

Sparsity in Machine Learning

EN.580.709 - Fall 2019

Supervised Learning

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We only get to measure the *empirical risk*,

$$\hat{R}_S(h) = \frac{1}{n} \sum_i L(h(\mathbf{x}_i), y_i)$$

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$$\min_{\boldsymbol{\beta}} \frac{1}{n} \sum_i^n (y_i - \boldsymbol{\beta}^T \mathbf{x}_i)^2 = \frac{1}{n} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2$$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \in \mathbb{R}^n, \quad \mathbf{X} = \begin{bmatrix} -\mathbf{x}_1^T - \\ -\mathbf{x}_2^T - \\ \vdots \\ -\mathbf{x}_n^T - \end{bmatrix} \in \mathbb{R}^{n \times m}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_n^T \end{bmatrix} \in \mathbb{R}^m$$

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- If $n < m$, infinite solutions. One possibility is the one with minimal ℓ_2 norm:

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Ridge (Regularized) Regression

$$\min_{\boldsymbol{\beta}} \mathcal{L} = \frac{1}{n} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \lambda \|\boldsymbol{\beta}\|_2^2$$

$$\Rightarrow \hat{\boldsymbol{\beta}} = \left(\frac{1}{n} \mathbf{X}^T \mathbf{X} + \lambda \mathbf{I} \right)^{-1} \left(\frac{1}{n} \mathbf{X}^T \mathbf{y} \right)$$

Polynomial Regression

Let $x \in \mathbb{R}$,

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$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \approx \begin{bmatrix} 1, \phi_1(x_1), \dots, \phi_m(x_1) \\ 1, \phi_1(x_2), \dots, \phi_m(x_2) \\ \vdots \\ 1, \phi_1(x_n), \dots, \phi_m(x_n) \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_m \end{bmatrix}$$

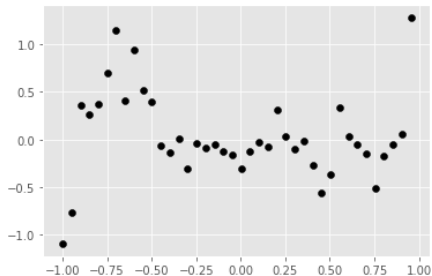
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$$y_i = h^*(x_i) + v_i, \quad v_i \sim \mathcal{N}(0, \sigma^2)$$



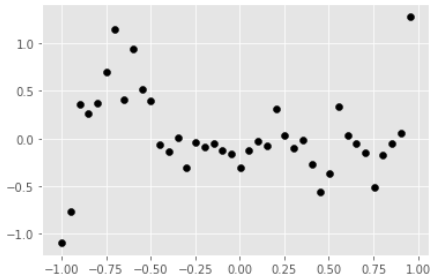
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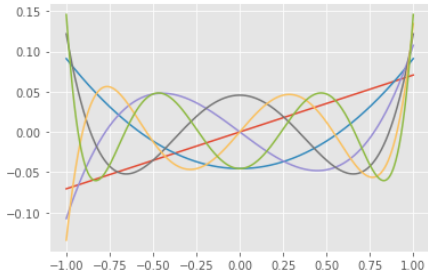
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$$\phi_j(x), \quad 1 \leq j \leq m$$



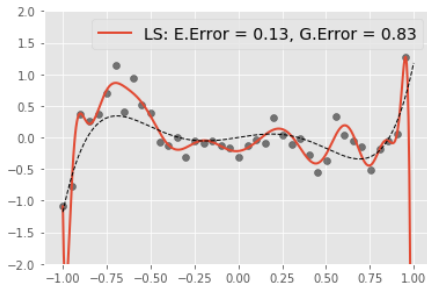
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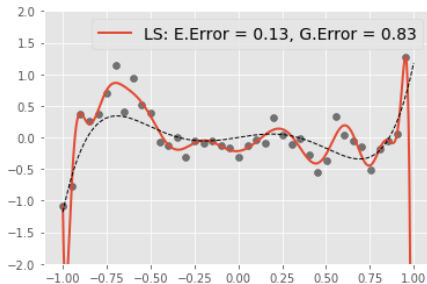
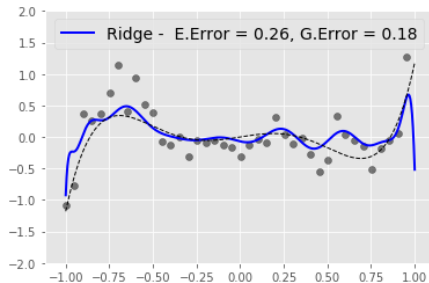
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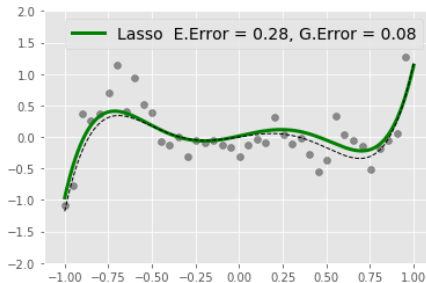
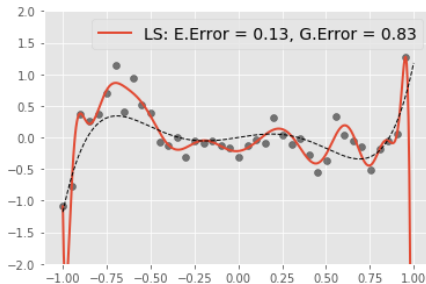
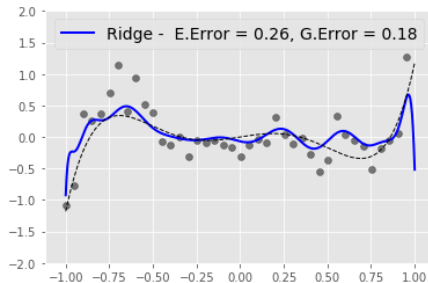
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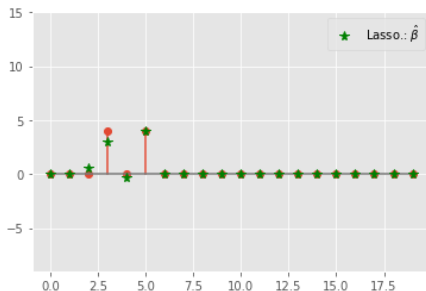
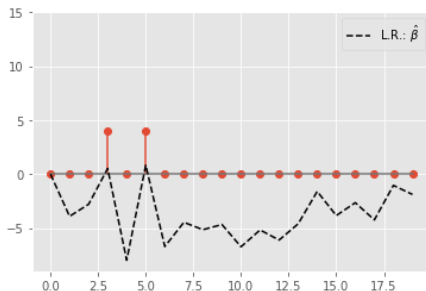
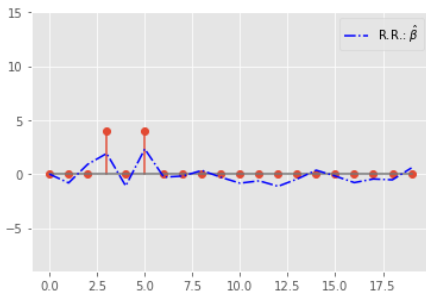
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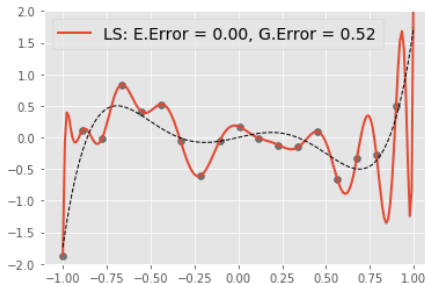
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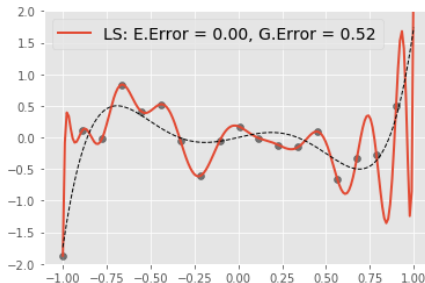
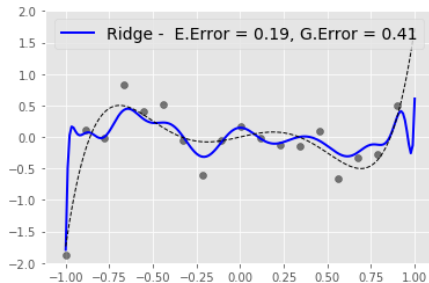
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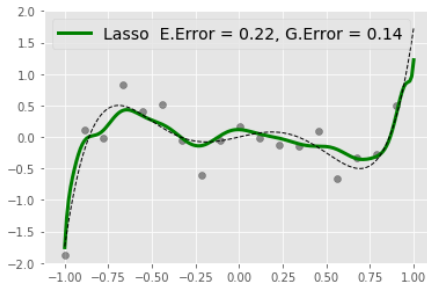
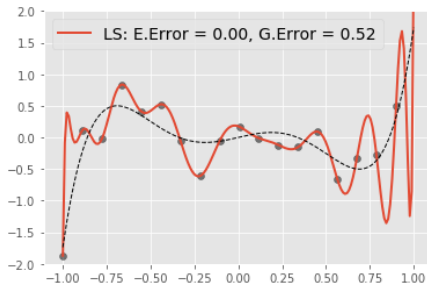
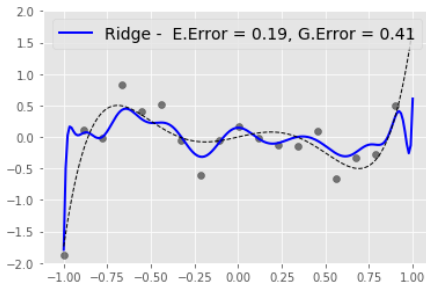
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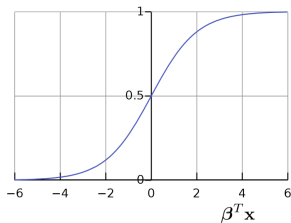
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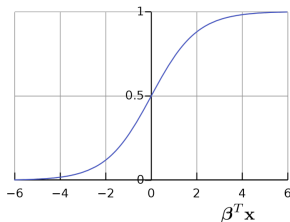


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Generalized Linear Models (GLM)

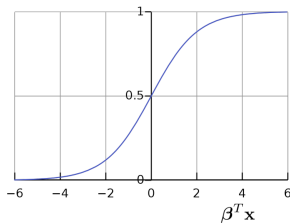
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For log. regression, $\mu(X) = P(Y = 1|X = \mathbf{x})$, and $g(u) = \log \frac{u}{1-u}$

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$$\hat{\beta} = \arg \max_{\beta} \sum_{i=1}^n y_i \beta^T \mathbf{x}_i - \log(1 + e^{\beta^T \mathbf{x}_i})$$

Logistic Regression

How do we fit β ? Maximize the (log) likelihood $P(\{y_i\}|\beta, \{x_i\})$:

$$\hat{\beta} = \arg \max_{\beta} \mathcal{L}(\beta)$$

$$\mathcal{L}(\beta) = \prod_{i=1}^n P(Y = y_i | \mathbf{x}_i) = \prod_{i=1}^n P(Y = 1 | \mathbf{x}_i)^{y_i} P(Y = 0 | \mathbf{x}_i)^{1-y_i}$$

$$\begin{aligned} \log \mathcal{L}(\beta) &= \sum_{i=1}^n y_i \log P(Y = 1 | \mathbf{x}_i) + (1 - y_i) \log P(Y = 0 | \mathbf{x}_i) \\ &= \sum_{i=1}^n y_i \log \frac{1}{1 + e^{-\beta^T \mathbf{x}}} + (1 - y_i) \log \frac{1}{1 + e^{\beta^T \mathbf{x}}} \end{aligned}$$

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Need for Regularization

Ridge ℓ_2 regularization:

$$\hat{\beta} = \arg \min_{\beta} -\log \mathcal{L}(\beta) + \lambda \|\beta\|_2^2$$

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Leukemia Dataset (lymphoblastic vs myeloid) $n = 35, p = 7128$!

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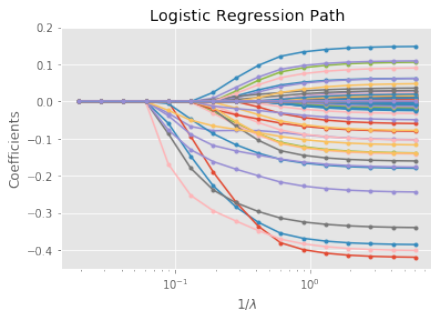
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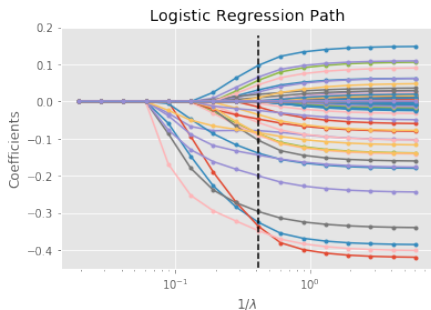
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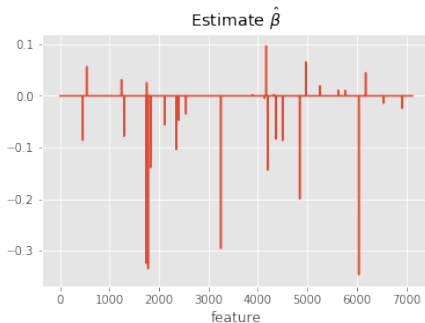
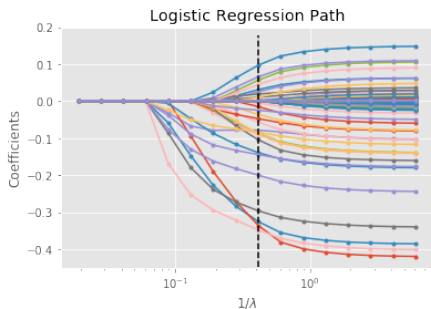
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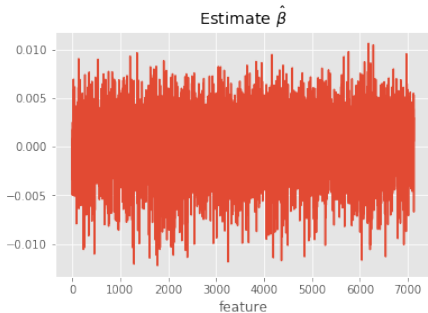
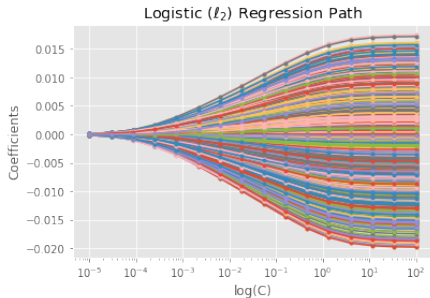
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- ℓ_2 Logistic Regression



Multi-class Logistic Regression

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- Multinomial likelihood

$$P(Y = k|\mathbf{x}) = \frac{e^{\beta_k^T \mathbf{x}}}{\sum_{l=1}^K e^{\beta_l^T \mathbf{x}}}; \quad K \text{ classifiers } \beta_l \in \mathbb{R}^m$$

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Multi-class Logistic Regression

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$$\frac{-1}{n} \sum_{i=1}^n \left[\sum_{k=1}^K 1_{[y_i=k]} (\beta_k^T \mathbf{x}_i) - \log \left(\sum_{k=1}^K e^{\beta_k^T \mathbf{x}_i} \right) \right] + \lambda \sum_{l=1}^K \|\beta_l\|_1$$

Digits Classification

Some samples from Dataset



Class 5



Class 0



Class 4



Class 1



Class 9



Class 2



Class 1



Class 3



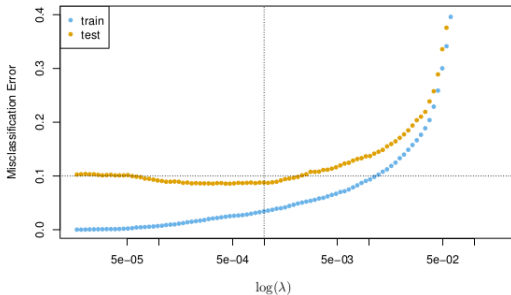
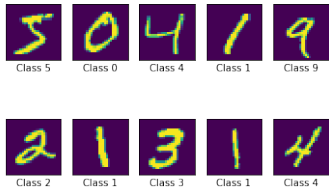
Class 1



Class 4

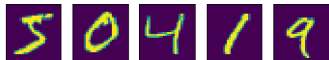
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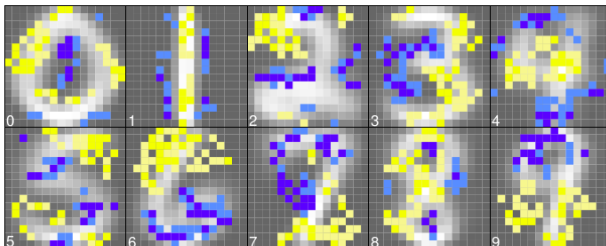
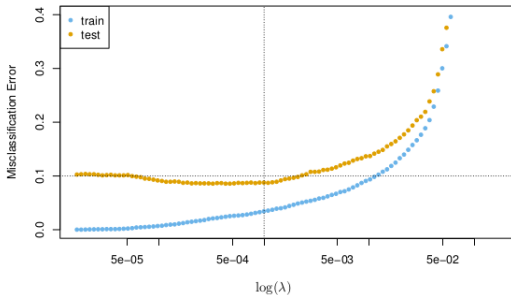
Class 2

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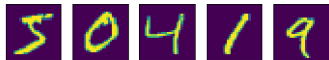
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Class 5

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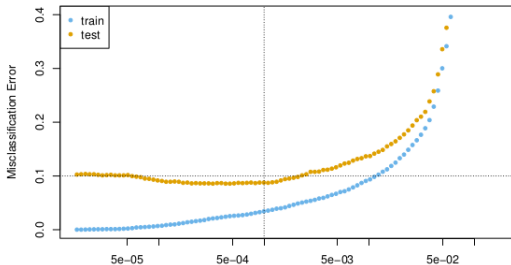
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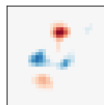
Class 1



Class 2



Class 3



Class 4



Class 5



Class 6



Class 7



Class 8



Class 9

Sparsity in Machine Learning

Part II

EN.580.709 - Fall 2019

Recall Lasso

- $\mathbf{y} \in \mathbb{R}^n$: response, $\mathbf{X} \in \mathbb{R}^{n \times m}$: predictors/features

$$\hat{\boldsymbol{\beta}} \in \arg \min_{\boldsymbol{\beta}} \frac{1}{2} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \lambda \|\boldsymbol{\beta}\|_1$$

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(why?)

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Elastic-Net

$$\hat{\boldsymbol{\beta}} \in \arg \min_{\boldsymbol{\beta}} \frac{1}{2} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \lambda \left(\alpha \|\boldsymbol{\beta}\|_1 + (1 - \alpha) \frac{1}{2} \|\boldsymbol{\beta}\|_2^2 \right)$$

Example

Let $Z_1, Z_2 \sim N(0, 1)$

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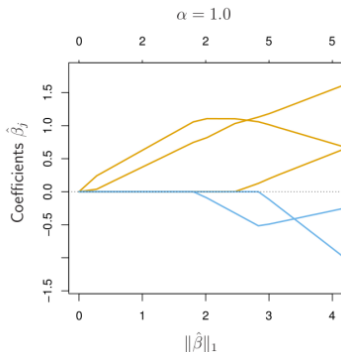
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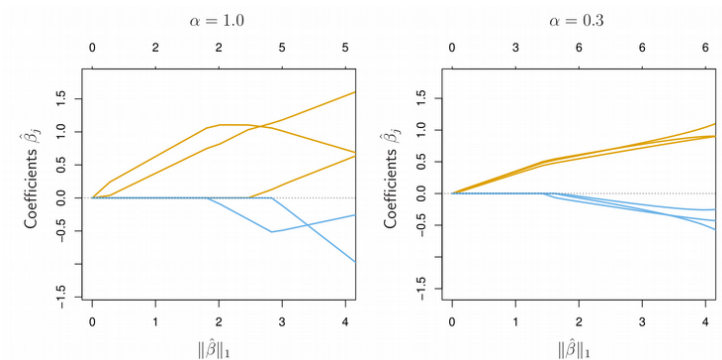
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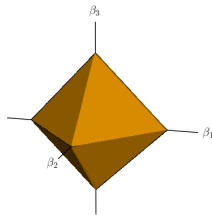
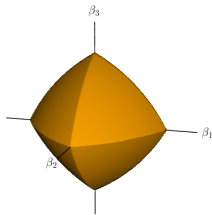
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The Elastic-Net Problem is Strictly Convex

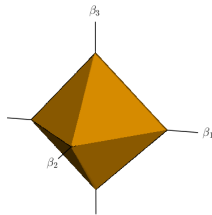
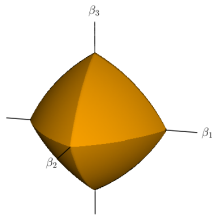
$$\min_{\boldsymbol{\beta}} \frac{1}{2} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \lambda \|\boldsymbol{\beta}\|_1 + \alpha \frac{1}{2} \|\boldsymbol{\beta}\|_2^2$$



(why?)

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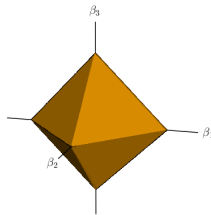
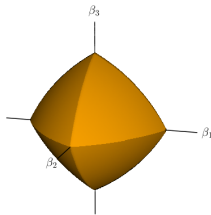
(why?)

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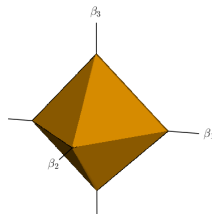
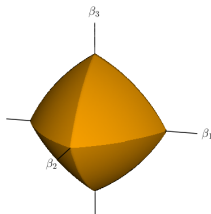
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- If \mathbf{X} : orthogonal $\Rightarrow \hat{\boldsymbol{\beta}} = \frac{1}{1+\alpha} S_{\lambda}(\mathbf{X}^T \mathbf{y})$
- If \mathbf{X} : redundant?

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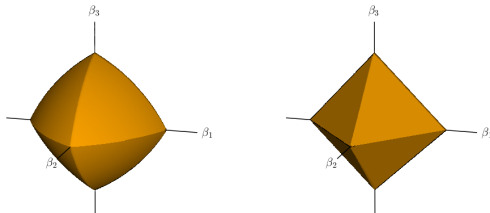
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$$\boldsymbol{\beta}^{k+1} = \text{prox}_{\lambda \|\cdot\|_1} (\boldsymbol{\beta}^k - \eta \nabla f(\boldsymbol{\beta}^k)) = S_{\lambda/c} \left(\boldsymbol{\beta}^k - \frac{1}{c} [\mathbf{X}^T (\mathbf{X} \boldsymbol{\beta}^k - \mathbf{y}) + \alpha \boldsymbol{\beta}^k] \right)$$

Leukemia type (AML/ALL) dataset - Golub et al, Science '90

- 38 training samples, 34 test samples, $m = 7129$ genes.
- Record the expression for sample i and gene j

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Leukemia classification example

Method	10-fold CV error	Test error	No. of genes
Golub UR	3/38	4/34	50
SVM RFE	2/38	1/34	31
PLR RFE	2/38	1/34	26
NSC	2/38	2/34	21
Elastic Net	2/38	0/34	45

UR: univariate ranking (Golub et al. 1999)

RFE: recursive feature elimination (Guyon et al. 2002)

SVM: support vector machine (Guyon et al. 2002)

PLR: penalized logistic regression (Zhu and Hastie 2004)

NSC: nearest shrunken centroids (Tibshirani et al. 2002)

Group Lasso

- What if there's some natural **grouping** in the problem, and we want to introduce this as a prior?
- Say, J groups, and each $\beta_j = [\beta_{j,1}, \dots, \beta_{j,m_j}]$

Group Lasso

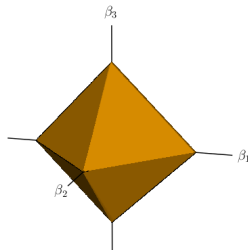
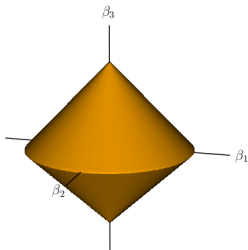
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- Let $\mathbf{Y} = [\mathbf{y}_1, \dots, \mathbf{y}_J]$: responses

$$\min_{\mathbf{B}} \|\mathbf{Y} - \mathbf{XB}\|_2^2 + \lambda \|\mathbf{B}\|_{1,2}; \quad \|\mathbf{B}\|_{1,2} = \sum_{i=1}^m \|\mathbf{B}_{i,:}\|_2$$

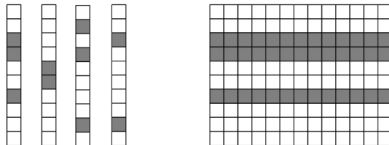
Group Lasso

- What if there's some natural **grouping** in the problem, and we want to introduce this as a prior?
- Say, J groups, and each $\beta_j = [\beta_{j,1}, \dots, \beta_{j,m_j}]$

$$\min_{\beta_j} \|\mathbf{y} - \sum_{j=1}^J \mathbf{X}_j \beta_j\|_2^2 + \lambda \sum_{j=1}^J \|\beta_j\|_2$$

- What if we have *different tasks* to predict [i.e. **multi-variate regression**]?
- Let $\mathbf{Y} = [\mathbf{y}_1, \dots, \mathbf{y}_J]$: responses

$$\min_{\mathbf{B}} \|\mathbf{Y} - \mathbf{XB}\|_2^2 + \lambda \|\mathbf{B}\|_{1,2}; \quad \|\mathbf{B}\|_{1,2} = \sum_{i=1}^m \|\mathbf{B}_{i,:}\|_2$$



Sparsity vs. joint sparsity

End of this Part

Where are we at?

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1. Sparsity in linear systems of equations

$$\min_{\mathbf{x}} \|\mathbf{y} - \mathbf{Ax}\|_2^2 \quad \text{s.t.} \quad \|\mathbf{x}\|_0 \leq k$$

2. Basis Pursuit and Compressed Sensing

$$\min_{\mathbf{x}} \|\mathbf{y} - \mathbf{Ax}\|_2^2 + \lambda \|\mathbf{x}\|_1$$

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$$\min_{\boldsymbol{\beta}} \sum_i^n \mathcal{L}(y_i, \mathbf{x}_i^T \boldsymbol{\beta}) + \lambda \|\boldsymbol{\beta}\|_p$$

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5. Dictionary Learning:

$$\min_{\mathbf{x}, \mathbf{A}} \sum_i^n \|\mathbf{y}_i - \mathbf{Ax}_i\|_2^2 \quad \text{s.t.} \quad \|\mathbf{x}_i\|_0 \leq k, \forall i$$

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4. Matrix spectral sparsity and robust PCA:

$$\min_{\mathbf{A}} \|\mathbf{X} - \mathbf{A}\| + \lambda \phi(\mathbf{A}) \quad \longleftrightarrow$$

5. Dictionary Learning:

$$\min_{\mathbf{x}, \mathbf{A}} \sum_i^n \|\mathbf{y}_i - \mathbf{A}\mathbf{x}_i\|_2^2 \quad \text{s.t.} \quad \|\mathbf{x}_i\|_0 \leq k, \forall i$$

Matrix Spectral Sparsity

EN.580.709 - Fall 2019

Eigenfaces

- Yale B Dataset



Eigenfaces

- Yale B Dataset



- Factoring Illumination



(a) mean face



(b) first eigenface



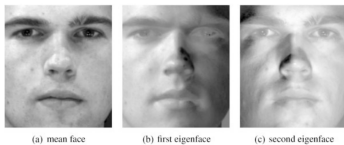
(c) second eigenface

Eigenfaces

- Yale B Dataset

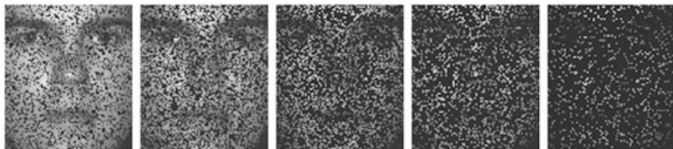


- Factoring Illumination



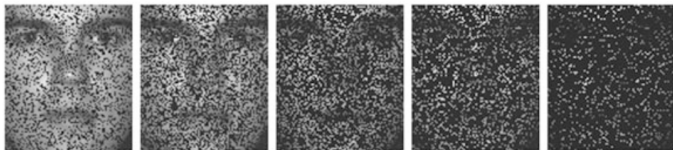
(a) Variation along the first eigenface

Matrix Completion

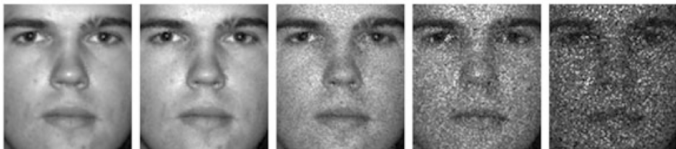


(a) Face images with (30, 50, 70, 80, 90)% percentage of missing entries

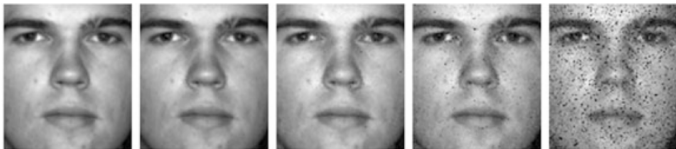
Matrix Completion



(a) Face images with (30, 50, 70, 80, 90)% percentage of missing entries



(c) Face images reconstructed by convex optimization with $\tau = 2 \times 10^4$



(d) Face images reconstructed by convex optimization with $\tau = 4 \times 10^5$

Robust PCA

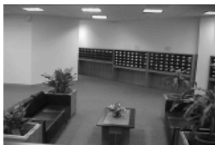
True Image



Training Image



Low-Rank ($\hat{\mathbf{L}}$)



Sparse ($\hat{\mathbf{S}}$)

