Master Degree in Artificial Intelligence
Statistical and Mathematical Methods for Artificial Intelligence

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Homework 4: MLE and MAP

Maximum Likelihood Estimation (MLE) and Maximum a Posteriori (MAP)

Suppose you are given a dataset $\mathbb{D} = \{X, Y\}$, where

$$X = [x^1 x^2 \dots x^N] \in \mathbb{R}^N \tag{1}$$

$$Y = [y^1 y^2 \dots y^N] \in \mathbb{R}^N, \tag{2}$$

and $x^i \in \mathbb{R}$, $y^i \in \mathbb{R}$, for any $i = 1, \dots, N$. Moreover, suppose that:

$$y^i = \theta_1 + \theta_2 x^i + \dots + \theta_K (x^i)^{K-1} + e^i \quad \forall i = 1, \dots, N, \tag{3}$$

where $e^i \sim \mathcal{N}(0, \sigma^2 I)$ is random Gaussian Noise and $\theta = (\theta_1, \dots, \theta_K)^T$. It is known that the Maximum Likelihood Estimation (MLE) approach works by defining the conditional probability of y given x, $p_\theta(y|x)$, and then optimizes the parameters θ to maximize this probability distribution over $\mathbb{D}$. Moreover, it is also known that this approach can be made equivalent to the deterministic approach to solve such problems (the Least Square method) by taking the negative-log of $p_\theta(y|x)$. Indeed, by assuming that the noise e^i is Gaussian for any i, we have:

$$p_\theta(y|x) = \mathcal{N}(f_\theta(x^i), \sigma^2 I) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(f_\theta(x) - y)^2}. \tag{4}$$

Thus,

$$p_\theta(Y|X) = \prod_{i=1}^N p_\theta(y^i|x^i) \implies$$

$$\theta_{MLE} = \arg\max_{\theta \in \mathbb{R}^s} p_\theta(Y|X) = \arg\min_{\theta \in \mathbb{R}^s} -\log p_\theta(Y|X) = \arg\min_{\theta \in \mathbb{R}^s} -\log \prod_{i=1}^N p_\theta(y^i|x^i) = \arg\min_{\theta \in \mathbb{R}^s} \sum_{i=1}^N -\log p_\theta(y^i|x^i) =$$

$$\arg\min_{\theta \in \mathbb{R}^s} \sum_{i=1}^N \frac{1}{2\sigma^2}(f_\theta(x^i) - y^i)^2 = \arg\min_{\theta \in \mathbb{R}^s} \sum_{i=1}^N \frac{1}{2\sigma^2} ||f_\theta(x^i) - y^i||_2^2.$$

If $f_\theta(x) = \theta_1 + \theta_2 x^i + \dots + \theta_K (x^i)^{K-1} = \sum_{j=1}^K \phi_j(x^i)\theta_j$, with $\phi_j(x) = x^{j-1}$, we already shown that the problem above becomes

$$\theta_{MLE} = \arg\min_{\theta \in \mathbb{R}^s} \frac{1}{2\sigma^2} (\Psi(X)\theta - y^i)^2, \tag{5}$$

where $\Psi(X)$ is the $N \times K$ Vandermond matrix associated with $X = [x^1 x^2 \dots x^N]$, i.e. the matrix whose j-th column is X^{j-1}, $\theta = (\theta_1, \dots, \theta_K)^T$ and $Y = (y^1, \dots, y^N)^T$.

Note that the above equation is equivalent to the function you optimized in the Exercise 3 of Lab3 with GD, with $A := \Phi(X)$, $x := \theta$ and $b := y$.

When it is unclear how to set the parameter K and it is impossible to use the error plot, it is required to use the Maximum A Posterior (MAP) approach. To show how it works, suppose that we know that the parameters are normally distributed $\theta \sim \mathcal{N}(0, \sigma_\theta^2 I)$. Then we can use the Bayes Theorem to express the A Posteriori probability on y given x and θ as

$$p(\theta|X,Y) = \frac{p(Y|X,\theta)p(\theta)}{p(Y|X)}. \tag{6}$$

The MAP solution searches for a set of parameters θ that maximizes $p(\theta|X,Y)$. Following the same reasoning as before,

$$\theta_{MAP} = \arg\max_\theta p(\theta|X,Y) = \arg\min_\theta \sum_{i=1}^N -\log p(\theta|x^i, y^i) = \arg\min_\theta \sum_{i=1}^N -\log p(y^i|x^i,\theta) - \log p(\theta). \tag{7}$$

Given the two optimization problem above, you are required to implement a program that compare the two solutions, that we will refer to as θ_{MLE} and θ_{MAP}. To do that:

1. Define a test problem in the following way:

   - Let the user fix a positive integer $K > 0$, and define $\theta_{true} = (1, 1, \dots, 1)^T$ (you can also consider different θ_{true});
   - Define an input dataset $X = [x^1 x^2 \dots x^N] \in \mathbb{R}^N$, where the x^i are N uniformly distributed datapoints in the interval $[a, b]$, where $a < b$ are values that the user can select;
   - Given a set of functions $\{\phi_1, \phi_2, \dots, \phi_K\}$, define the Generalized Vandermonde matrix $\Phi(X) \in \mathbb{R}^{N\times K}$, whose element in position i, j is $\phi_j(x^i)$. In particular, write a function defining the classical Vandermonde matrix where $\phi_j(x) = x^{j-1}$;
   - Given a variance $\sigma^2 > 0$ defined by the user, compute $Y = \Phi(X)\theta_{true} + e$, where $e \sim \mathcal{N}(0, \sigma^2 I)$ is Gaussian distributed noise with variance σ^2. Try the following experiments for different values of σ^2. Note that the test problem defined in this way is very similar to what we did to define a test problem in the first Lab.

2. We now built a dataset $\mathbb{D} = \{X, Y\}$ such that $\theta_{true} = (1, 1, \dots, 1)^T \in \mathbb{R}^K$ is the best solution to the least squares problem $\Phi(X)\theta \approx Y$.

3. Pretend not to know the correct value of K. The first task is to try to guess it and use it to approximate the true solution θ_{true} by MLE and MAP. To do that:

   - Write a function that takes as input the training data $\mathbb{D} = (X, Y)$ and K and returns the MLE solution (with Gaussian assumption) $\theta_{MLE} \in \mathbb{R}^K$ for that problem. Note that the loss function can be optimized by GD, SGD or Normal Equations.
   - Write a function that takes as input a set of K-dimensional parameter vector θ and a test set $\mathcal{TE} = \{X_{test}, Y_{test}\}$ and returns the average absolute error of the polynomial regressor $f_\theta(x)$ over X_{test}, computed as:

     $$\frac{1}{N_{test}} ||f_\theta(X_{test}) - Y_{test}||_2^2. \tag{8}$$

   - For different values of K, plot the training datapoints and the test datapoints with different colors and visualize (as a continuous line) the learnt regression model $f_{\theta_{MLE}}(x)$. Comment the results.
   - For increasing values of K, use the functions defined above to compute the training and test error, where the test set is generated by sampling N_{test} new points on the same interval $[a, b]$ of the training set and generating the corresponding Y_test with the same procedure of the training set. Plot the two errors with respect to K. Comment the results.
   - Write a function that takes as input the training data $\mathbb{D} = (X, Y)$, K and $\lambda > 0$ and returns the MAP solution (with Gaussian assumption) $\theta_{MAP} \in \mathbb{R}^K$ for that problem. Note that the loss function can be optimized by GD, SGD or Normal Equations.

- ~~For K lower, equal and greater than the correct degree of the test polynomial, plot the training atapoints and the test datapoints with different colors, and visualize (as a continuous line) the learnt regression model $f_{\theta_{MAP}}(x)$ with different values of λ. Comment the results.~~
- For K being way greater than the correct degree of the polynomial, compute the MLE and MAP solution. Compare the test error of the two, for different values of λ (in the case of MAP).
- For K greater than the true degree of the polynomial, define $Err(\theta) = \frac{||\theta - \theta_{true}||_2}{||\theta_{true}||_2}$, where θ_{true} has been padded with zeros to match the shape of θ. Compute $Err(\theta_{MLE})$ and $Err(\theta_{MAP})$ for increasing values of K and different values of λ.
- Compare the results obtained by increasing the number N of datapoints.
- Compare the results obtained by the three algorithms GD, SGD and Normal Equations.

Note: when the value of a parameter is not explicitly specified, you can set it as you want. Suggestion: repeat for different values of the parameter.