^{[\ell-1]}$

$$\mathrm{d}Z^{[\ell]} = \mathrm{d}A^{[\ell]} \cdot g'^{[\ell]}(Z^{[\ell]})$$
$$\mathrm{d}W^{[\ell]} = \frac{1}{m} \mathrm{d}Z^{[\ell]} \cdot A^{[\ell-1]T}$$
$$\mathrm{d}\vec{b}^{[\ell]} = \frac{1}{m} \sum_i \mathrm{d}Z_i^{[\ell]}$$
$$\mathrm{d}A^{[\ell-1]} = W^{[\ell]T} \cdot \mathrm{d}Z^{[\ell]}$$

2.3 Improving model

Cross validation: split data into training and test, use test data to determine how well the model generalizes

2.3.1 Fixing high bias/variance

High bias (underfit): J_{train} high, $J_{train} \approx J_{cv}$
High variance (overfit): J_{train} may be low, $J_{cv} \gg J_{train}$
High bias and high variance: J_{train} high, $J_{cv} \gg J_{train}$
How to fix:

1. Get more training examples (fix high variance)
2. Try smaller sets of features (fix high variance)
3. Add more features (fix high bias)
4. Add polynomial features (fix high bias)
5. Decrease λ (fix high bias)
6. Increase λ (fix high variance)

Neural networks and bias/variance
If J_{train} is high, make the network larger
If J_{cv} is high, get more data

2.3.2 Adding data

Data augmentation: add data with distortions (ex. distorted letters in a letter recognition program)

2.4 Decision trees