#### CSci 8980: ML at Large Scale and High Dimensions

Instructor: Arindam Banerjee

January 29, 2014

Instructor: Arindam Banerjee The LASSC

• Given training data  $(y_i, \mathbf{x}_i), i = 1, \dots, n, \mathbf{x}_i \in \mathbb{R}^p$ 

э

/₽ ► < ∃ ►

- Given training data  $(y_i, \mathbf{x}_i), i = 1, \dots, n, \mathbf{x}_i \in \mathbb{R}^p$
- Ordinary least squares (OLS)

$$\hat{\beta} = \operatorname{argmin}_{\beta \in \mathbb{R}^p} \sum_{i=1}^n (y_i - \beta^T \mathbf{x}_i)^2$$

- Given training data  $(y_i, \mathbf{x}_i), i = 1, \dots, n, \mathbf{x}_i \in \mathbb{R}^p$
- Ordinary least squares (OLS)

$$\hat{\beta} = \operatorname{argmin}_{\beta \in \mathbb{R}^p} \sum_{i=1}^n (y_i - \beta^T \mathbf{x}_i)^2$$

• Issues/challenges with OLS

- Given training data  $(y_i, \mathbf{x}_i), i = 1, \dots, n, \mathbf{x}_i \in \mathbb{R}^p$
- Ordinary least squares (OLS)

$$\hat{\beta} = \operatorname{argmin}_{\beta \in \mathbb{R}^p} \sum_{i=1}^n (y_i - \beta^T \mathbf{x}_i)^2$$

- Issues/challenges with OLS
  - Accuracy: low bias, high variance

- Given training data  $(y_i, \mathbf{x}_i), i = 1, \dots, n, \mathbf{x}_i \in \mathbb{R}^p$
- Ordinary least squares (OLS)

$$\hat{\beta} = \operatorname{argmin}_{\beta \in \mathbb{R}^p} \sum_{i=1}^n (y_i - \beta^T \mathbf{x}_i)^2$$

- Issues/challenges with OLS
  - Accuracy: low bias, high variance
  - Interpretation: All coefficients are non-zero

- Given training data  $(y_i, \mathbf{x}_i), i = 1, \dots, n, \mathbf{x}_i \in \mathbb{R}^p$
- Ordinary least squares (OLS)

$$\hat{\beta} = \operatorname{argmin}_{\beta \in \mathbb{R}^p} \sum_{i=1}^n (y_i - \beta^T \mathbf{x}_i)^2$$

- Issues/challenges with OLS
  - Accuracy: low bias, high variance
  - Interpretation: All coefficients are non-zero
  - Cannot determine small subsets with strong effects

- Given training data  $(y_i, \mathbf{x}_i), i = 1, \dots, n, \mathbf{x}_i \in \mathbb{R}^p$
- Ordinary least squares (OLS)

$$\hat{\beta} = \operatorname{argmin}_{\beta \in \mathbb{R}^p} \sum_{i=1}^n (y_i - \beta^T \mathbf{x}_i)^2$$

- Issues/challenges with OLS
  - Accuracy: low bias, high variance
  - Interpretation: All coefficients are non-zero
  - Cannot determine small subsets with strong effects
- Shrinking coefficients

- Given training data  $(y_i, \mathbf{x}_i), i = 1, \dots, n, \mathbf{x}_i \in \mathbb{R}^p$
- Ordinary least squares (OLS)

$$\hat{\beta} = \operatorname{argmin}_{\beta \in \mathbb{R}^p} \sum_{i=1}^n (y_i - \beta^T \mathbf{x}_i)^2$$

- Issues/challenges with OLS
  - Accuracy: low bias, high variance
  - Interpretation: All coefficients are non-zero
  - Cannot determine small subsets with strong effects
- Shrinking coefficients
  - Increases bias, lowers variance, improves accuracy

- Given training data  $(y_i, \mathbf{x}_i), i = 1, \dots, n, \mathbf{x}_i \in \mathbb{R}^p$
- Ordinary least squares (OLS)

$$\hat{\beta} = \operatorname{argmin}_{\beta \in \mathbb{R}^p} \sum_{i=1}^n (y_i - \beta^T \mathbf{x}_i)^2$$

- Issues/challenges with OLS
  - Accuracy: low bias, high variance
  - Interpretation: All coefficients are non-zero
  - Cannot determine small subsets with strong effects
- Shrinking coefficients
  - Increases bias, lowers variance, improves accuracy
- Alternatives

- Given training data  $(y_i, \mathbf{x}_i), i = 1, \dots, n, \mathbf{x}_i \in \mathbb{R}^p$
- Ordinary least squares (OLS)

$$\hat{\beta} = \operatorname{argmin}_{\beta \in \mathbb{R}^p} \sum_{i=1}^n (y_i - \beta^T \mathbf{x}_i)^2$$

- Issues/challenges with OLS
  - Accuracy: low bias, high variance
  - Interpretation: All coefficients are non-zero
  - Cannot determine small subsets with strong effects
- Shrinking coefficients
  - Increases bias, lowers variance, improves accuracy
- Alternatives
  - Subset selection: Unstable, sensitive to small changes

- Given training data  $(y_i, \mathbf{x}_i), i = 1, \dots, n, \mathbf{x}_i \in \mathbb{R}^p$
- Ordinary least squares (OLS)

$$\hat{\beta} = \operatorname{argmin}_{\beta \in \mathbb{R}^p} \sum_{i=1}^n (y_i - \beta^T \mathbf{x}_i)^2$$

- Issues/challenges with OLS
  - Accuracy: low bias, high variance
  - Interpretation: All coefficients are non-zero
  - Cannot determine small subsets with strong effects
- Shrinking coefficients
  - Increases bias, lowers variance, improves accuracy
- Alternatives
  - Subset selection: Unstable, sensitive to small changes
  - Ridge regression: Shrinks coefficients, but not to 0

$$ullet$$
 Let  $\hateta^0$  be the OLS solution, and  $t_0=\sum_{j=1}^p|\hateta^0|$ 

æ

<ロト <部ト < 注ト < 注ト

- Let  $\hat{\beta}^0$  be the OLS solution, and  $t_0 = \sum_{i=1}^p |\hat{\beta}^0|$
- The non-negative garotte estimator (Breiman, 1996)

$$(\hat{\alpha}, \hat{c}) = \operatorname*{argmin}_{(\alpha, c)} \sum_{i=1}^{n} (y_i - \alpha - \sum_j c_j \hat{\beta}_j^0 x_{ij})^2 \text{ s.t.} c_j \ge 0, \sum_j c_j \le t$$

- Let  $\hat{\beta}^0$  be the OLS solution, and  $t_0 = \sum_{j=1}^p |\hat{\beta}^0|$
- The non-negative garotte estimator (Breiman, 1996)

$$(\hat{\alpha}, \hat{c}) = \operatorname*{argmin}_{(\alpha, c)} \sum_{i=1}^{n} (y_i - \alpha - \sum_j c_j \hat{\beta}_j^0 x_{ij})^2 \text{ s.t.} c_j \ge 0, \sum_j c_j \le t$$

• Relies on OLS  $\hat{\beta}^0$ : may be problematic in certain settings

- Let  $\hat{\beta}^0$  be the OLS solution, and  $t_0 = \sum_{j=1}^p |\hat{\beta}^0|$
- The non-negative garotte estimator (Breiman, 1996)

$$(\hat{lpha}, \hat{c}) = \operatorname*{argmin}_{(lpha, c)} \sum_{i=1}^{n} (y_i - lpha - \sum_j c_j \hat{eta}_j^0 x_{ij})^2 ext{ s.t.} c_j \ge 0, \sum_j c_j \le t$$

- Relies on OLS  $\hat{\beta}^0$ : may be problematic in certain settings
- Least absolute shrinkage and selection operator (LASSO)

$$(\hat{\alpha}, \hat{\beta}) = \operatorname{argmin}_{(\alpha, \beta)} \sum_{i=1}^{n} (y_i - \alpha - \sum_j \beta_j x_{ij})^2 \text{ s.t. } \sum_j |\beta_j| \le t$$

- Let  $\hat{\beta}^0$  be the OLS solution, and  $t_0 = \sum_{j=1}^p |\hat{\beta}^0|$
- The non-negative garotte estimator (Breiman, 1996)

$$(\hat{lpha}, \hat{c}) = \operatorname*{argmin}_{(lpha, c)} \sum_{i=1}^{n} (y_i - lpha - \sum_j c_j \hat{eta}_j^0 x_{ij})^2 ext{ s.t.} c_j \ge 0, \sum_j c_j \le t$$

- Relies on OLS  $\hat{\beta}^0$ : may be problematic in certain settings
- Least absolute shrinkage and selection operator (LASSO)

$$(\hat{\alpha}, \hat{\beta}) = \operatorname{argmin}_{(\alpha, \beta)} \sum_{i=1}^{n} (y_i - \alpha - \sum_j \beta_j x_{ij})^2 \text{ s.t. } \sum_j |\beta_j| \le t$$

• Parameter  $t < t_0$  will cause shrinkage

- Let  $\hat{\beta}^0$  be the OLS solution, and  $t_0 = \sum_{j=1}^p |\hat{\beta}^0|$
- The non-negative garotte estimator (Breiman, 1996)

$$(\hat{lpha}, \hat{c}) = \operatorname*{argmin}_{(lpha, c)} \sum_{i=1}^{n} (y_i - lpha - \sum_j c_j \hat{eta}_j^0 x_{ij})^2 ext{ s.t.} c_j \ge 0, \sum_j c_j \le t$$

- Relies on OLS  $\hat{\beta}^0$ : may be problematic in certain settings
- Least absolute shrinkage and selection operator (LASSO)

$$(\hat{\alpha}, \hat{\beta}) = \operatorname{argmin}_{(\alpha, \beta)} \sum_{i=1}^{n} (y_i - \alpha - \sum_j \beta_j x_{ij})^2 \text{ s.t. } \sum_j |\beta_j| \le t$$

- Parameter  $t < t_0$  will cause shrinkage
  - Some coefficients will become 0

• Design matrix  $X \in \mathbb{R}^{n \times p}$ , assume  $X^T X = I \in \mathbb{R}^{p \times p}$ 

- Design matrix  $X \in \mathbb{R}^{n \times p}$ , assume  $X^T X = I \in \mathbb{R}^{p \times p}$
- Best subset selection picks k largest coefficients

- Design matrix  $X \in \mathbb{R}^{n \times p}$ , assume  $X^T X = I \in \mathbb{R}^{p \times p}$
- Best subset selection picks k largest coefficients
- $\bullet\,$  For a suitable constant  $\gamma,$  the LASSO solution is

 $\hat{\beta}_j = \operatorname{sign}(\hat{\beta}_j^0)(|\hat{\beta}_j^0| - \gamma)_+$ 

- Design matrix  $X \in \mathbb{R}^{n \times p}$ , assume  $X^T X = I \in \mathbb{R}^{p \times p}$
- Best subset selection picks k largest coefficients
- For a suitable constant  $\gamma$ , the LASSO solution is  $\hat{\beta}_i = \operatorname{sign}(\hat{\beta}_i^0)(|\hat{\beta}_i^0| - \gamma)_+$
- Ridge regression shrinks the coefficients

$$\hat{eta}^{\mathsf{ridge}}_j = rac{1}{1+\gamma}\hat{eta}^{\mathsf{0}}_j$$

- Design matrix  $X \in \mathbb{R}^{n \times p}$ , assume  $X^T X = I \in \mathbb{R}^{p \times p}$
- Best subset selection picks k largest coefficients
- For a suitable constant  $\gamma$ , the LASSO solution is  $\hat{\beta}_i = \operatorname{sign}(\hat{\beta}_i^0)(|\hat{\beta}_i^0| - \gamma)_+$
- Ridge regression shrinks the coefficients

$$\hat{eta}^{\mathsf{ridge}}_j = rac{1}{1+\gamma}\hat{eta}^{\mathsf{0}}_j$$

Garotte estimates

$$\hat{eta}_j^{ ext{garotte}} = \left(1 - rac{\gamma}{(\hat{eta}_j^0)^2}
ight)_+ \hat{eta}_j^0$$



Shrinkage due to (a) subset selection, (b) ridge regression, (c) the lasso, and (b) the garotte

 $(\beta - \hat{\beta}^0)^T X^T X (\beta - \hat{\beta}^0)$ 

 $(\beta - \hat{\beta}^0)^T X^T X (\beta - \hat{\beta}^0)$ 

• Level sets of the contour intersects with  $L_q$  norm ball

 $(\beta - \hat{\beta}^0)^T X^T X (\beta - \hat{\beta}^0)$ 

Level sets of the contour intersects with L<sub>q</sub> norm ball
 q = 2: Ridge regression, shrinkage but no sparsity

 $(\beta - \hat{\beta}^0)^T X^T X (\beta - \hat{\beta}^0)$ 

- Level sets of the contour intersects with  $L_q$  norm ball
  - q = 2: Ridge regression, shrinkage but no sparsity
  - q = 1: Lasso, shrinkage and sparsity

 $(\beta - \hat{\beta}^0)^T X^T X (\beta - \hat{\beta}^0)$ 

- Level sets of the contour intersects with  $L_q$  norm ball
  - q = 2: Ridge regression, shrinkage but no sparsity
  - q = 1: Lasso, shrinkage and sparsity
- Ridge vs Lasso: Can the sign change from OLS estimate?

## Geometry of LASSO: p = 2



Estimation in (a) the lasso, and (b) ridge regression

# Geometry of LASSO: p > 2



Sign change in LASSO vs OLS is possible for p > 2

#### Example: Regularization Path



Shrinkage of parameters over  $s = \frac{t}{\sum_{j} \hat{\beta}_{j}^{0}}$ 

$$(\hat{\alpha}, \hat{\beta}) = \operatorname{argmin}_{(\alpha, \beta)} \sum_{i=1}^{n} (y_i - \alpha - \sum_j \beta_j x_{ij})^2 + \lambda \sum_j |\beta_j|$$

æ

$$(\hat{\alpha}, \hat{\beta}) = \operatorname{argmin}_{(\alpha, \beta)} \sum_{i=1}^{n} (y_i - \alpha - \sum_j \beta_j x_{ij})^2 + \lambda \sum_j |\beta_j|$$

• Cross-validation over  $\lambda$  (or t)

$$(\hat{\alpha}, \hat{\beta}) = \operatorname{argmin}_{(\alpha, \beta)} \sum_{i=1}^{n} (y_i - \alpha - \sum_j \beta_j x_{ij})^2 + \lambda \sum_j |\beta_j|$$

- Cross-validation over  $\lambda$  (or t)
  - Pick the value that leads to smallest error

$$(\hat{\alpha}, \hat{\beta}) = \operatorname{argmin}_{(\alpha, \beta)} \sum_{i=1}^{n} (y_i - \alpha - \sum_j \beta_j x_{ij})^2 + \lambda \sum_j |\beta_j|$$

- Cross-validation over  $\lambda$  (or t)
  - Pick the value that leads to smallest error
- Resampling based estimates, e.g., stability selection

• General regression problem formulation

- General regression problem formulation
  - Constrained version

$$\hat{eta} = \operatorname*{argmin}_{eta} L(y, X, eta) \text{ s.t. } \|eta\|_1 \leq t$$

## Generalized Regression Models

- General regression problem formulation
  - Constrained version

$$\hat{eta} = \operatorname*{argmin}_{eta} \ L(y, X, eta) \ ext{ s.t. } \|eta\|_1 \leq t$$

Regularized version

$$\hat{eta} = \operatorname*{argmin}_{eta} \ L(y, X, eta) + \lambda \|eta\|_1$$

## Generalized Regression Models

- General regression problem formulation
  - Constrained version

$$\hat{eta} = \operatorname*{argmin}_{eta} \ L(y, X, eta) \ ext{ s.t. } \|eta\|_1 \leq t$$

Regularized version

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} L(y, X, \beta) + \lambda \|\beta\|_1$$

• The other constrained version

$$\hat{eta} = \operatorname*{argmin}_eta \|eta\|_1 \;\; ext{s.t.} \; L(y, X, eta) \leq a$$

## Generalized Regression Models

- General regression problem formulation
  - Constrained version

$$\hat{eta} = \operatorname*{argmin}_eta \ L(y, X, eta) \ \ ext{s.t.} \ \|eta\|_1 \leq t$$

Regularized version

$$\hat{eta} = \operatorname*{argmin}_{eta} L(y, X, eta) + \lambda \|eta\|_1$$

• The other constrained version

$$\hat{eta} = \mathop{\mathrm{argmin}}\limits_eta \|eta\|_1 \;\; ext{s.t.} \; L(y, X, eta) \leq a$$

• Examples: logistic regression, generalized linear models, etc.

- General regression problem formulation
  - Constrained version

$$\hat{eta} = \operatorname*{argmin}_eta \ L(y, X, eta) \ \ ext{s.t.} \ \|eta\|_1 \leq t$$

Regularized version

$$\hat{eta} = \operatorname*{argmin}_{eta} L(y, X, eta) + \lambda \|eta\|_1$$

• The other constrained version

$$\hat{eta} = \operatorname*{argmin}_eta \|eta\|_1 \;\; ext{s.t.} \; L(y, X, eta) \leq a$$

- Examples: logistic regression, generalized linear models, etc.
- We will consider efficient algorithms for such general problems

• Consider orthonormal design  $X^T X = I$ , so Lasso estimate is

$$\hat{eta}_j = \mathsf{sign}(\hat{eta}_j^0)(|\hat{eta}_j^0|-\gamma)_+$$

- Consider orthonormal design  $X^T X = I$ , so Lasso estimate is  $\hat{\beta}_i = \operatorname{sign}(\hat{\beta}_i^0)(|\hat{\beta}_i^0| - \gamma)_+$
- Let  $\beta$  be the 'true' parameter:

$$y = \beta^T \mathbf{x} + \epsilon, \ \epsilon \sim N(0, \sigma^2)$$

- Consider orthonormal design  $X^T X = I$ , so Lasso estimate is  $\hat{\beta}_i = \operatorname{sign}(\hat{\beta}_i^0)(|\hat{\beta}_i^0| - \gamma)_+$
- Let  $\beta$  be the 'true' parameter:

$$y = \beta^T \mathbf{x} + \epsilon, \ \epsilon \sim N(0, \sigma^2)$$

Consider risk

$$R(\hat{\beta},\beta) = E \|\hat{\beta} - \beta\|^2$$

- Consider orthonormal design  $X^T X = I$ , so Lasso estimate is  $\hat{\beta}_i = \operatorname{sign}(\hat{\beta}_i^0)(|\hat{\beta}_i^0| - \gamma)_+$
- Let  $\beta$  be the 'true' parameter:

$$y = \beta^T \mathbf{x} + \epsilon, \ \epsilon \sim N(0, \sigma^2)$$

Consider risk

$$R(\hat{\beta},\beta) = E \|\hat{\beta} - \beta\|^2$$

• Let  $R_{DP}$  be the loss of the 'optimal' predictor  $T_{DP}(\hat{\beta}^0, \delta) = (\delta_j \hat{\beta}_j^0), \quad \delta_j = I(|\beta_j| > \sigma) \in \{0, 1\}$ 

- Consider orthonormal design  $X^T X = I$ , so Lasso estimate is  $\hat{\beta}_i = \operatorname{sign}(\hat{\beta}_i^0)(|\hat{\beta}_i^0| - \gamma)_+$
- Let  $\beta$  be the 'true' parameter:

$$y = \beta^T \mathbf{x} + \epsilon, \ \epsilon \sim N(0, \sigma^2)$$

Consider risk

$$R(\hat{\beta},\beta) = E \|\hat{\beta} - \beta\|^2$$

- Let  $R_{DP}$  be the loss of the 'optimal' predictor  $T_{DP}(\hat{\beta}^0, \delta) = (\delta_j \hat{\beta}_j^0), \quad \delta_j = I(|\beta_j| > \sigma) \in \{0, 1\}$
- $T_{DP}$  needs knowledge of  $\beta$ , not practical

• Hard threshold estimator 
$$\tilde{\beta}_j = \hat{\beta}_j^0 I(|\hat{\beta}_j^0| > \gamma)$$

æ

• Hard threshold estimator  $\tilde{\beta}_j = \hat{\beta}_j^0 I(|\hat{\beta}_j^0| > \gamma)$ • Has risk  $R(\tilde{\beta}, \beta) \le (2 \log p + 1)(\sigma^2 + R_{DP})$ 

- Hard threshold estimator  $\tilde{\beta}_j = \hat{\beta}_j^0 I(|\hat{\beta}_j^0| > \gamma)$ 
  - Has risk  $R( ilde{eta},eta) \leq (2\log p + 1)(\sigma^2 + R_{DP})$
  - Threshold  $\gamma = \sigma (2 \log n)^{1/2}$  to get smallest asymptotic risk

- Hard threshold estimator β<sub>j</sub> = β<sup>0</sup><sub>j</sub>I(|β<sup>0</sup><sub>j</sub>| > γ)
   Has risk R(β, β) ≤ (2 log p + 1)(σ<sup>2</sup> + R<sub>DP</sub>)
   Threshold γ = σ(2 log n)<sup>1/2</sup> to get smallest asymptotic risk
- Soft threshold estimator  $\hat{\beta}_j = \operatorname{sign}(\hat{\beta}_j^0)(|\hat{\beta}_j^0| \gamma)_+$

- Hard threshold estimator  $\tilde{\beta}_j = \hat{\beta}_j^0 I(|\hat{\beta}_j^0| > \gamma)$ 
  - Has risk  $R( ilde{eta},eta) \leq (2\log p + 1)(\sigma^2 + R_{DP})$
  - Threshold  $\gamma = \sigma (2 \log n)^{1/2}$  to get smallest asymptotic risk
- Soft threshold estimator  $\hat{\beta}_j = \text{sign}(\hat{\beta}_j^0)(|\hat{\beta}_j^0| \gamma)_+$ 
  - With  $\gamma = \sigma (2 \log n)^{1/2}$ , has same behavior

- Hard threshold estimator  $\tilde{\beta}_j = \hat{\beta}_j^0 I(|\hat{\beta}_j^0| > \gamma)$ 
  - Has risk  $R( ilde{eta},eta) \leq (2\log p + 1)(\sigma^2 + R_{DP})$
  - Threshold  $\gamma = \sigma (2 \log n)^{1/2}$  to get smallest asymptotic risk
- Soft threshold estimator  $\hat{\beta}_j = \operatorname{sign}(\hat{\beta}_j^0)(|\hat{\beta}_j^0| \gamma)_+$ 
  - With  $\gamma = \sigma (2 \log n)^{1/2}$ , has same behavior
- General design matrices

- Hard threshold estimator  $\tilde{\beta}_j = \hat{\beta}_j^0 I(|\hat{\beta}_j^0| > \gamma)$ 
  - Has risk  $R( ilde{eta},eta) \leq (2\log p + 1)(\sigma^2 + R_{DP})$
  - Threshold  $\gamma = \sigma (2\log n)^{1/2}$  to get smallest asymptotic risk
- Soft threshold estimator  $\hat{\beta}_j = \operatorname{sign}(\hat{\beta}_j^0)(|\hat{\beta}_j^0| \gamma)_+$ 
  - With  $\gamma = \sigma (2 \log n)^{1/2}$ , has same behavior
- General design matrices
  - Lasso estimator continues to have good properties

- Hard threshold estimator  $\tilde{\beta}_j = \hat{\beta}_j^0 I(|\hat{\beta}_j^0| > \gamma)$ 
  - Has risk  $R( ilde{eta},eta) \leq (2\log p + 1)(\sigma^2 + R_{DP})$
  - Threshold  $\gamma = \sigma (2 \log n)^{1/2}$  to get smallest asymptotic risk
- Soft threshold estimator  $\hat{\beta}_j = \operatorname{sign}(\hat{\beta}_j^0)(|\hat{\beta}_j^0| \gamma)_+$ 
  - With  $\gamma = \sigma (2 \log n)^{1/2}$ , has same behavior
- General design matrices
  - Lasso estimator continues to have good properties
  - · Generalized to other sparsity inducing norms



 $L_q$  norm level sets: (a) q = 4, (b) q = 2, (c) q = 1, (d) q = 0.5, (e) q = 0.1

э