RIDGE and LASSO regularization for regression

- Some algorithms perform naturally feature selection
 - for example Decision Trees, Boosting
- Other algorithms have difficulty with correlated features
 - for example Naive Bayes, Regression
- Some algorithms have difficulty with too many features

- Task(label) Independent, Model independent
 - Dimensionality reduction, clustering
 - PCA
- Filter Methods: Task dependent, Model independent
 - compute correlation among pairs of features
 - compute correlation of feature with labels
- Wrapper methods: Task dependent, Model dependent
 - try subsets of features with a given ML algorithm, pick a "best" subset

- Task dependent, Model dependent
- Select one feature at a time, dynamically
 - depending on how previous features do

set of features initial empty, $S = \emptyset$ repeat while improvement $> \epsilon$

for each feature $f \notin S$

performance $(S \cup \{f\}) = \operatorname{performance}(\operatorname{model}, \operatorname{trained} \operatorname{on} S \cup \{f\})$ end for

$$f_{new} = \operatorname{argmax}_{f} \text{ performance}(S \cup \{f\})$$

improvement = performance $(S \cup \{f_{new}\})$ - performance (S)
 $S = S \cup \{f_{new}\}$
end repeat

- Free coefficients (unconstrained) can result in problems
 - features canceling each other
 - features overwhelming each other
 - large complexity with no generalization benefit
- Solution : constrain the coefficients

- Regression: same as before, a linear predictor

$$h_w(x) = w^0 + x^T w = w^0 + \sum_j x^j w^j$$

- Regularized regression means add a "complexity" penalty in the objective
 - the objective contains the traditional least square (to be minimized)
 - but also R(w) a notion of complexity (to be minimized)
- λ tradeoffs the complexity for the objective

$$\min_{(w_0,w)\in\mathcal{R}^{d+1}} \left[\frac{1}{2N} \sum_{i=1}^{N} (y_i - w_0 - x_i^T w)^2 + \frac{\lambda}{N} R(w) \right]$$

Regularization for regression

- RIDGE penalty : L2 norm
 - causes all w coefficients to be small

 $L_2 \text{ norm } R(w) = \frac{1}{2} ||w||_2^2 = \frac{1}{2} \sum_{j=1}^d w^{j2}$

- LASSO penalty: L1 norm
 - causes some coefficients to be 0 (feature selection) $L_1 \text{ norm } R(w) = ||w||_1 = \sum_{j=1}^d |w^j|$
- "elastic-net" : mixture of L1 and L2 norms

 $R_{\beta}(w) = (1-\beta)\frac{1}{2}||w||_{2}^{2} + \beta||w||_{1} = \sum_{j=1}^{d} \left[\frac{1}{2}(1-\beta)w^{j2} + \beta|w^{j}|\right]$

Digits dataset

- can be written as constrained optimization
 - a direct correspondence between λ and t
 - solved by taking derivatives with Lagrangian Multipliers

$$\hat{w}^{ridge} = \arg\min_{w} \sum_{i=1}^{N} (y_i - w^0 - \sum_{j=1}^{d} x_i^j w^j)^2$$

subject to
$$\sum_{j=1}^{d} w^{j2} \le t$$

RIDGE vs LASSO

Figure 1: Source: Figure 3.11 of [4] Estimation picture for LASSO (left) and RIDGE (right). Solid areas are for regions of constraints $|w^1| + |w^2| \le t$ (LASSO, left) and $(w^1)^2 + (w^2)^2 \le t$ (RIDGE, right). Red ellipses are the contours of the objective, here the least square function.



- the solution w will be in the feasible region (solid blue)

RIDGE vs LASSO

- RIDGE penalty for linear regression is essentially a regression problem with bigger matrices
 - Z = matrix data; n=number of data points, p=number of dimensions/features

The ℓ_2 criterion is the RSS for the augmented data set:

$$\mathbf{Z}_{\lambda} = \begin{pmatrix} z_{1,1} & z_{1,2} & z_{1,3} & \cdots & z_{1,p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ z_{n,1} & z_{n,2} & z_{n,3} & \cdots & z_{n,p} \\ \sqrt{\lambda} & 0 & 0 & \cdots & 0 \\ 0 & \sqrt{\lambda} & 0 & \cdots & 0 \\ 0 & 0 & \sqrt{\lambda} & \ddots & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & \sqrt{\lambda} \end{pmatrix}; \ \mathbf{y}_{\lambda} = \begin{pmatrix} y_{1} \\ \vdots \\ y_{n} \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

So:

$$\mathbf{Z}_{\lambda} = \begin{pmatrix} \mathbf{Z} \\ \sqrt{\lambda} \mathbf{I}_{p} \end{pmatrix} \mathbf{y}_{\lambda} = \begin{pmatrix} \mathbf{y} \\ \mathbf{0} \end{pmatrix}$$

- like regression, admits analytical solution

$$\begin{aligned} (\mathbf{Z}_{\lambda}^{\top}\mathbf{Z}_{\lambda})^{-1}\mathbf{Z}_{\lambda}^{\top}y_{\lambda} &= \left((\mathbf{Z}^{\top},\sqrt{\lambda}\mathbf{I}_{p}) \left(\begin{array}{c} \mathbf{Z} \\ \sqrt{\lambda}\mathbf{I}_{p} \end{array} \right) \right)^{-1} (\mathbf{Z}^{\top},\sqrt{\lambda}\mathbf{I}_{p}) \left(\begin{array}{c} \mathbf{y} \\ \mathbf{0} \end{array} \right) \\ &= (\mathbf{Z}^{\top}\mathbf{Z}+\lambda\mathbf{I}_{p})^{-1}\mathbf{Z}^{\top}\mathbf{y}, \end{aligned}$$

- LASSO does not have an analytical solution
- RIDGE regularized regression can be solved with Gradient Descent : simply add a term to the gradient
 - same for RIDGE-Logistic regression
- LASSO can be solved via quadratic programming
 - or via approximation schemas like "forward stagewise"

Logistic Regression with RIDGE

$$h_w(\mathbf{x}) = g(w\mathbf{x}) = \frac{1}{1 + e^{-w\mathbf{x}}} = \frac{1}{1 + e^{-\sum_d w^d x^d}}$$

- like before, Logistic Regression optimizes max log likelihood of data
 - but now we add the L2 RIDGE penalty

$$\max_{w_0,w} \frac{1}{N} \sum_{i=1}^{N} \left[y_i \log(P(y=1|x_i) + (1-y_i) \log(P(y=0|x_i)) \right] - \frac{\lambda}{N} R(w)$$
$$\max_{w_0,w} \frac{1}{N} \sum_{i=1}^{N} \left[y_i \log h_w(x) + (1-y_i) \log(1-h_w(x)) \right] - \frac{\lambda}{2N} \sum_{j=1}^{d} w^{j2}$$

- to use Gradient Descent we differentiate for each component j
 - gradient same as the one for logistic regression, except adding the differential of RIDGE penalty

$$\frac{\delta J}{\delta w^j} = \frac{1}{N} \sum_{i=1}^N (y_i - h_w(x_i)) x_i^j + \frac{\lambda}{N} w^j$$

- The differential gives the Gradient Descend rule

$$\begin{split} w^{0} &:= w^{0} - \alpha \frac{1}{N} \sum_{i=1}^{N} (h_{w}(x_{i}) - y_{i}) x_{i}^{0} \\ w^{j} &:= w^{j} - \alpha \big[\frac{1}{N} \sum_{i=1}^{N} (h_{w}(x_{i}) - y_{i}) x_{i}^{j} + \frac{\lambda}{N} w^{j} \big] \text{ for any } j = 1:d \end{split}$$

