

**Problem Set 2**

Fall 2016

**Issued:** Thurs, September 8, 2016      **Due:** Tuesday, September 20, 2016

**Note:** Hand in hard copy at the start of class.

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**Relevant materials:** Lectures plus course reader (Chap. 6 and 8).

**Problem 2.1**

*Polynomial regression and model selection:* Suppose that you are given a vector of responses  $y \in \mathbb{R}^n$  and covariates  $t \in \mathbb{R}^n$ , and your goal is to fit a polynomial model of degree  $D$  to the data.

- (a) Show how, with a suitable choice of features, this problem can formulated as a form of linear prediction.
- (b) Write a routine to do a least-squares fit of a polynomial function of degree  $D$ , including a constant term, to data vectors  $y$  and  $t$ , each of length  $n$ . Using the data in `y.dat` and `t.dat`, fit polynomials of degree  $D \in \{1, 2, \dots, n-1\}$ . Letting  $f_D$  denote the fitted polynomial of degree  $D$ , plot the the mean-squared error  $R(D) = \frac{1}{n} \sum_{i=1}^D (y_i - f_D(t_i))^2$  versus the degree  $D$ .
- (c) How does the MSE behave as a function of  $D$ , and why? What is special about the degree  $n - 1$  fit? What happens if you try to fit a polynomial of degree  $n$ ? (Try to do so using a direct method, such as matrix inverse, to compute the least-squares fit.) Explain why.
- (d) Using the new response vector  $\tilde{y} \in \mathbb{R}^n$  given in `yfresh.dat`, compute the average squared error  $\tilde{R}(D) = \frac{1}{n} \sum_{i=1}^n (\tilde{y}_i - f_D(t_i))^2$  of your fits from (b). Why do you think that this plot is *qualitatively* different from the part from part (b)? What does this tell you how the fitted degree  $D$  should be chosen? (The problem of choosing the “right” degree is known as the *model selection problem*.)
- (e) Using the MSE’s  $R(D)$  obtained in part (b), compute the adjusted quantities

$$F(D) = R(D) + \frac{\sigma^2 D \log n}{n} \quad \text{with } \sigma = 0.25.$$

On the same plots, over the range  $D \in \{2, \dots, 9\}$ , plot the functions  $\tilde{R}(D)$  and  $F(D)$ . How are the minimizing arguments of the two functions related? Why is this an interesting observation?

- (f) **(BONUS:)** Consider the model selection rule

$$\hat{D} = \arg \min_{D \in \{1, 2, \dots, n-1\}} F(D).$$

Prove something interesting and non-trivial about this rule as  $n \rightarrow +\infty$ , assuming that the data is drawn i.i.d. from a model of the form  $y = f_{D^*}(t) + w$ , where  $f_{D^*}$  is a fixed polynomial of degree  $D^*$  on the interval  $[-1, 1]$ , the covariate  $t \sim \text{Uni}[-1, 1]$ , and  $w \sim N(0, \sigma^2)$ , independent of  $t$ .

### Problem 2.2

*Exponential families and conjugate duality:* Recall the one-dimensional exponential family  $p_\eta(y) = h(y)e^{\eta y - A(\eta)}$ , where  $A(\eta) = \log \left( \int_{\mathcal{Y}} h(y)e^{\eta y} dy \right)$  (Think of the integral over  $\mathcal{Y}$  as a sum for discrete random variables.)

- (a) Prove that  $A$  is a convex function.  
 (b) The Kullback-Leibler divergence between distributions  $p_\eta$  and  $p_{\tilde{\eta}}$  is given by

$$D(p_\eta \| p_{\tilde{\eta}}) = \mathbb{E}_\eta \left[ \log \frac{p_\eta(Y)}{p_{\tilde{\eta}}(Y)} \right],$$

where  $\mathbb{E}_\eta$  denotes expectations under  $p_\eta$ . Express the KL divergence in terms of  $A$  and its derivative  $A'$ .

- (c) The conjugate dual of  $A$  is defined as  $A^*(t) := \sup_{\eta \in \mathbb{R}} \{ \eta t - A(\eta) \}$ . Compute the conjugate duals for:  
 (i) Bernoulli random variable (logistic model)  
 (ii) Gaussian random variable (as discussed in class)  
 (iii) Poisson random variable  
 (d) Prove that the conjugate dual  $A^*$  is always a convex function.

### Problem 2.3

*Maximum likelihood and exponential families:* Recall the one-dimensional exponential family from the previous problem, and suppose that we are given  $n$  i.i.d. samples  $\{y_i\}_{i=1}^n$  samples.

- (a) Give a simple expression for the maximum likelihood estimate  $\hat{\eta}$  that involves the inverse function of the derivative  $A'$  and the sample mean  $\frac{1}{n} \sum_{i=1}^n y_i$ . (The inverse function exists under suitable regularity conditions.)
- (b) Use part (a) to compute closed-form estimates for the MLE in the { Gaussian, Poisson, Bernoulli } models.
- (c) Suppose that we had an infinite number of samples ( $n = \infty$ ), all drawn from the distribution  $p_{\eta^*}$  where  $\eta^*$  is the unknown true parameter. By taking suitable expectations, show that the MLE is given by

$$\hat{\eta} = \arg \min_{\eta \in \mathbb{R}} \left\{ A(\eta) - A(\eta^*) - A'(\eta^*)(\eta - \eta^*) \right\}.$$

- (d) Now assume that  $A$  is strictly convex. Prove that  $\hat{\eta} = \eta^*$  in the infinite data limit from (c).

#### Problem 2.4

*Generalized linear models and stochastic gradient:*

- (a) Write out the stochastic gradient updates (using a single sample per round) for solving the GLM maximum likelihood problem.
- (b) Make your updates explicit for the Poisson and logistic cases.
- (c) Using the data in `Xone.dat` and `yone.dat`, use your code (with a step size decaying as  $1/t$ ) to fit a logistic model to the data. Compute the probabilities  $\mathbb{P}[y_i = 1 \mid x_i; \hat{\theta}]$  based on your fitted vector  $\hat{\theta}$ , and plot a histogram of these probabilities.
- (d) Repeat the same for the data in `Xtwo.dat` and `ytwo.dat`. Comment on the differences between the histograms, and what it suggests about the accuracy of the fits.
- (e) Via maximum likelihood, fit a 2-component Gaussian mixture model to each of the two data sets. **Note:** You are given the labels in `yone.dat` and `ytwo.dat`.
- (f) Examine the connection between the fitted logistic vector  $\hat{\theta}$  from parts (c) and (d), and the fitted mean vectors in part (e). What does this tell you?