Introduction to

Machine Learning and Data Mining

(Học máy và Khai phá dữ liệu)

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Contents

- Introduction to Machine Learning & Data Mining
- **Supervised learning**
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Linear regression: introduction

- **Regression problem:** learn a function $y = f(\mathbf{x})$ from a given training data $\mathbf{D} = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_M, y_M)\}$ such that $y_i \cong f(\mathbf{x}_i)$ for every i
  - Each observation of $\mathbf{x}$ 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/feature/variate*.
  - Bold characters denote vectors.
- Linear model: if $f(\mathbf{x})$ is assumed to be of linear form

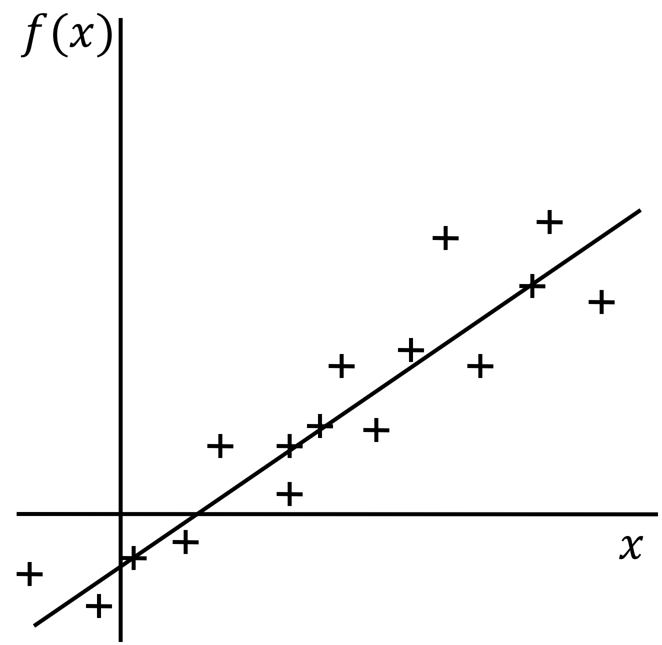
$$f(\mathbf{x}) = w_0 + w_1x_1 + \ldots + w_nx_n$$

  - $w_0, w_1, \ldots, w_n$ are the regression coefficients/weights. w_0 sometimes is called "*bias*".
- Note: learning a linear function is equivalent to learning the coefficient 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*: c_x
    (but unknown for future data)
  - *Prediction* by our system:

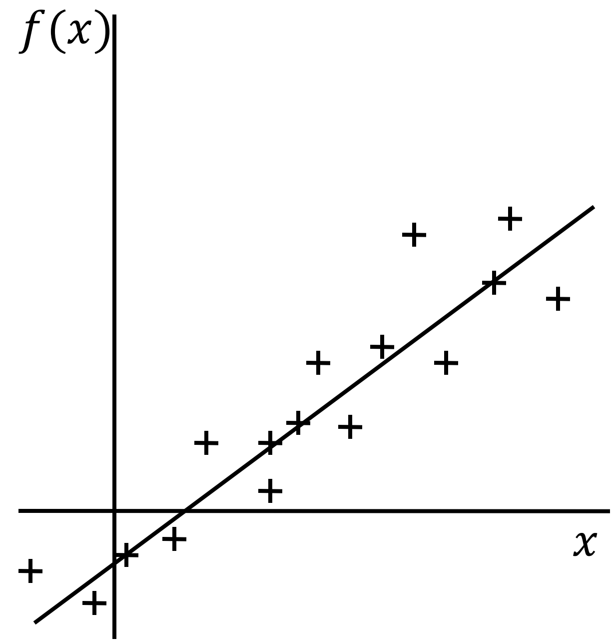
$$y_x = w_0 + w_1 x_1 + \ldots + w_n x_n$$

  - We often expect $y_x \cong c_x$.
- Prediction for future observation $\mathbf{z} = (z_1, z_2, \ldots, z_n)^T$
  - Use the previously learned function to make prediction

$$f(\mathbf{z}) = w_0 + w_1 z_1 + \ldots + w_n z_n$$

Learning a regression function

- Learning goal: *learn a function f* such that its prediction in the future is the best.*
  - Its generalization is best.
- Difficulty: infinite number of functions
  - How can we learn?
  - Is function f better than g?
- Use a measure
  - *Loss function* or *generalization error* are often used to guide learning.



Loss function

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

$$r(\mathbf{x}) = [c_x - f^*(\mathbf{x})]^2 = (c_x - w_0 - w_1x_1 - \ldots - w_nx_n)^2$$

  - The *expected loss* over the whole space:

$$E = \mathbf{E}_x[r(\mathbf{x})] = \mathbf{E}_x[c_x - f^*(\mathbf{x})]^2$$

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

Cost, risk

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

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

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

- Empirical loss (residual sum of squares):

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

  - RSS/M is an approximation to $\mathbf{E}_x[r(\mathbf{x})]$.

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

Methods: ordinary least squares (OLS)

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

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

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

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

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

  - Where **A** is the data matrix of size Mx(n+1), whose the i^{th} row is $\mathbf{A}_i = (1, x_{i1}, x_{i2}, \ldots, x_{in})$; $\mathbf{B}^{-1}$ is the inversion of matrix **B**; $\mathbf{y} = (y_1, y_2, \ldots, y_M)^T$.
  - Note: we assume that $\mathbf{A}^T\mathbf{A}$ is invertible.

Methods: OLS

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

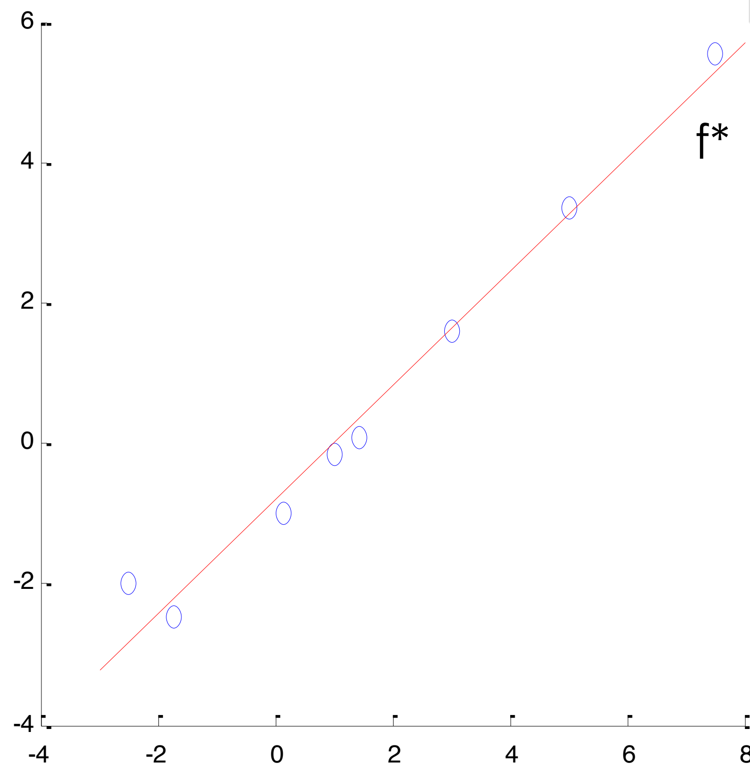
$$\boldsymbol{w}^* = (\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T\boldsymbol{y}$$

  - Where **A** is the data matrix of size Mx(n+1), whose the i^{th} row is $\mathbf{A}_i = (1, x_{i1}, x_{i2}, \ldots, x_{in})$; $\mathbf{B}^{-1}$ is the inversion of matrix **B**; $\mathbf{y} = (y_1, y_2, \ldots, y_M)^T$.
  - Note: we assume that $\mathbf{A}^T\mathbf{A}$ is invertible.
- Prediction for a new **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



$f^*(x) = 0.81x - 0.78$

Methods: limitations of OLS

- OLS cannot work if $\mathbf{A}^T\mathbf{A}$ is not invertible
  - If some columns (attributes/features) of $\mathbf{A}$ are dependent, then $\mathbf{A}$ will be singular and therefore $\mathbf{A}^T\mathbf{A}$ is not invertible.
- OLS requires considerable computation due to the need of computing a matrix inversion.
  - Intractable for the very high dimensional problems.
- OLS very likely tends to overfitting, because the learning phase just focuses on minimizing errors on the training data.

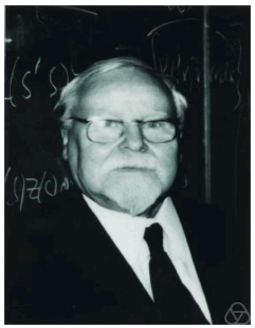
Methods: Ridge regression (1)

- Given **D** = {($\mathbf{x}_1$, y_1), ($\mathbf{x}_2$, y_2), …, ($\mathbf{x}_M$, y_M)}, we solve for:

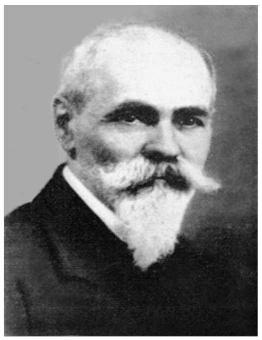
$$f^* = \arg\min_{f \in \boldsymbol{H}} RSS(f) + \lambda \|\boldsymbol{w}\|_2^2$$

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

  - Where $\mathbf{A}_i$ = (1, x_{i1}, x_{i2}, …, x_{in}) is composed from $\mathbf{x}_i$; and λ is a regularization constant (λ> 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 regression (2)

- Problem (2) is equivalent to the following:

$$w^* = \arg\min_{\boldsymbol{w}} \sum_{i=1}^{M} (y_i - \boldsymbol{A}_i \boldsymbol{w})^2 \qquad (3)$$

Subject to $\sum_{j=0}^{n} w_j^2 \leq t$

  - 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 regression (3)

- 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 Mx(n+1), whose the i^{th} row is $\mathbf{A}_i = (1, x_{i1}, x_{i2}, \ldots, x_{in})$; $\mathbf{B}^{-1}$ is the inversion of matrix **B**; $\mathbf{y} = (y_1, y_2, \ldots, y_M)^T$; $\mathbf{I}_{n+1}$ 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.
  - But error in the training data might be greater than OLS.
- Note: *the predictiveness of Ridge depends heavily on the choice of the hyperparameter* λ.

Methods: Ridge regression (4)

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

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

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

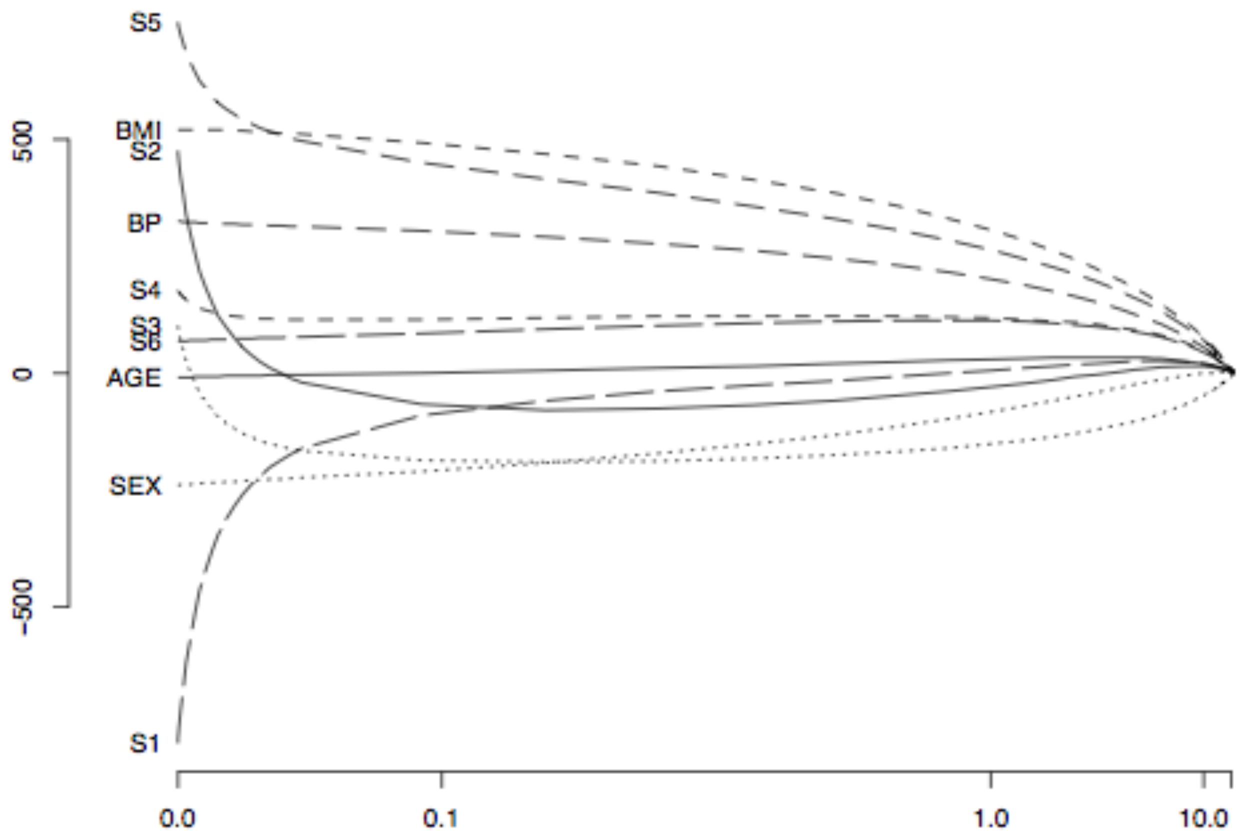
An example of using Ridge and OLS

- 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

- **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:

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

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

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

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

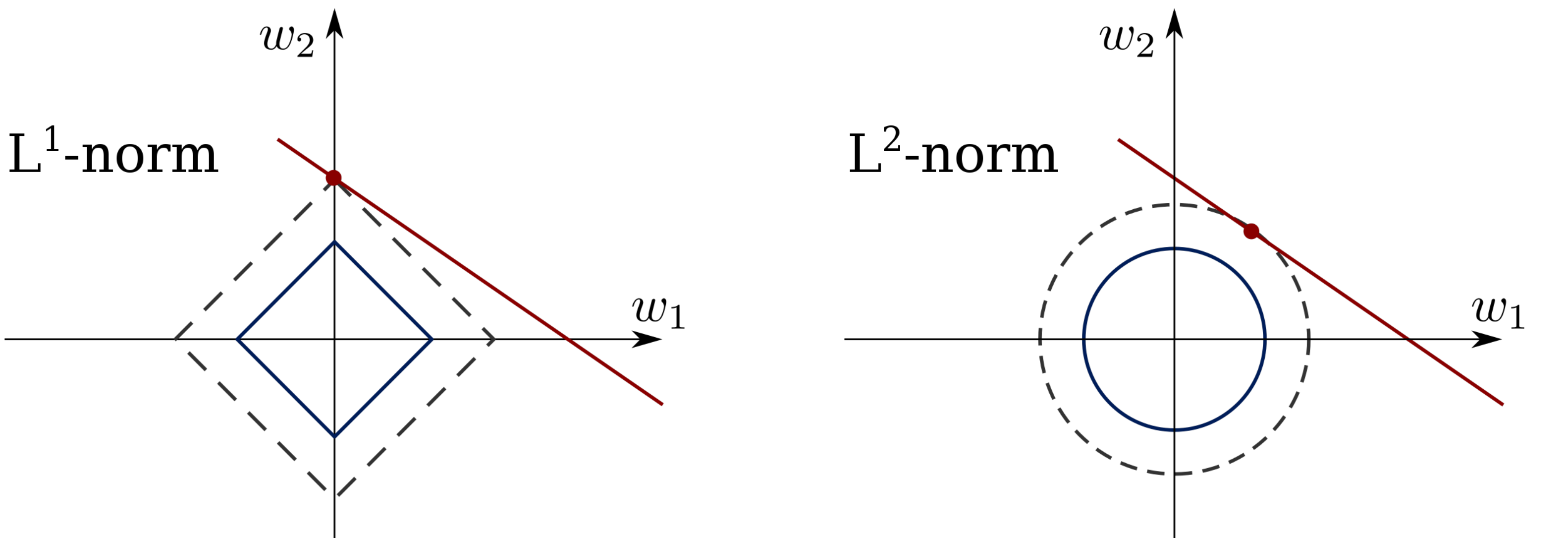
- Equivalently:

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

- 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



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

- Trevor Hastie, Robert Tibshirani, Jerome Friedman. *The Elements of Statistical Learning*. Springer, 2009.
- Tibshirani, Robert (1996). "Regression Shrinkage and Selection via the lasso". *Journal of the Royal Statistical Society. Series B (methodological)*. Wiley. 58 (1): 267–88.

Exercises

- Derive the solution of (1) and (2) in details.
- Derive the solution of (2) when removing w_0 from the penalty term.