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CS109

Lecture Notes #22
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Gradient Ascent

Based on a chapter by Chris Piech

Maximum Likelihood Refresher

Our first algorithm for estimating parameters is called Maximum Likelihood Estimation (MLE). The central idea behind MLE is to select that parameters (θ) that make the observed data the most likely.

The data that we are going to use to estimate the parameters are going to be n independent and identically distributed (IID) samples: $X_1, X_2, \ldots X_n$.

Likelihood

First we define the likelihood of our data give parameters θ:

$$L(\theta) = \prod_{i=1}^{n} f(X_i|\theta)$$

This is the probability of all of our data. It evaluates to a product because all X_i are independent. Now we chose the value of θ that maximizes the likelihood function. Formally $\hat{\theta} = \underset{\theta}{\operatorname{argmax}}\ L(\theta)$.

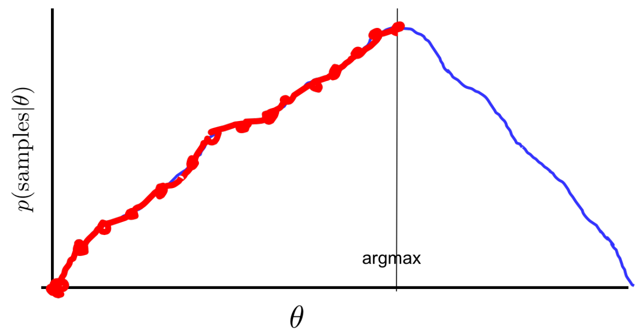
A cool property of argmax is that since log is a monotonic function, the argmax of a function is the same as the argmax of the log of the function! That's nice because logs make the math simpler. Instead of using likelihood, you should instead use log likelihood: $LL(\theta)$.

$$LL(\theta) = \log \prod_{i=1}^{n} f(X_i|\theta) = \sum_{i=1}^{n} \log f(X_i|\theta)$$

To use a maximum likelihood estimator, first write the log likelihood of the data given your parameters. Then chose the value of parameters that maximize the log likelihood function. Argmax can be computed in many ways. Most require computing the first derivative of the function.

Gradient Ascent Optimization

In many cases we can't solve for argmax mathematically. Instead we use a computer. To do so we employ an algorithm called gradient ascent (a classic in optimization theory). The idea behind gradient ascent is that if you continuously take small steps in the direction of your gradient, you will eventually make it to a local maxima.



Start with theta as any initial value (often 0). Then take many small steps towards a local maxima. The new theta after each small step can be calculated as:

$$\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \frac{\partial LL(\theta^{\text{old}})}{\partial \theta_j}$$

Where "eta" (η) is the magnitude of the step size that we take. If you keep updating θ using the equation above you will (often) converge on good values of θ. As a general rule of thumb, use a small value of η to start. If ever you find that the function value (for the function you are trying to argmax) is decreasing, your choice of η was too large. Here is the gradient ascent algorithm in pseudo-code:

```
Initialize: θj = 0 for all 0 ≤ j ≤ m

Repeat many times:
    gradient[j] = 0 for all 0 ≤ j ≤ m

    Calculate all gradient[j]'s based on data
    and current setting of theta

    θj += η * gradient[j] for all 0 ≤ j ≤ m
```

Linear Regression Lite

MLE is an algorithm that can be used for any probability model with a derivable likelihood function. As an example lets estimate the parameter θ in a model where there is a random variable Y such that $Y = \theta X + Z$, $Z \sim N(0, \sigma^2)$ and X is an unknown distribution.

In the case where you are told the value of X, θX is a number and $\theta X + Z$ is the sum of a gaussian and a number. This implies that $Y|X \sim N(\theta X, \sigma^2)$. Our goal is to chose a value of θ that maximizes the probability IID: $(X_1, Y_1), (X_2, Y_2), \ldots (X_n, Y_n)$.

We approach this problem by first finding a function for the log likelihood of the data given θ. Then we find the value of θ that maximizes the log likelihood function. To start, use the PDF of a Normal to express the probability of $Y|X,\theta$:

$$f(Y_i|X_i,\theta) = \frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(Y_i-\theta X_i)^2}{2\sigma^2}}$$

Now we are ready to write the likelihood function, then take its log to get the log likelihood function:

$$\begin{aligned}
L(\theta) &= \prod_{i=1}^{n} f(Y_i, X_i|\theta) && \text{Let's break up this joint}\\
&= \prod_{i=1}^{n} f(Y_i|X_i,\theta)f(X_i) && f(X_i) \text{ is independent of } \theta\\
&= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(Y_i-\theta X_i)^2}{2\sigma^2}} f(X_i) && \text{Substitute in the definition of } f(Y_i|X_i)
\end{aligned}$$

$$\begin{aligned}
LL(\theta) &= \log L(\theta)\\
&= \log \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(Y_i-\theta X_i)^2}{2\sigma^2}} f(X_i) && \text{Substitute in } L(\theta)\\
&= \sum_{i=1}^{n} \log \frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(Y_i-\theta X_i)^2}{2\sigma^2}} + \sum_{i=1}^{n} \log f(X_i) && \text{Log of a product is the sum of logs}\\
&= n \log \frac{1}{\sqrt{2\pi}} - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(Y_i-\theta X_i)^2 + \sum_{i=1}^{n} \log f(X_i)
\end{aligned}$$

Remove positive constant multipliers and terms that don't include θ. We are left with trying to find a value of θ that maximizes:

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}} \left[-\sum_{i=1}^{n}(Y_i-\theta X_i)^2\right]$$

To solve this argmax we are going to use Gradient Ascent. In order to do so we first need to find the derivative of the function we want to argmax with respect to θ.

$$\begin{aligned}
\frac{\partial}{\partial\theta}\left[-\sum_{i=1}^{n}(Y_i-\theta X_i)^2\right] &= -\sum_{i=1}^{n}\frac{\partial}{\partial\theta}(Y_i-\theta X_i)^2\\
&= -\sum_{i=1}^{n} 2(Y_i-\theta X_i)(-X_i)\\
&= \sum_{i=1}^{n} 2(Y_i-\theta X_i)(X_i)
\end{aligned}$$

This first derivative can be plugged into gradient ascent to give our final algorithm:

```
Initialize: θ = 0

Repeat many times:
    gradient = 0
    For each training example (x, y):
        gradient += 2(y - θ x)(x)
    θ += η * gradient
```

Towards Linear Regression

In our Linear Regression Lite model, we made two large simplifying assumptions: (1) our X is 1-dimensional, and (2) the linear relationship between Y and X does not have an intercept term.

Linear Regression in general seeks to find a linear relationship between Y and $\boldsymbol{X} = (X_1, X_2, \ldots, X_m)$ as follows:

$$Y = \theta_0 + \theta_1 X_1 + \theta_2 X_2 \ldots \theta_m X_M + Z,$$

where $Z \sim \mathcal{N}(0, \sigma^2)$, a Gaussian noise, and θ_0 is the intercept term.

We will cover multidimensional =datapoints in a few classes, but as an exercise for now, try to run gradient ascent for the case when our X is 1-dimensional and the linear relationship has an intercept term θ_0:

$$Y = \theta_0 + \theta_1 X + Z.$$

Your optimization objective can be computed as:

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}} \left[- \sum_{i=1}^{n} (Y_i - (\theta_1 X_i + \theta_0))^2 \right]$$

Start by computing the gradient for θ_0. The gradient for θ_1 has already been computed for you:

$$\frac{\partial}{\partial \theta_1} \left[- \sum_{i=1}^{n} (Y_i - (\theta_1 X_i + \theta_0))^2 \right] = \sum_{i=1}^{n} 2(Y_i - (\theta_1 X_i + \theta_0))(X_i)$$