Due: Fri. 11/8/2019, 2:00 PM

1. For a regression problem with 2 features, consider the effect of different regularizers and different amounts of regularization, graphically as described below. You may do this by hand, or you may use a computer to assist you if you prefer.

Assume the unconstrained objective function is $f_{obj}(\underline{w}) = \frac{1}{N} RSS(\underline{w}, \mathcal{D}_i)$. For simplicity, in this problem we assume $w_0 = 0$, consistent with a dataset that has been standardized in both x and y. Consider 10 different datasets $\mathcal{D}_1, \mathcal{D}_2, \cdots, \mathcal{D}_{10}$, each resulting in an unconstrained (unregularized) minimum at $\hat{\underline{w}}_{lin}^{(i)}$ given by:

$$\mathcal{D}_{1}: \ \underline{\hat{w}}_{lin}^{(1)} = (10,0), \quad \mathcal{D}_{2}: \ \underline{\hat{w}}_{lin}^{(2)} = (10,2), \quad \mathcal{D}_{3}: \ \underline{\hat{w}}_{lin}^{(3)} = (10,4),$$

$$\mathcal{D}_{4}: \ \underline{\hat{w}}_{lin}^{(4)} = (10,6), \quad \mathcal{D}_{5}: \ \underline{\hat{w}}_{lin}^{(5)} = (8,6), \quad \mathcal{D}_{6}: \ \underline{\hat{w}}_{lin}^{(6)} = (8,8),$$

$$\mathcal{D}_{7}: \ \underline{\hat{w}}_{lin}^{(7)} = (6,8), \quad \mathcal{D}_{8}: \ \underline{\hat{w}}_{lin}^{(8)} = (6,10), \quad \mathcal{D}_{9}: \ \underline{\hat{w}}_{lin}^{(9)} = (4,10), \quad \mathcal{D}_{10}: \ \underline{\hat{w}}_{lin}^{(10)} = (2,10)$$

Assume the shape of $RSS(\underline{w}, \mathcal{D}_i)$ = constant curves in 2D weight space are circles (special case of ellipses), for simplicity.

In each regularizer case given below, make a plot in 2D weight space, showing:

- (i) the 10 unregularized-minimum points $\hat{\underline{w}}_{lin}^{(i)}$ given above,
- (ii) the region that satisfies the given regularizer constraint, and
- (iii) the resulting 10 regularized minimum points, i.e., solution of

$$\underline{\hat{w}}_{\text{reg}}^{(i)} = \arg\min_{\underline{w}} f_{obj}(\underline{w}, \mathcal{D}_i) \quad \text{s.t. } \Omega(\underline{w}) \leq C .$$

for each *i*. Also show or justify how you found the resulting $\hat{\underline{w}}_{reg}^{(i)}$. (Showing your method for one or two points in each regularizer case, should be sufficient.)

(iv) Also, answer: how many of the resulting $\underline{\hat{w}}_{reg}^{(i)}$, $i = 1, 2, \dots, 10$, are more sparse than the corresponding $\underline{\hat{w}}_{lin}^{(i)}$? For the purpose of this problem, define sparsity as the number of components $\hat{w}_{i}^{(i)}$ that have value 0, for a given i.

Tip: For cases in which there are more than one possible $\underline{\hat{w}}_{reg}^{(i)}$ for a given dataset and a given constraint, pick any one.

- (a) L2 regularization: $\Omega(\underline{w}) = ||\underline{w}||_2^2$, $C = 2^2$.
- (b) L1 regularization: $\Omega(\underline{w}) = ||\underline{w}||_1$, C = 2.
- (c) Lp regularization (based on p-norm): $\Omega(\underline{w}) = |\underline{w}|_p^p$, as $p \to \infty$, C = 1.

Hint: if you're not sure of the shape of $\left\| \underline{w} \right\|_p^p = 1$, try plotting it numerically for increasing p, e.g. p = 4,10,100.

- (d) Repeat (a), except with $C = 5^2$.
- (e) Repeat (b), except with C = 5.
- 2. Suppose you develop and optimize a machine learning system, starting with setting aside a test dataset \mathcal{D}_{Test} , and using the remaining data points as the set \mathcal{D}' . Your hypothesis set is \mathcal{H}_1 , and you use \mathcal{D}' as a training set to find its best hypothesis h_{g1} . Let $d_{VC}(\mathcal{H}_1) = d_{VC}^{(1)}$, $N' = |\mathcal{D}'|$, and $N_{Test} = |\mathcal{D}_{Test}|$. When you are finished, you pull out the test set and calculate $E_{Test}(h_{g1})$. In this problem, all generalization bounds are with tolerance δ (with probability $\geq 1 \delta$).
 - (a) Draw a flow chart (like we did in Lecture 16, p. 6, and like AML Fig. 4.11), that shows the dataset usage, hypothesis set, and procedure.
 - (b) Give an inequality for the generalization bound based on the training error $E_{\mathcal{D}'} \Big(h_{g1} \Big)$, and the generalization bound based on the test-set error $E_{Test} \Big(h_{g1} \Big)$.

Afterwards, independently of the results you got above, you think of a different approach that you also want to try. So you start the process all over again, setting aside the same test set \mathcal{D}_{Test} . You define a hypothesis set \mathcal{H}_2 for your model. Let $d_{VC}(\mathcal{H}_2) = d_{VC}^{(2)}$.

In this case, however, you also use some model selection to choose the optimum number of features in a feature selection process. So you split \mathcal{D}' into a training set \mathcal{D}_{Tr} and a validation set \mathcal{D}_{Val} , that are disjoint. You use \mathcal{D}_{Tr} to train each model (based on a given number of features d), and use model selection to compare different values of d, with $d = 1, 2, 3, \dots, d_{\max}$, in which d_{\max} is the maximum number

of features you try. You choose the best number of features by comparing $E_{Val}\left(h_{g2}^{(d)}\right)$ for each value of d. Let $N_{Tr}=\left|\mathcal{D}_{Tr}\right|$, and $N_{Val}=\left|\mathcal{D}_{Val}\right|$.

- (c) Draw a flow chart (like we did in Lecture 16, p. 6, and like AML Fig. 4.11), that shows the dataset usage, hypothesis sets, parameter values *d*, and procedure, for this second approach only.
- (d) Give:
 - (i) An inequality for the generalization bound based on the training-set error $E_{Tr}\left(h_{g2}^{(d)}\right)$ for a given number of features d;
 - (ii) An inequality for the generalization bound based on the validation-set error $E_{Val}\left(h_{g2}^{(d^*)}\right)$ for the optimal number of features d^* ;
 - (iii) An inequality for the generalization bound based on the test-set error $E_{\mathcal{D}_{Test}}\left(h_{g2}^{(d^*)}\right)$ for the best hypothesis $h_{g2}^{(d^*)}$.

Finally, you compare the best results from the 2 systems you developed, and pick the one with the lower test-set error.

(e) Give an inequality for the generalization bound based on the test-set error $E_{Test}(h_g^*)$ for the best hypothesis h_g^* .

Hint: what is the effective hypothesis set used by \mathcal{D}_{Test} to pick between the two machine-learning systems you developed?