Tutorials 4 & 5

CS 337 Artificial Intelligence & Machine Learning

Sunday 26th September, 2021

Problem 1. Weighted Linear Regression

Consider a data set in which each data point y_i is associated with a weighting factor r_i , so that the sum-square error function becomes

$$\frac{1}{2} \sum_{i=1}^{m} r_i (y_i - w^T \phi(x_i))^2$$

Find an expression for the solution w^* that minimizes this error function. The weights r_i 's are known before hand. (Exercise 3.3 of Pattern Recognition and Machine Learning, Christopher Bishop).

Problem 2. Locally Weighted Kernel Regression

In problem 1, we discussed weighted regression. In this problem, we will deal with weighted regression, with the weights obtained using some kernel K(.,.). Given a training set of points $\mathcal{D} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_i, y_i), \dots, (\mathbf{x}_n, y_n)\}$, we predict a regression function $f(x') = (\mathbf{w}^{\top} \phi(x') + b)$ for each test (or query point) x' as follows:

$$(\mathbf{w}', b') = \underset{\mathbf{w}, b}{\operatorname{argmin}} \sum_{i=1}^{n} K(x', x_i) (y_i - (\mathbf{w}^{\top} \phi(x_i) + b))^2$$

- 1. If there is a closed form expression for (\mathbf{w}', b') and therefore for f(x') in terms of the known quantities, derive it.
- 2. How does this model compare with linear regression and k-nearest neighbor regression? What are the relative advantages and disadvantages of this model?
- 3. In the one dimensional case (that is when $\phi(x) \in \Re$), graphically try and interpret what this regression model would look like, say when K(.,.) is the linear kernel¹.

Problem 3. Redoing the Kernel Ridge Regression Problem: Let $\mathcal{D} = \langle (\mathbf{x}_1, y_1), \dots, (\mathbf{x}_m, y_m) \rangle$ such that each $y_j \in \Re$. Let $\phi(\mathbf{x}) = [\phi_1(\mathbf{x}), \dots, \phi_n(\mathbf{x})]$ be a vector of basis functions. Consider the linear regression function $f(\mathbf{x}) = \phi^T(\mathbf{x})\mathbf{w}$ with \mathbf{w} obtained either as a least squares or

¹Hint: What would the regression function look like at each training data point?

ridge regression estimate. Show that, using either of these estimates for \mathbf{w} , the regression function can be written in the (so-called *kernelized*) form $f(\mathbf{x}) = \sum_{i=1}^{m} \alpha_i K(\mathbf{x}, \mathbf{x}_i) y_i$ where

 $K(\mathbf{x}, \mathbf{x}_i) = \phi^T(\mathbf{x})\phi(\mathbf{x}_i)$ is a function of \mathbf{x} and \mathbf{x}_i only and independent of any of the \mathbf{y}_i 's and \mathbf{x}_j for all $j \neq i$. Each α_i can be a function of the entire dataset \mathcal{D} .

Hint: Use the following Matrix Identity that holds for any matrices P, B and R with compatible dimensions such that R and $BPB^T + R$ are invertible:

$$(P^{-1} + B^T R^{-1} B)^{-1} B^T R^{-1} = P B^T (B P B^T + R)^{-1}$$

Problem 4. Equivalent Kernelized Representation (Post-midsem):

Throughout this question, let $0 . Consider a data set <math>\mathcal{D} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_m, y_m)\}$ of m points and a feature function $\phi(\mathbf{x}) \subseteq \Re^n$. Let $f(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + b$. You have seen linear regression with various regularizations of the form:

$$\sum_{i=1}^{m} (y_i - \phi^T(\mathbf{x}_i)\mathbf{w})^2 + \lambda \left(\sum_{j=1}^{n} |w_j|^p\right)$$
(1)

Now consider a somewhat complementary setting:

$$\sum_{i=1}^{m} (y_i - \phi^T(\mathbf{x}_i)\mathbf{w})^p + \lambda \left(\sum_{j=1}^{n} |w_j|^2\right)$$
(2)

- 1. Do these forms have an equivalent kernelized representation: $f(\mathbf{x}) = \phi^T(\mathbf{x})\mathbf{w}^* + b = \sum_{i=1}^m \alpha_i K(\mathbf{x}, \mathbf{x}^{(i)})$? How would you prove?
- 2. Contrast the two descriptions for their capabilities.

Problem 5. More on Kernel Perceptron:

Recall the proof for convergence of the perceptron update algorithm. Now can this proof be extended to the kernel perceptron?

Recall that Kernelized perceptron is specified as:

$$f(x) = sign\left(\sum_{i} \alpha_{i}^{*} y_{i} K(x, x_{i})\right)$$

The perceptron update algorithm for the Kernelized version is:

- INITIALIZE: $\alpha = zeroes()$
- REPEAT: for $\langle x_i, y_i \rangle$

- If
$$sign\left(\sum_{j} \alpha_{j} y_{j} K(x_{j}, x_{j})\right) \neq y_{i}$$

- then,
$$\alpha_i = \alpha_i + 1$$

Problem 6. Kernel Logistic Regression: Intuition (and optional Rigorous proof)

Recall the Regularized (Logistic) Cross-Entropy Loss function (minimized wrt $\mathbf{w} \in \Re^p$):

$$E\left(\mathbf{w}\right) = -\left[\frac{1}{m}\sum_{i=1}^{m} \left(y^{(i)}\log f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right) + \left(1 - y^{(i)}\right)\log\left(1 - f_{\mathbf{w}}\left(\mathbf{x}^{(i)}\right)\right)\right)\right] + \frac{\lambda}{2m}\|\mathbf{w}\|_{2}^{2}$$
(3)

Now intuitively show that minimizing the following dual kernelized objective² (minimized wrt $\alpha \in \Re^m$) is equivalent to minimizing the regularized cross-entropy loss function:

$$E_D(\alpha) = \left[\sum_{i=1}^m \left(\sum_{j=1}^m -y^{(i)} K\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) \alpha_j + \frac{\lambda}{2} \alpha_i K\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) \alpha_j \right) + \log \left(1 + \exp \sum_{j=1}^m \alpha_j K\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) \right) \right]$$
(4)

where, decision function $f_{\mathbf{w}}(\mathbf{x}) = \frac{1}{1 + \exp\left(-\sum_{j=1}^{m} \alpha_{j} \mathbf{K}\left(\mathbf{x}, \mathbf{x}^{(j)}\right)\right)}$ How would you prove this

very rigorously (optional)?

Problem 7. Effect of increasing λ in Ridge Regression

Consider the ridge regression problem

$$\widehat{\mathbf{w}}_{ridge} = \underset{\mathbf{w}}{\operatorname{argmin}} ||\Phi^T \mathbf{w} - \mathbf{y}||^2 + \frac{\lambda}{2} ||\mathbf{w}||^2$$

for any $\lambda \geq 0$. Recall the purpose for which the regularization term $\frac{\lambda}{2}||\mathbf{w}||^2$ was introduced in linear regression.

Let \mathbf{w}_1 be the optimal solution to this problem when $\lambda = \lambda_1$ and let \mathbf{w}_2 be the optimal solution to this problem when $\lambda = \lambda_2$. Let $\lambda_2 < \lambda_1$.

Which of the following statements is correct?

- 1. $||\mathbf{w}_2|| \le ||\mathbf{w}_1||$ (that is, $||\widehat{\mathbf{w}}_{ridge}||$ will not increase as λ decreases towards 0).
- 2. $||\mathbf{w}_2|| \ge ||\mathbf{w}_1||$ (that is, $||\widehat{\mathbf{w}}_{ridge}||$ will not decrease as λ decreases towards 0).
- 3. none of these

Prove your answer. Why does increase in λ reduce the curvature of the solution obtained via ridge regression?

Problem 8. Are these Valid Kernels? Consider the space of all possible subsets A of a given fixed set D. Prove/disprove the following functions are valid Kernels:

- 1. $K(A_1, A_2) = |A_1 \cap A_2|$
- 2. $K(A_1, A_2) = 2^{|A_1 \cap A_2|}$

where A_1, A_2 are subsets of D and |B| is the cardinality of |B| or the number of elements in B.

²http://perso.telecom-paristech.fr/~clemenco/Projets_ENPC_files/kernel-log-regression-svm-boosting.pdf