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Introduction to
Machine Learning and Data Mining

IT3190

Lecture: Linear Regression

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Regression

- There is an *unknown* function y^* that maps each **x** to a number $y^*(\boldsymbol{x})$
  - In practice, we can collect some pairs: ($\mathbf{x}_i$, y_i), where $y_i = y^*(\boldsymbol{x}_i)$.
  - Each observation of **x** is represented by a vector in an n-dimensional space, e.g., $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{in})^T$. Each dimension represents an *attribute (thuộc tính) or feature (đặc trưng) or variate*.
  - Bold characters denote vectors or matrices.
- **Regression problem:** learn a function y = f(**x**) from a given training set **D** = $\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_M, y_M)\}$ such that $y_i \cong f(\boldsymbol{x}_i)$ for every i

Linear regression (Hồi quy tuyến tính)

- Linear model: assume that $y^*(\boldsymbol{x})$ can be well approximated by

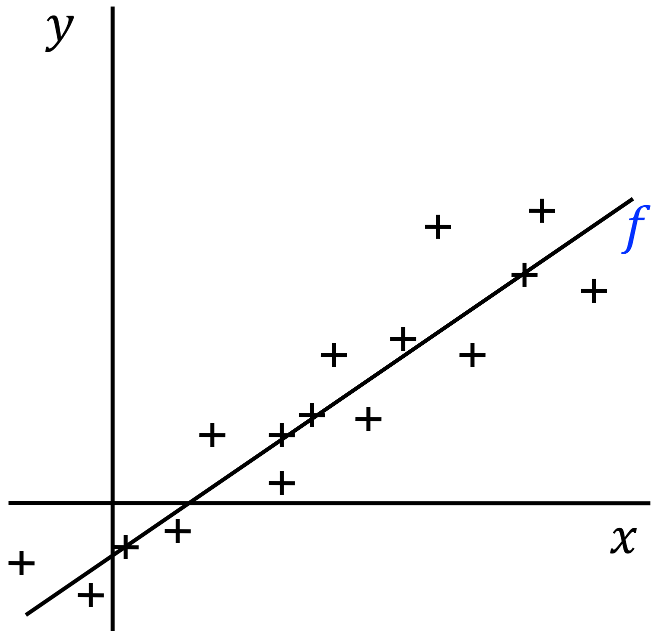
$$f(\mathbf{x},\mathbf{w}) = w_0 + w_1x_1 + \ldots + w_nx_n$$

  - $w_0, w_1, \ldots, w_n$ are the regression coefficients/weights. w_0 sometimes is called "*bias*".
  - In other words, we use a hyperplane to approximate the unknown function.
  - $f(\mathbf{x},\mathbf{w})$ may not be linear in $\mathbf{x}$.
- *Note:* learning a linear model is equivalent to finding the weight vector $\mathbf{w} = (w_0, w_1, \ldots, w_n)^T$.

Linear regression: example

- What is the best function?

x	y
0.13	-0.91
1.02	-0.17
3.17	1.61
-2.76	-3.31
1.44	0.18
5.28	3.36
-1.74	-2.46
7.93	5.56
...	...



Prediction

- For each observation $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$
  - The *true output*: $y^*(\boldsymbol{x})$ (but unknown for future data)
  - *Prediction* by our linear model:

$$y_x = w_0 + w_1x_1 + \ldots + w_nx_n$$

  - We often expect $y_x \cong y^*(\boldsymbol{x})$.

- Prediction for a future observation $\mathbf{z} = (z_1, z_2, \ldots, z_n)^T$
  - Use the learned function to make prediction

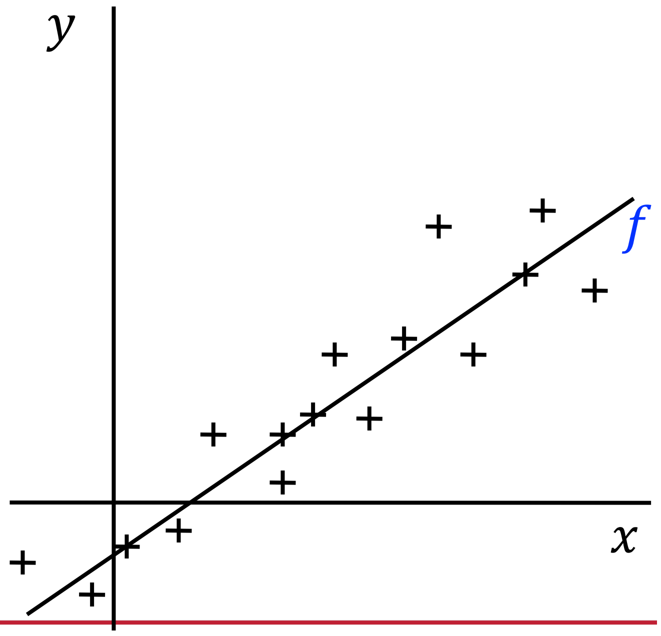
$$f(\mathbf{z},\mathbf{w}) = w_0 + w_1z_1 + \ldots + w_nz_n$$

Learning a regression function

- Learning goal: *learn a function f* such that its prediction in the future is the best.*
  - Its generalization is the best.
- Difficulty: infinite number of functions

$$\boldsymbol{H} = \{\, f(\boldsymbol{x}, \boldsymbol{w}) \colon \boldsymbol{w} = (w_0, w_1, \dots, w_n) \in \mathbb{R}^{n+1} \}$$

  - How can we learn?
  - Is function f better than g?
- Use a measure
  - *Loss function* is often used to guide learning.



Loss function

- The *error/loss* of the prediction for an example **x** = $(x_1, x_2, \ldots, x_n)^T$:

$$r(f,\boldsymbol{x}) = [y^*(\boldsymbol{x}) - f(\boldsymbol{x},\boldsymbol{w})]^2$$

Cost, risk

- The *expected loss (risk) of f* over the whole space:

$$E = \boldsymbol{E}_x[r(f,\boldsymbol{x})] = \boldsymbol{E}_x[y^*(\boldsymbol{x}) - f(\boldsymbol{x},\boldsymbol{w})]^2$$

($\mathbf{E}_x$ is the expectation over **x**)

- About the loss/cost: $r(f,\boldsymbol{x})$
  - Square loss is used above. Other loss functions can be used, e.g.
    - *Absolute loss:* $|y^*(\boldsymbol{x}) - f(\boldsymbol{x},\boldsymbol{w})|$
    - *Hinge loss:* $\max\{0, 1 - y^*(\boldsymbol{x})\, f(\boldsymbol{x},\boldsymbol{w})\}$
    - …

Loss function

- The goal of learning is to find f* that minimizes the expected loss:

$$f^* = \arg\min_{f \in \boldsymbol{H}} \boldsymbol{E}_x[r(f, \boldsymbol{x})]$$

  - For linear model: **H** is the space of functions of linear form.
- But we cannot work directly with this problem during the learning phase.
  (Why?)

Empirical loss

- We can observe a data set **D** = {($\mathbf{x}_1$, y_1), ($\mathbf{x}_2$, y_2), …, ($\mathbf{x}_M$, y_M)}, and have to learn f from **D**.

- Residual sum of squares:

$$RSS(f) = \sum_{i=1}^{M} \left(y_i - f(\boldsymbol{x}_i, \boldsymbol{w})\right)^2 = \sum_{i=1}^{M} (y_i - w_0 - w_1 x_{i1} - \cdots - w_n x_{in})^2$$

- Empirical loss (lỗi thực nghiệm): $L(f, \mathbf{D}) = \frac{1}{M} RSS(f)$
  - $L(f, \mathbf{D})$ is an approximation of $\mathbf{E}_x[r(\mathbf{x})]$.

- $|L(f, \mathbf{D}) - \boldsymbol{E}_x[r(\boldsymbol{x})]|$ is often known as *generalization error* (lỗi tổng quát hoá) of *f*.

- Many learning algorithms base on this RSS or its variants.

Methods: ordinary least squares (OLS)

- Given **D**, we find f* that minimizes RSS:

$$f^* = \arg\min_{f \in \boldsymbol{H}} RSS(f) \tag{1}$$

$$\Leftrightarrow \boldsymbol{w}^* = \arg\min_{\mathbf{w}} \sum_{i=1}^{M} (y_i - w_0 - w_1 x_{i1} - \cdots - w_n x_{in})^2$$

- This method is often known as *ordinary least squares (OLS, bình phương tối thiểu).*
- Find **w*** by taking the gradient of RSS and solving the equation RSS'=0. We have:

$$\boldsymbol{w}^* = (\boldsymbol{A}^T \boldsymbol{A})^{-1} \boldsymbol{A}^T \boldsymbol{y}$$

  - Where $\mathbf{A}$ is the data matrix of size $M \times (n+1)$, where the i^{th} row is $\mathbf{A_i} = (1, x_{i1}, x_{i2}, \dots, x_{in})$; $\mathbf{B}^{-1}$ is the inversion of matrix $\mathbf{B}$; $\mathbf{y} = (\mathrm{y}_1, \mathrm{y}_2, \dots, \mathrm{y}_\mathrm{M})^\mathrm{T}$.
  - Note: we assume that **A**^{T}**A** is invertible (ma trận **A**^{T}**A** khả nghịch).

Methods: OLS

- Input: $\mathbf{D} = \{(\mathbf{x}_1, \mathrm{y}_1), (\mathbf{x}_2, \mathrm{y}_2), \ldots, (\mathbf{x}_\mathrm{M}, \mathrm{y}_\mathrm{M})\}$
- Output: $\boldsymbol{w}^*$
- Learning: compute

$$\boldsymbol{w}^* = (\boldsymbol{A}^T \boldsymbol{A})^{-1} \boldsymbol{A}^T \boldsymbol{y}$$

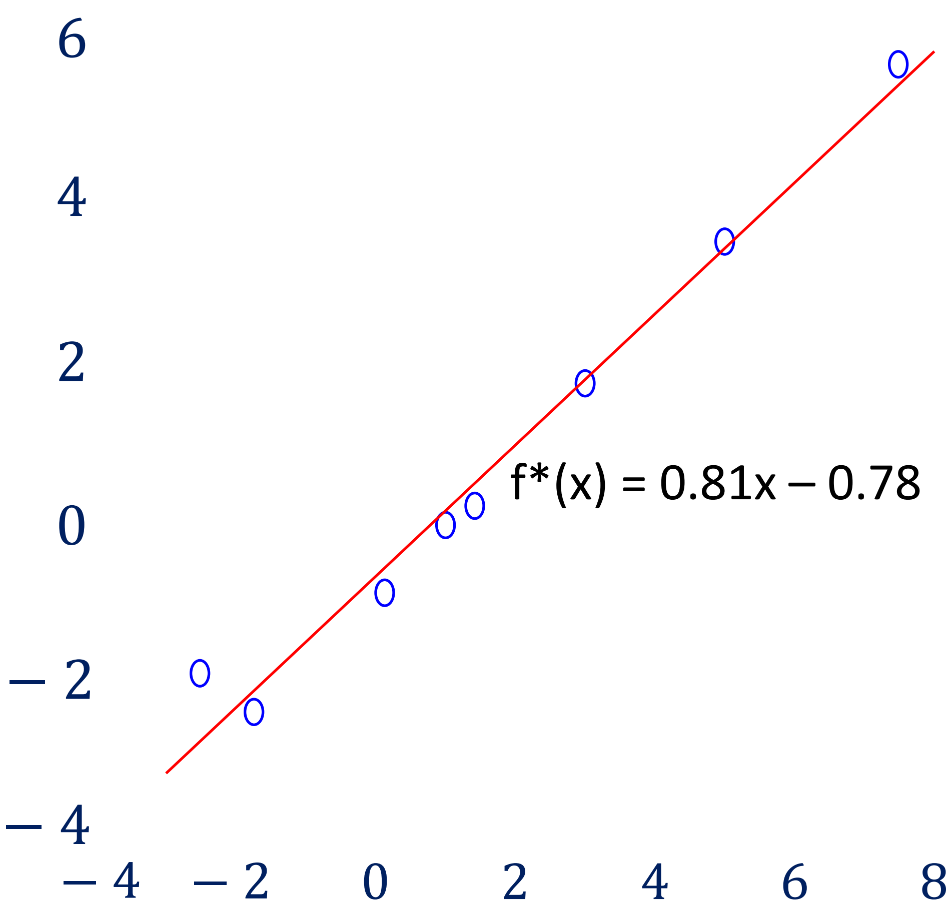
  - Where $\mathbf{A}$ is the data matrix of size $M \times (n+1)$, where the i^{th} row is $\mathbf{A}_\mathbf{i} = (1, x_{i1}, x_{i2}, \ldots, x_{in})$; $\mathbf{B}^{-\mathbf{1}}$ is the inversion of matrix $\mathbf{B}$;

    $\mathbf{y} = (\mathrm{y}_1, \mathrm{y}_2, \ldots, \mathrm{y}_\mathrm{M})^\mathrm{T}$.
  - Note: we assume that $\boldsymbol{A}^T \boldsymbol{A}$ is invertible.

- Prediction for a new $\mathbf{x}$: $y_x = w_0^* + w_1^* x_1 + \cdots + w_n^* x_n$

Methods: OLS example

x	y
0.13	-1
1.02	-0.17
3	1.61
-2.5	-2
1.44	0.1
5	3.36
-1.74	-2.46
7.5	5.56



Methods: limitations of OLS

- OLS cannot work if $\mathbf{A}^T\mathbf{A}$ is not invertible
  - If some columns (attributes/features) of **A** are dependent, then **A** will be singular and therefore $\mathbf{A}^T\mathbf{A}$ is not invertible.
    (Nếu một vài cột của A phụ thuộc tuyến tính thì A sẽ không khả nghịch)
- OLS requires considerable computation due to the need of computing a matrix inversion.
  - Intractable for the very high dimensional problems.
- OLS likely tends to overfitting, because the learning phase just focuses on minimizing the error of the training data.

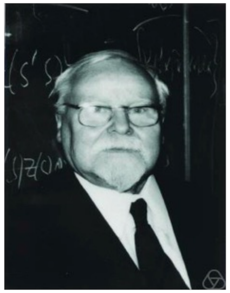
Methods: Ridge

- Given **D** = {(**x**$_1$, y$_1$), (**x**$_2$, y$_2$), …, (**x**$_M$, y$_M$)}, we solve for:

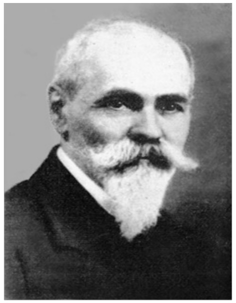
$$f^* = \arg\min_{f \in \boldsymbol{H}} RSS(f) + \lambda \|\boldsymbol{w}\|_2^2$$

$$\Leftrightarrow \boldsymbol{w}^* = \arg\min_{\mathbf{w}} \sum_{i=1}^{M} (y_i - \boldsymbol{A}_i \boldsymbol{w})^2 + \lambda \sum_{j=0}^{n} w_j^2 \qquad (2)$$

  - Where λ is a regularization constant ($\lambda > 0$), $\|\boldsymbol{w}\|_2$ is the L^2 norm.



Tikhonov, smoothing an ill-posed problem



Zaremba, model complexity minimization

Bayes: priors over parameters

Andrew Ng: need no maths, but it prevents overfitting!

Methods: Ridge

- Problem (2) is equivalent to the following:

$$w^* = \arg\min_{\boldsymbol{w}} \sum_{i=1}^{M} (y_i - \boldsymbol{A}_i \boldsymbol{w})^2 \quad \text{Subject to } \sum_{j=0}^{n} w_j^2 \leq t \qquad (3)$$

  - for some constant *t*.

- The **regularization/penalty** term: $\lambda ||\boldsymbol{w}||_2^2$
  - Limits the magnitute/size of **w*** (i.e., reduces the search space for f*).
  - Helps us to trade off between *the fitting of f on **D*** and *its generalization* on future observations.

Methods: Ridge

- We solve for **w*** by taking the gradient of the objective function in (2), and then zeroing it. Therefore we obtain:

$$\boldsymbol{w}^* = (\boldsymbol{A}^T\boldsymbol{A} + \lambda\boldsymbol{I}_{n+1})^{-1}\boldsymbol{A}^T\boldsymbol{y}$$

  - Where **A** is the data matrix of size $M\times(n+1)$, where the i^{th} row is $\mathbf{A}_i = (1, x_{i1}, x_{i2}, \ldots, x_{in})$; $\mathbf{y} = (y_1, y_2, \ldots, y_M)^T$; $\mathbf{I}_{n+1}$ is the identity matrix of size $n+1$.
- Compared with OLS, Ridge can
  - Avoid the cases of singularity, unlike OLS. Hence Ridge always works.
  - Reduce overfitting.
  - Increase the error for the training set.
- Note: *the predictiveness of Ridge depends heavily on the choice of* λ.

Methods: Ridge

- Input: $\mathbf{D} = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_M, y_M)\}$ and $\lambda > 0$
- Output: $\mathbf{w}^*$
- Learning: compute

$$\boldsymbol{w}^* = (\boldsymbol{A}^T\boldsymbol{A} + \lambda \boldsymbol{I}_{n+1})^{-1}\boldsymbol{A}^T\boldsymbol{y}$$

- Prediction for a new $\mathbf{x}$:

$$y_x = w_0^* + w_1^* x_1 + \cdots + w_n^* x_n$$

- *Note:* to avoid some negative effects of the magnitude of y on covariates $\mathbf{x}$, one should remove w_0 from the penalty term in (2). In this case, the solution of $\mathbf{w}^*$ should be modified slightly.

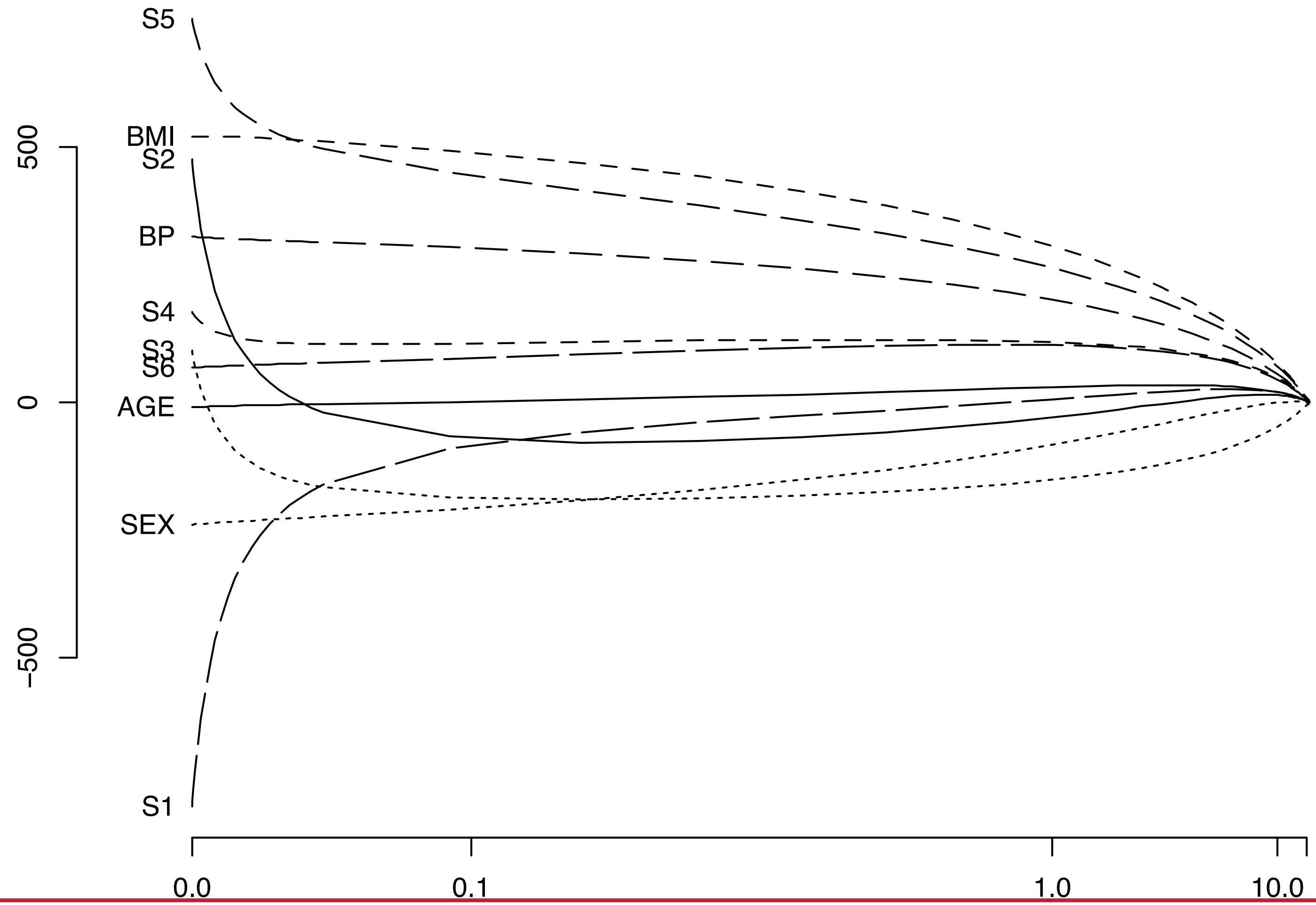
An example of using Ridge and OLS

- The training set **D** contains 67 observations on prostate cancer, each was represented with 8 attributes. Ridge and OLS were learned from **D**, and then predicted 30 new observations.

w	Ordinary Least Squares	Ridge
0	2.465	2.452
lcavol	0.680	0.420
lweight	0.263	0.238
age	−0.141	−0.046
lbph	0.210	0.162
svi	0.305	0.227
lcp	−0.288	0.000
gleason	−0.021	0.040
pgg45	0.267	0.133
Test RSS	**0.521**	**0.492**

Effects of λ in Ridge regression

- $\mathbf{W}^*$ = (w_0, S1, S2, S3, S4, S5, S6, AGE, SEX, BMI, BP) changes as the regularization constant λ changes.



LASSO

- Ridge regression use L^2 norm for regularization:

$$\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} \sum_{i=1}^{M} (y_i - \boldsymbol{A}_i\boldsymbol{w})^2, \text{ subject to } \sum_{j=0}^{n} w_j^2 \le t \quad (3)$$

- Replacing L^2 by L^1 norm will result in LASSO:

$$\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} \sum_{i=1}^{M} (y_i - \boldsymbol{A}_i\boldsymbol{w})^2$$

$$\text{Subject to } \sum_{j=0}^{n} |w_j| \le t$$

- Equivalently:

$$w^* = \arg\min_{\boldsymbol{w}} \sum_{i=1}^{M} (y_i - \boldsymbol{A}_i\boldsymbol{w})^2 + \lambda\|\boldsymbol{w}\|_1 \quad (4)$$

- This problem is non-differentiable → the training algorithm should be more complex than Ridge.

LASSO: regularization role

- The regularization types lead to different domains for **w**.
- LASSO often produces **sparse** solutions, i.e., many components of **w** are zero.
  - Shinkage and selection at the same time

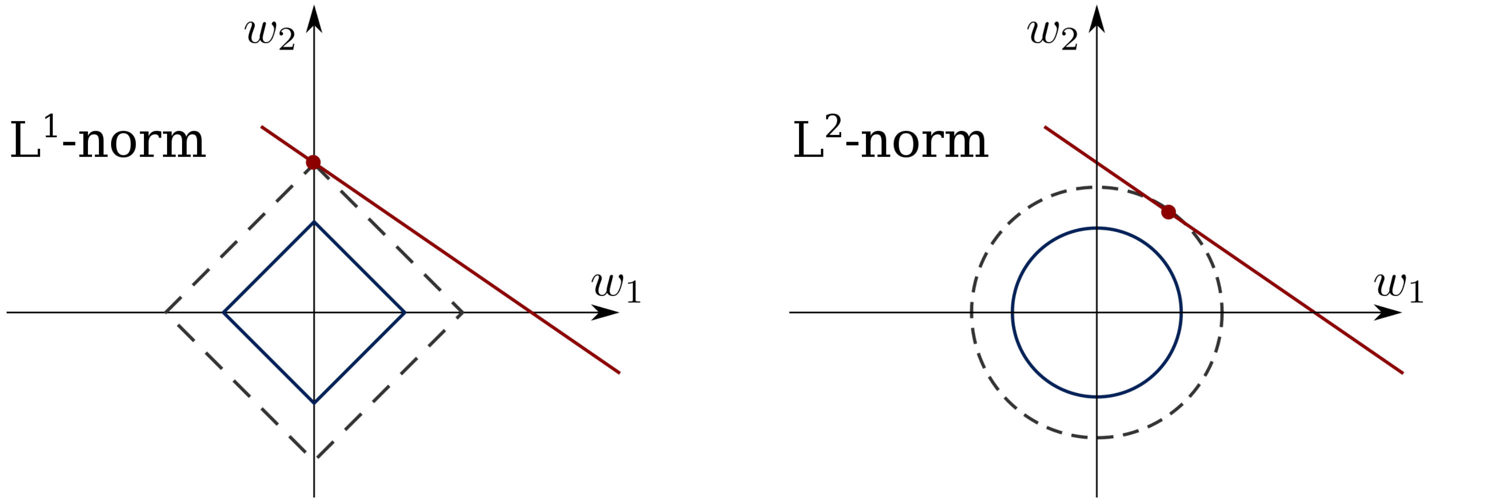


Figure by Nicoguaro - Own work, CC BY 4.0, https://commons.wikimedia.org/w/index.php?curid=58258966

OLS, Ridge, and LASSO

- The training set **D** contains 67 observations on prostate cancer, each was represented with 8 attributes. OLS, Ridge, and LASSO were trained from **D**, and then predicted 30 new observations.

w	Ordinary Least Squares	Ridge	LASSO
0	2.465	2.452	2.468
lcavol	0.680	0.420	0.533
lweight	0.263	0.238	0.169
age	−0.141	−0.046	
lbph	0.210	0.162	0.002
svi	0.305	0.227	0.094
lcp	−0.288	0.000	
gleason	−0.021	0.040	
pgg45	0.267	0.133	
Test RSS	**0.521**	**0.492**	**0.479**

Some weights are 0
→ some attributes may not be important

References

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