Foundations of Machine Learning CentraleSupélec — Fall 2017

7. Regularized linear regression

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Practical matters

• Class representatives (délégués de classe)

HW04

Assume p random variables X_1, \ldots, X_p , conditionally independent given Y. Y is a discrete random variable that can take one of K values $\{y_1, \ldots, y_K\}$, corresponding to K classes. We suppose that each X_j is distributed normally:

$$p(X_j = u|Y = y_k) = \frac{1}{\sigma_{jk}\sqrt{2\pi}} \exp\left(\frac{-(u - \mu_{jk})^2}{2\sigma_{jk}^2}\right).$$

Let us assume that the variance is independent of the class k and the feature j, i.e. $\sigma_{jk} = \sigma$. We observe n datapoints $\{x^1, \ldots, x^n\}$ and their labels $\{y^1, \ldots, y^n\}$. Derive the maximum likelihood estimator for μ_{jk} .

What is known? What are the parameters to be estimated?

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Maximum likelihood estimation

- Find θ such that X is the most likely to be drawn.
- Likelihood of θ given the i.i.d. sample \mathcal{X} : $\ell(\theta|\mathcal{X}) = p(\mathcal{X}|\theta) = p(\boldsymbol{x}^1|\theta)p(\boldsymbol{x}^2|\theta)\dots p(\boldsymbol{x}^n|\theta)$
- Log likelihood: $\mathcal{L}(\theta|\mathcal{X}) = \log \ell(\theta|\mathcal{X}) = \log p(\boldsymbol{x}^1|\theta) + \dots + \log p(\boldsymbol{x}^n|\theta)$
- Maximum likelihood estimation (MLE):

$$\theta^* = \arg\max_{\theta} \mathcal{L}(\theta|\mathcal{X})$$

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$$\left|\mu_{jk}^* = rg\max_{\mu_{jk}} \sum_{i=1}^n \log p(X_j = x_j^i | \mu_{jk}, \sigma)
ight|$$
 when Y=y_k

• Log likelihood:

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For feature j, class k

$$\mu_{jk}^* = \arg\max_{\mu_{jk}} \sum_{i=1}^n \log p(X_j = x_j^i | \mu_{jk}, \sigma) \quad \text{when Y=y}_k$$

$$= \frac{1}{\sigma_{jk}\sqrt{2\pi}} \exp\left(\frac{-(u-\mu_{jk})^2}{2\sigma_{jk}^2}\right)$$

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$$= \frac{1}{\sigma_{jk} \sqrt{2\pi}} \exp\left(\frac{-(x_j^i - \mu_{jk})^2}{2\sigma_{jk}^2}\right)^{I_{ik}}$$

Learning objectives

- Understand regularization as a means to control model complexity.
- Define Lasso, ridge regression, elastic net.
- Understand the role of the I1 and I2 norms in regularization
- Interpret solution paths for Lasso and ridge regression.

Regression setting

$$x_j^i \in \mathbb{R}$$
$$y^i \in \mathbb{R}$$

features variables descriptors regressors attributes p

observations samples camples data points

data matrix design matrix

X

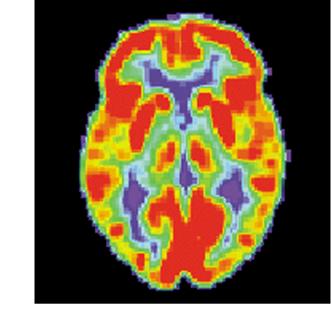
outcome target label

У

Large p, small n

neuroimaging

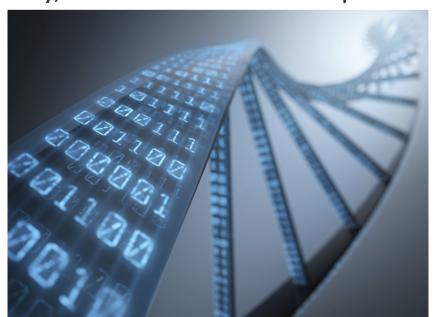
thousands of brain regions / pixels / voxels much fewer patients

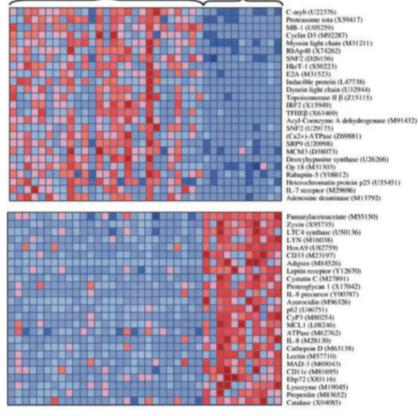


AML

genetics and genomics

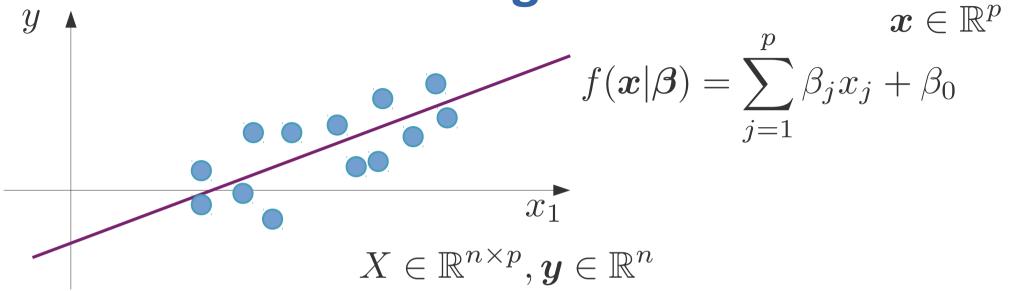
thousands of genes, millions of SNPs.. usually, at best thousands of patients





ALL

Linear regression



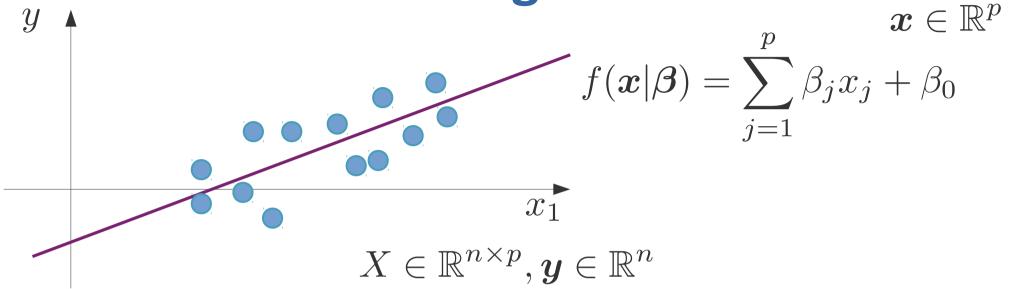
Least-squares fit (equivalent to MLE under the assumption of Gaussian noise):

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} (\boldsymbol{y} - X\boldsymbol{\beta})^{\top} (\boldsymbol{y} - X\boldsymbol{\beta}) = (X^{\top}X)^{-1}X^{\top}\boldsymbol{y}$$

Solution uniquely defined when ?



Linear regression



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Solution uniquely defined when $X^{\top}X$ invertible.

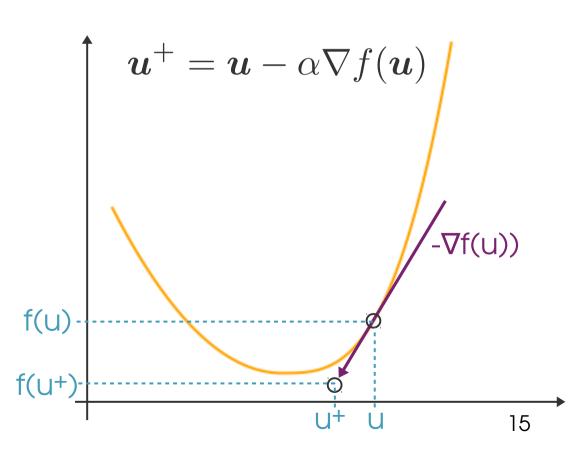
When X^TX not inversible

$$(X^{\top}X)\hat{\beta} = X^{\top}y$$

- Pseudo-inverse
- Linear system of p equations:

Numerical methods

- Gaussian elimination
- LU decomposition
- Gradient descent



Properties of the least-squares fit estimate

- Unbiased $\mathbb{E}[\hat{oldsymbol{eta}}] = oldsymbol{eta}$
- Explicit form $\hat{\beta} = (X^{\top}X)^{-1}X^{\top}y$ Computational time

Properties of the least-squares fit estimate

- Unbiased $\mathbb{E}[\hat{oldsymbol{eta}}] = oldsymbol{eta}$
- Explicit form $\hat{\boldsymbol{\beta}} = (X^{\top}X)^{-1}X^{\top}\boldsymbol{y}$
- Computational time: $\mathcal{O}(p^3 + np)$

computation of
$$(X^{\top}X)^{-1}=\mathcal{O}(p^3)$$
 computation of $X^{\top}\boldsymbol{y}=\mathcal{O}(np)$

•
$$\mathbf{p} > \mathbf{n}$$
: $X^{\top} X$

• p > n: $X^{\top}X$ not invertible

- p > n: $X^{T}X$ not invertible
 - Use a pseudo-inverse M $(X^{\top}X)M(X^{\top}X)=(X^{\top}X)$
 - Multiple possible solutions
 - High variance of the estimator.

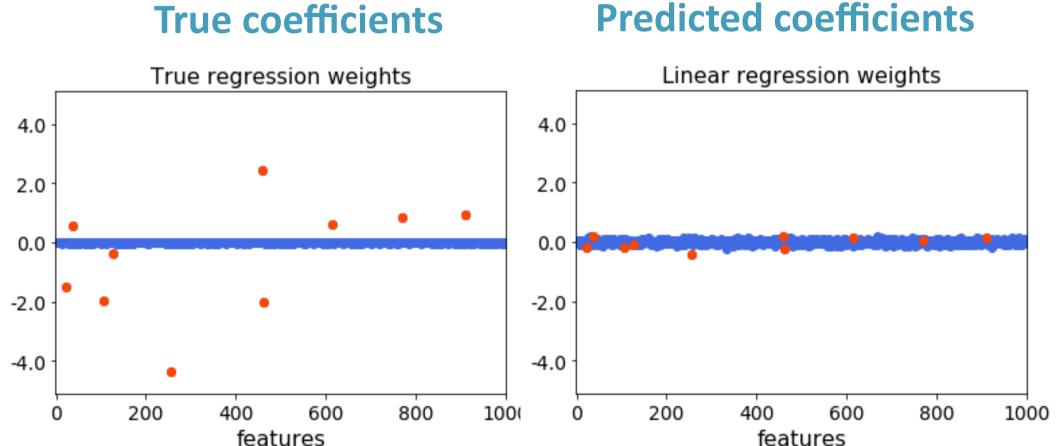
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 - High variance of the estimator.
- Multicollinearity: $X^{T}X$ not invertible
- Large p reduces interpretability of the model

Would prefer a small subset of features with strong effects (= large coefficients).

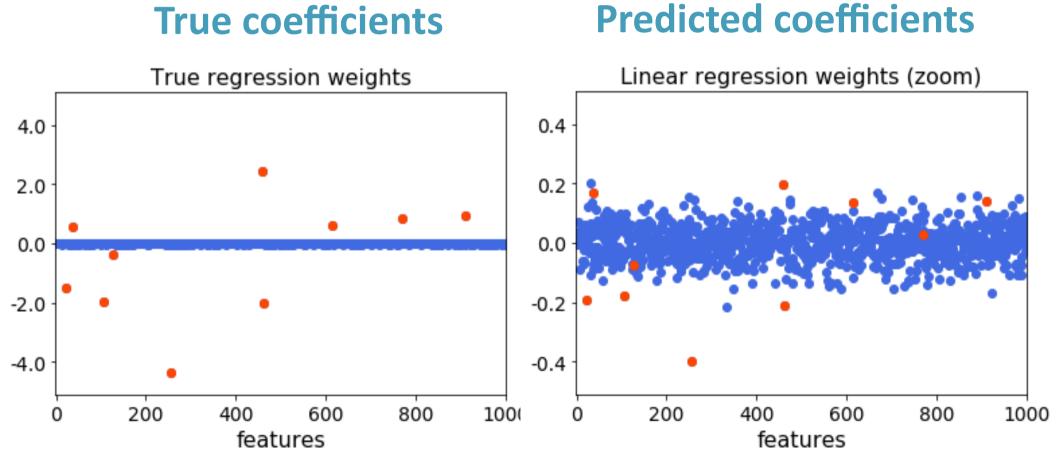
Linear regression when p >> n

Simulated data: p=1000, n=100, 10 causal features



Linear regression when p >> n

Simulated data: p=1000, n=100, 10 causal features



Regularization

Regularization

Minimize

Prediction error + λ penalty on model complexity

- Biased estimator when $\lambda \neq 0$.
- Trade bias for a smaller variance.
- λ can be set by cross-validation.

- Simpler model ≈ fewer parameters
 - → shrinkage: drive the coefficients of the parameters towards 0.

Sum-of-squares penalty

$$\hat{\boldsymbol{\beta}}_{\text{ridge}} = \arg\min_{\boldsymbol{\beta}} ||y - X\boldsymbol{\beta}||_2^2 + \lambda ||\boldsymbol{\beta}||_2^2$$

• Ridge regression estimator: ?



Sum-of-squares penalty

$$\hat{\beta}_{\text{ridge}} = \arg\min_{\beta} ||y - X\beta||_2^2 + \lambda ||\beta||_2^2$$

Ridge regression estimator:

$$\hat{\boldsymbol{\beta}}_{\text{ridge}} = (X^{\top}X + \lambda I)^{-1}X^{\top}\boldsymbol{y}$$
if $(X^{\top}X + \lambda I)$ invertible.

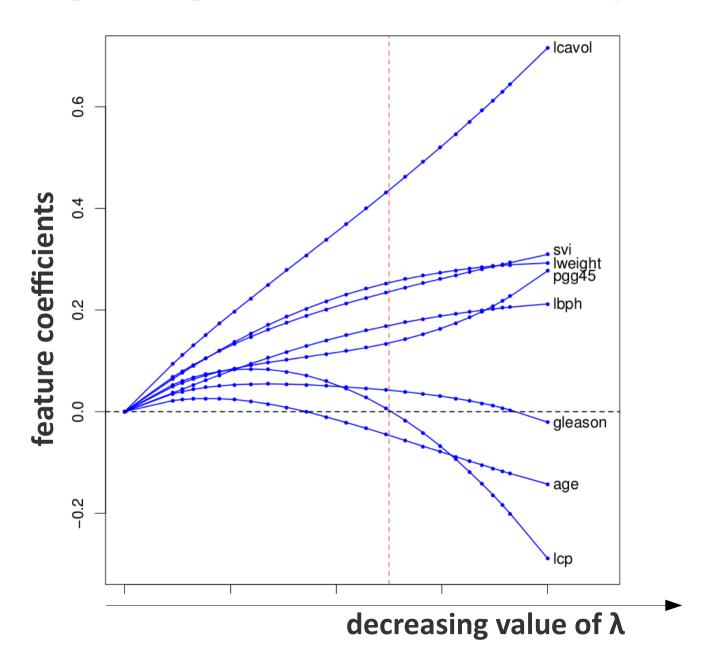
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 if $(X^{\top}X + \lambda I)$ invertible. Always!

Ridge regression solution path



Standardization

• Multiply x_j by a constant:



For ridge regression

Standardization

- Multiply x_i by a constant:
 - For standard linear regression:

$$\hat{\beta}_j \to \frac{1}{c}\hat{\beta}_j$$

 $\hat{\beta}_{j} \rightarrow \frac{1}{c}\hat{\beta}_{j}$ – For ridge regression:



Standardization

- Multiply x_i by a constant:
 - For standard linear regression:

$$\hat{\beta}_j \to \frac{1}{c}\hat{\beta}_j$$

- For ridge regression:
 - Not so clear, because of the penalization term λeta_j^2
- Need to standardize the features

$$\tilde{x}_{j}^{i} = \frac{x_{j}^{i}}{\sqrt{\frac{1}{n} \sum_{i=1}^{n} (x_{j}^{i} - \bar{x}_{j})^{2}}}$$

average value of x_i

Grouped selection:

- correlated variables get similar weights
- identical variables get identical weights
- Ridge regression shrinks coefficients towards 0 but does not result in a sparse model.

Sparsity:

- many coefficients get a weight of 0
- they can be eliminated from the model.

Lasso

Lasso

L1 penalty

$$||\boldsymbol{\beta}||_1 = \sum_{j=1}^p |\beta_p|$$

$$\hat{\beta}_{\text{lasso}} = \arg\min_{\beta} ||y - X\beta||_2^2 + \lambda ||\beta||_1$$

- aka basis pursuit (signal processing)
- no closed-form solution
- Equivalent to

$$\hat{\boldsymbol{\beta}}_{\text{lasso}} = \arg\min_{\boldsymbol{\beta}} ||y - X\boldsymbol{\beta}||_2^2 \text{ s.t. } ||\boldsymbol{\beta}||_1 \le t$$

for a unique one-to-one match between t and λ .

Optimization problem:

Lasso

L1 penalty

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QP: maximize a quadratic form under linear constraints.

Geometric interpretation

Minimize $f(\beta)$ under the constraint $g(\beta) \leq 0$

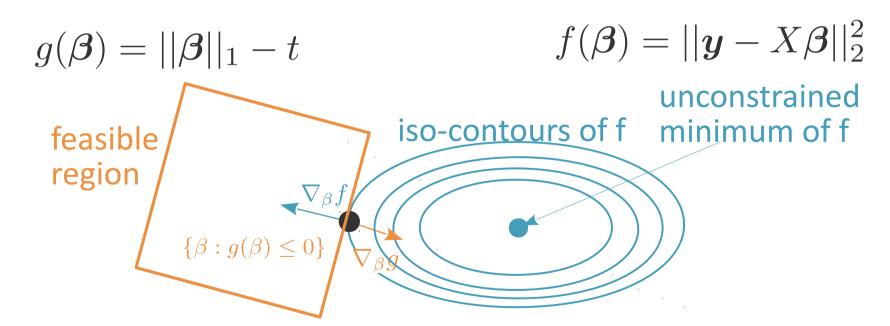
$$g(\boldsymbol{\beta}) = ||\boldsymbol{\beta}||_1 - t$$

$$f(\boldsymbol{\beta}) = ||\boldsymbol{y} - X\boldsymbol{\beta}||_2^2$$

Geometric interpretation

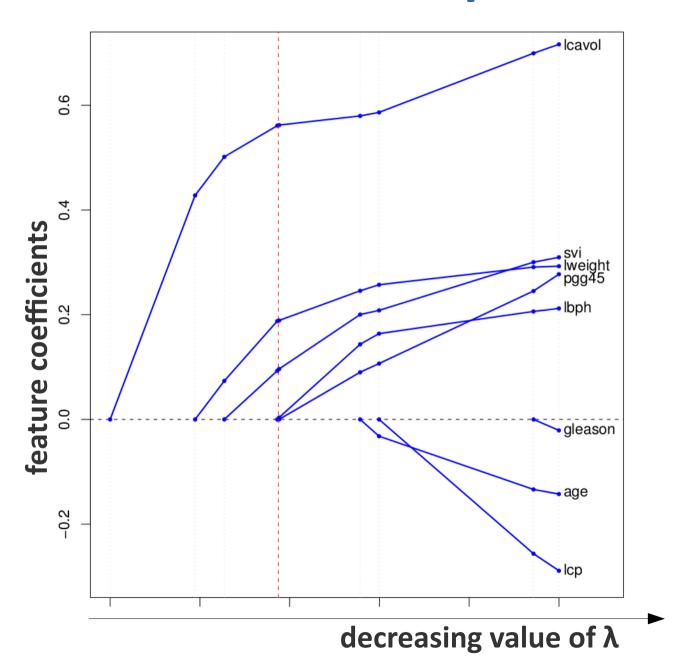
Minimize $f(\beta)$ under the constraint $g(\beta) \leq 0$

- Case 1: the unconstrained minimum lies in the feasible region.
- Case 2: it does not.



The gradient is orthonormal to the iso-contours and points towards the direction of maximum increase.

Lasso solution path



Forward stepwise regression

- Build model sequentially, adding one variable at a time
 - Start with the intercept
 - At each step, add the variable that most improves the fit
 - Stop when $||\beta||_1 \le t$
- Greedy solution

At each step, add "only as much of a variable as needed"

1. Standardize the predictors to have mean zero and unit norm. Start with the residual $\mathbf{r} = \mathbf{y} - \bar{\mathbf{y}}, \, \beta_1, \beta_2, \dots, \beta_p = 0$.

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- 2. Find the predictor \mathbf{x}_j most correlated with \mathbf{r} .
- 3. Move β_j from 0 towards its least-squares coefficient $\langle \mathbf{x}_j, \mathbf{r} \rangle$, until some other competitor \mathbf{x}_k has as much correlation with the current residual as does \mathbf{x}_i .

$$\beta_{j} \leftarrow \beta_{j} + \alpha \frac{1}{\sum_{i=1}^{n} (x_{j}^{i})^{2}} \sum_{i=1}^{n} x_{j}^{i} r^{i}$$

$$= \beta_{j} + \alpha (x_{j}^{\top} x_{j})^{-1} x_{j}^{\top} r$$

$$= \beta_{j} + \alpha \langle x_{j}^{\top}, x_{j} \rangle^{-1} \langle x_{j}, r \rangle$$

$$r = (y - \bar{y}) - \beta_{j} x_{j}$$

step size

- 1. Standardize the predictors to have mean zero and unit norm. Start with the residual $\mathbf{r} = \mathbf{y} \bar{\mathbf{y}}, \, \beta_1, \beta_2, \dots, \beta_p = 0$.
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- 4. Move β_j and β_k in the direction defined by their joint least squares coefficient of the current residual on $(\mathbf{x}_j, \mathbf{x}_k)$ until some other competitor \mathbf{x}_l has as much correlation with the current residual.

$$r = (y - \bar{y}) - \beta_j x_j - \beta_k x_k$$

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Maximum number of steps: max(n-1, p)

Approaches to dimensionality reduction

Feature selection

Choose m < p features, ignore the remaining (p-m)

Filtering approaches

Apply a statistical measure to assign a score to each feature (correlation, χ^2 -test).

Wrapper approaches

Search problem: Find the best set of features for a given predictive model.

Embedded approaches

Simultaneously fit a model and learn which features should be included.

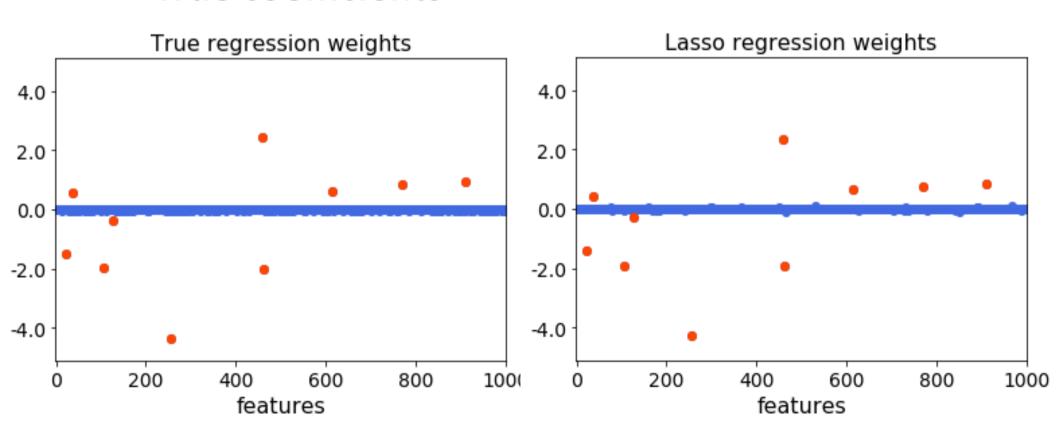
All these feature selection approaches are supervised.

Linear regression when p >> n

Simulated data: p=1000, n=100, 10 causal features

True coefficients

Predicted coefficients



Elastic Net

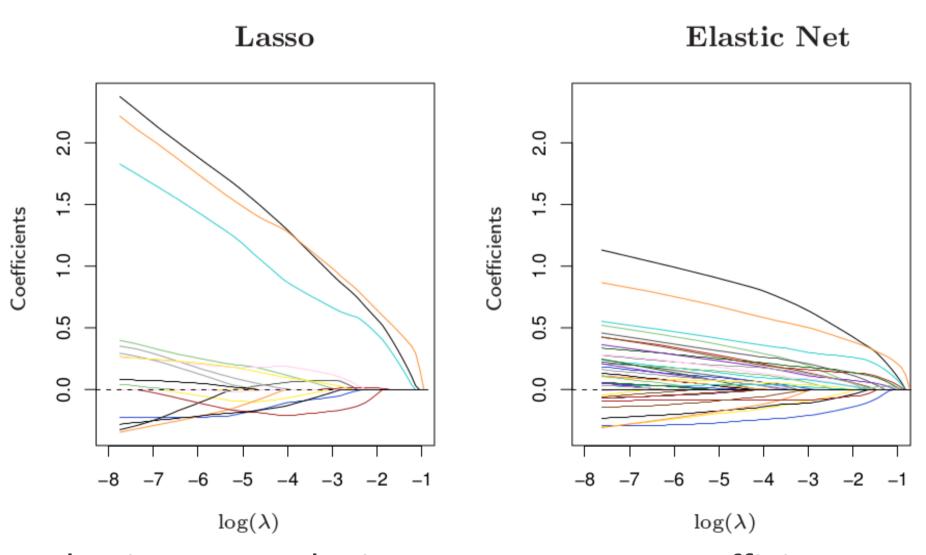
Elastic Net

Combine lasso and ridge regression

$$\hat{\beta}_{\text{enet}} = \arg\min_{\beta} ||y - X\beta||_2^2 + \lambda \left(\alpha ||\beta||_2^2 + (1 - \alpha)||\beta||_1\right)$$

- Select variables like the lasso.
- Shrinks together coefficients of correlated variables like the ridge regression.

E.g. Leukemia data



Elastic Net results in more non-zero coefficients than Lasso, but with smaller amplitudes.

Lq-norm regularization

Lq-norm regularization

$$\hat{oldsymbol{eta}} = rg \min_{oldsymbol{eta}} ||Y - Xoldsymbol{eta}||_2^2 + \lambda ||oldsymbol{eta}||_q^q \qquad ||oldsymbol{eta}||_q = \left(\sum_{j=1}^p |eta_j|^q
ight)^{1/q}$$

Equivalently:

$$\hat{\boldsymbol{\beta}} = \arg\min_{\beta} ||Y - X\boldsymbol{\beta}||_2^2 \text{ s. t. } ||\boldsymbol{\beta}||_q^q \le s$$

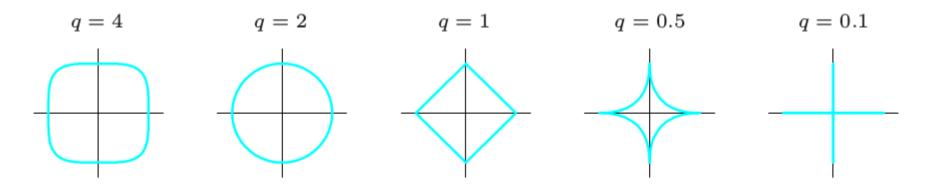
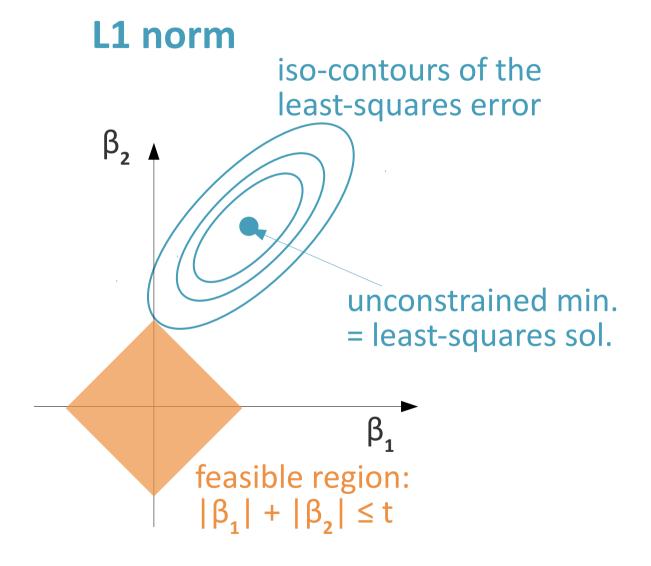
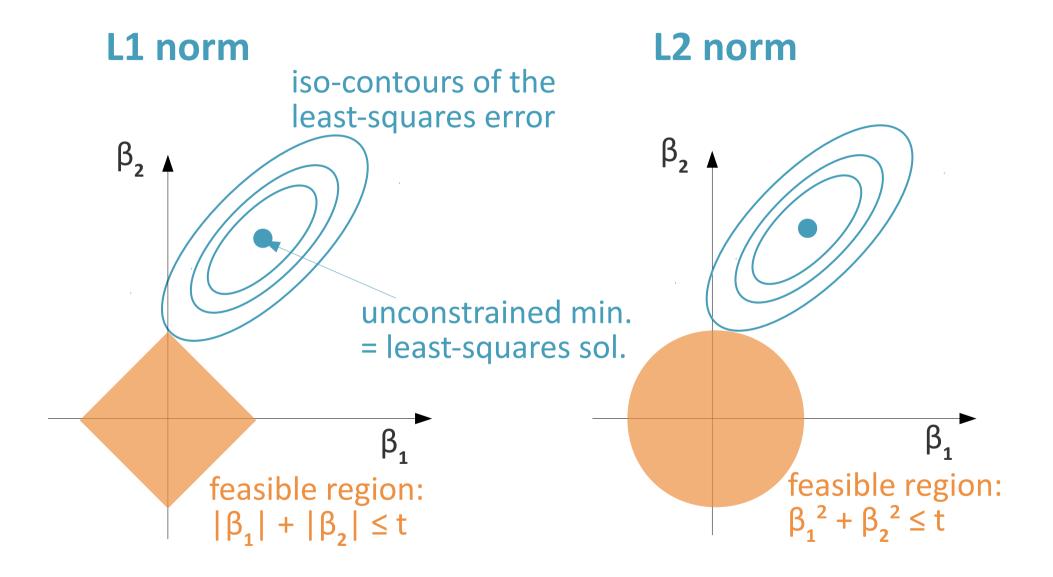


FIGURE 3.12. Contours of constant value of $\sum_{j} |\beta_{j}|^{q}$ for given values of q.

Lasso vs. ridge



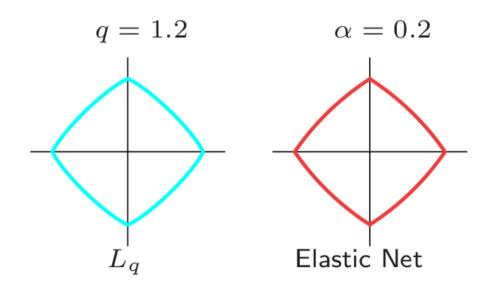
Lasso vs. ridge



Elastic net

Elastic penalty

$$\hat{\beta} = \arg\min_{\beta} ||y - X\beta||_{2}^{2} + \lambda \left(\alpha ||\beta||_{2}^{2} + (1 - \alpha)||\beta||_{1}\right)$$



Structured regularization

Group lasso

Use K predefined groups of variables that are known to "work" together and expected to be either all active or all inactive together.

E.g.: genes belonging to the same biological pathway.

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} ||y - \sum_{k=1}^{K} X_k \boldsymbol{\beta}_k||_2^2 + \lambda \sum_{k=1}^{K} \sqrt{p_k} ||\boldsymbol{\beta}_k||_2$$
 Size of group k

Features belonging to group k

Other examples of structured penalties

Overlapping groups

Jacob et al. (2009). Group lasso with overlap and graph lasso. *ICML*.

Graphs

Li & Li (2010). Variable selection and regression analysis for graph-structured covariates with an application to genomics. *Ann. App. Stats.*

Trees

Zhao et al. (2006). Grouped and hierarchical model selection through composite absolute penalties. *Ann. Stat.*

Multiple related tasks

Obozinski et al. (2006). Multitask feature selection. *Technical Report, UC Berkeley.*

Minimize SSE + λ x regularizer

Ridge

- gives similar weights to similar variables
- not very sparse
- analytical solution

Lasso

- randomly picks one of several correlated variables
- sparse
- LAR algorithm

Elastic net

- selects variables like the lasso
- shrinks together the coefficients of correlated variables.
- Many other regularizers are possible

Lp norms, groups, graphs, trees...

References

- A Course in Machine Learning. http://ciml.info/dl/v0_99/ciml-v0_99-all.pdf
 - Regularization: Chap 7.2–7.3
- The Elements of Statistical Learning. http://web.stanford.edu/~hastie/ElemStatLearn/
 - Regularization: Chap 10.12
 - Ridge regression: Chap 3.4.1
 - Lasso: Chap 3.4.2
 - LAR: Chap 3.4.4
 - Elastic Net: Chap 4.2

Lab 5

Logistic regression with no scaling

AUC = 0.642

```
# Logistic regression (no regularization, no scaling)
from sklearn import linear model
clf logreg = linear model.\overline{\text{LogisticRegression}}(C=1e6) # large C = no regularization
# Train the model
clf logreq.fit(Xtr, ytr)
# Predict on the test set
# Predicted probabilities of belonging to the positive class
pos idx = list(clf logreg.classes ).index(1)
ypred logreg = clf logreg.predict proba(Xte)[:, pos idx]
# Predicted binary labels
ypred logreg b = np.where(ypred logreg > 0.5, 1, 0)
from sklearn import metrics
print("No regularization: accuracy = %.3f" % metrics.accuracy score(yte, ypred logreg b))
print("AUC = %.3f" % (metrics.roc auc score(yte, ypred logreg)))
No regularization: accuracy = 0.636
```

Logistic regression with scaling

AUC = 0.859

```
# Logistic regression (no regularization, scaling)
clf_logreg_s = linear_model.LogisticRegression(C=1e6)

# Train the model
clf_logreg_s.fit(Xtr_scaled, ytr)

# Predict on the test set
# Predicted probabilities of belonging to the positive class
pos_idx = list(clf_logreg_s.classes_).index(1)
ypred_logreg_s = clf_logreg_s.predict_proba(Xte_scaled)[:, pos_idx]
# Predicted binary labels
ypred_logreg_s_b = np.where(ypred_logreg_s > 0.5, 1, 0)

print("Scaled, no regularization: accuracy = %.3f" % metrics.accuracy_score(yte, ypred_logreg_s_b))
print("AUC = %.3f" % (metrics.roc_auc_score(yte, ypred_logreg_s)))

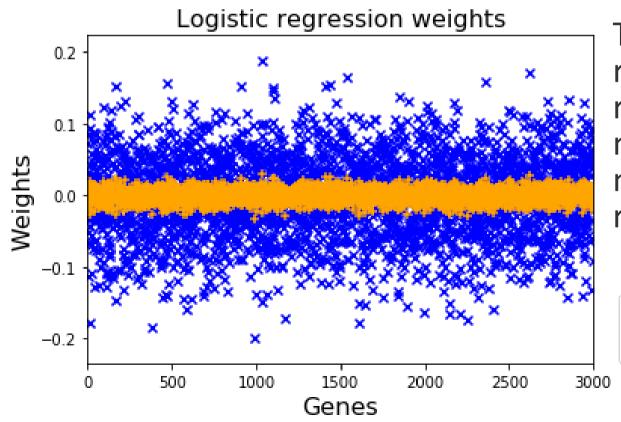
Scaled, no regularization: accuracy = 0.782
```

L2-regularized logistic regression with scaling

The performance did not change.

AUC = 0.858

• Did the regression coefficients change?



The coefficients of the regularized logistic regression have a smaller magnitude than those of the non-regularized logistic regression.

- Logistic regression
- L2-regularized logistic regression

Optimization of the parameter C

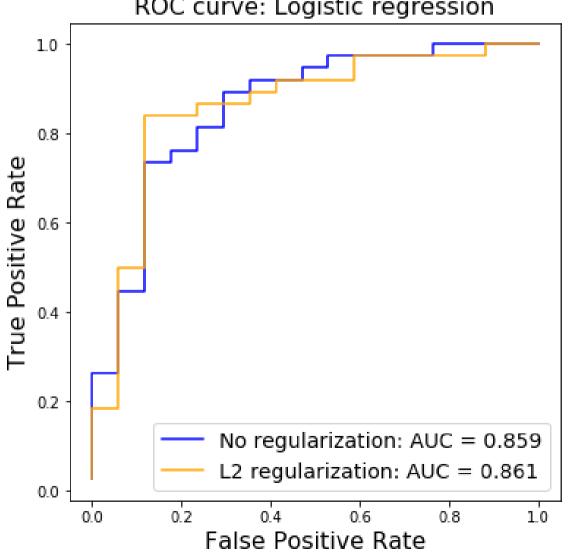
```
# Optimize cvalue
classifier = linear model.LogisticRegression(penalty='l2')
param grid = {'C': cvalues list}
clf logreg l2 s opt = model selection.GridSearchCV(classifier, param grid, cv=3)
# Train the model
clf logreg l2 s opt.fit(Xtr scaled, ytr)
# index of the positive class
pos idx = list(clf logreg l2 s opt.best estimator .classes ).index(1)
# predict probability of being positive
ypred logreg l2 s opt = clf logreg l2 s opt.best estimator .predict proba(Xte scaled)[:, pos idx]
# predict binary label
vpred logreg l2 s opt b = np.where(<math>vpred logreg l2 s opt > 0.5, 1, 0)
cvalue opt = clf logreg l2 s opt.best estimator .C
print("Scaled, l2 regularization (C=%.2e): accuracy = %.3f" % (cvalue opt,
                                                                metrics.accuracy score(yte,
                                                                                       ypred logreg l2 s opt b)))
print("AUC = %.3f" % (metrics.roc auc score(yte, ypred logreg l2 s opt)))
Scaled, l2 regularization (C=3.79e-04): accuracy = 0.818
```

- Now C = 0.000379 (smaller), ie λ has increased. There is *more* regularization. We expect smaller regression coefficients.
- The performance has slightly improved

AUC = 0.861

plt.xlabel('False Positive Rate', fontsize=16)
plt.ylabel('True Positive Rate', fontsize=16)
plt.title('ROC curve: Logistic regression', fon
plt.legend(fontsize=14)

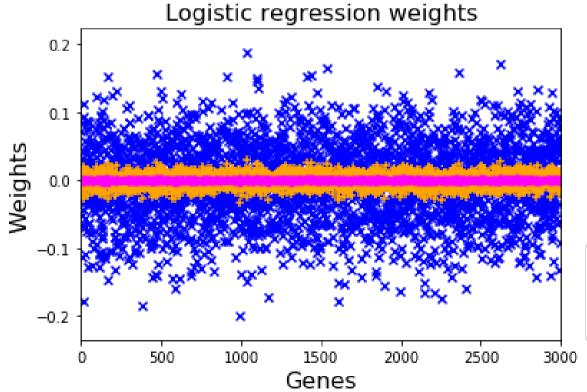
 The ROC curves are not very different from each other (the AUC are quite close to each other as well).



```
# Effect of l2-regularization on the weights
num features = X clf.shape[1]
plt.scatter(range(num features), clf logreg s.coef ,
            color='blue', marker='x', label='Logistic regression')
plt.scatter(range(num features), clf logreg l2 s.coef ,
            color='orange', marker='+', label='L2-regularized logistic regression')
plt.scatter(range(num features), clf logreg l2 s opt.best estimator .coef ,
            color='magenta', marker='.', label='L2-regularized logistic regression (opt)')
plt.xlabel('Genes', fontsize=16)
plt.ylabel('Weights', fontsize=16)
plt.title('Logistic regression weights', fontsize=16)
plt.legend(fontsize=14, loc=(1.05, 0))
plt.xlim([0, num features])

    As expected, the

                                                      optimized 12-
             Logistic regression weights
```



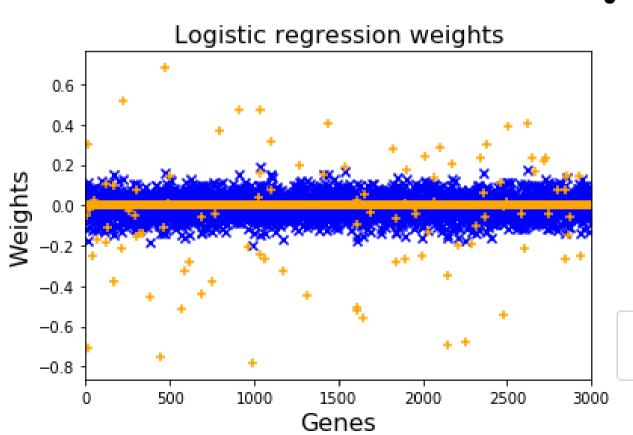
 As expected, the optimized I2regularized logistic regression has coefficients of even smaller magnitude than the non-optimized one.

- Logistic regression
- L2-regularized logistic regression
- L2-regularized logistic regression (opt)

L1-regularized logistic regression with scaling

```
cvalue = 10.
clf logreg l1 s = linear model.LogisticRegression(C=cvalue, penalty='l1')
# train model
clf logreg l1 s.fit(Xtr scaled, ytr)
# index of the positive class
pos idx = list(clf logreg l1 s.classes ).index(1)
# predict the probability of belonging to the positive class
vpred logreg l1 s = clf logreg l1 s.predict proba(Xte scaled)[:, pos idx]
# predict binary labels
ypred logreg l1 s b = np.where(ypred logreg l1 s > 0.5, 1, 0)
print("Scaled, l1 regularization (C=%.2e): accuracy = %.3f" % (cvalue,
                                                               metrics.accuracy score(yte,
                                                                                       ypred logreg l1 s b)))
print("AUC = %.3f" % (metrics.roc auc score(yte, ypred logreg l1 s)))
Scaled, l1 regularization (C=1.00e+01): accuracy = 0.727
AUC = 0.748
```

- The performance is now noticeably worse!
- What are the regression coefficients like?



 It looks like many coefficients are equal to zero.

Logistic regression

L1-regularized logistic regression

The non-regularized logistic regression uses 3000 features The L2-regularized logistic regression uses 3000 features The L1-regularized logistic regression uses 106 features Number of features discarded by the L1-regularization: 2894

- Indeed, the performance got worse but the l1regularized model only uses 106 features!
- Notice that if you train the l1-regularized logistic regression you very likely get a different performance and a different number of features: the l1 regularization is unstable.

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ROC curve: Logistic regression 1.0 0.8 True Positive Rate 0.6 0.4 0.2 No regularization: AUC = 0.859L2 regularization: AUC = 0.861

• The ROC curve of the l1-regularized logistic regression is quite below the other curves, confirming a worse performance.

False Positive Rate

0.4

0.0

0.0

0.2

L1 regularization: AUC = 0.776

0.8

1.0

0.6

- For me, the optimal value of C is 88.6
- A larger C means a smaller λ , hence less regularization. I am expecting *more* non-zero weights (i.e. selected features).
- Indeed, my l1-regularized model with optimized C uses 289 features. These 289 features include the previous features (remember the lasso regularization path: once a feature is included it stays included).

