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ĐẠI HỌC BÁCH KHOA HÀ NỘI

HANOI UNIVERSITY OF SCIENCE AND TECHNOLOGY

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Machine Learning

IT3190E

Lecture: Regularization

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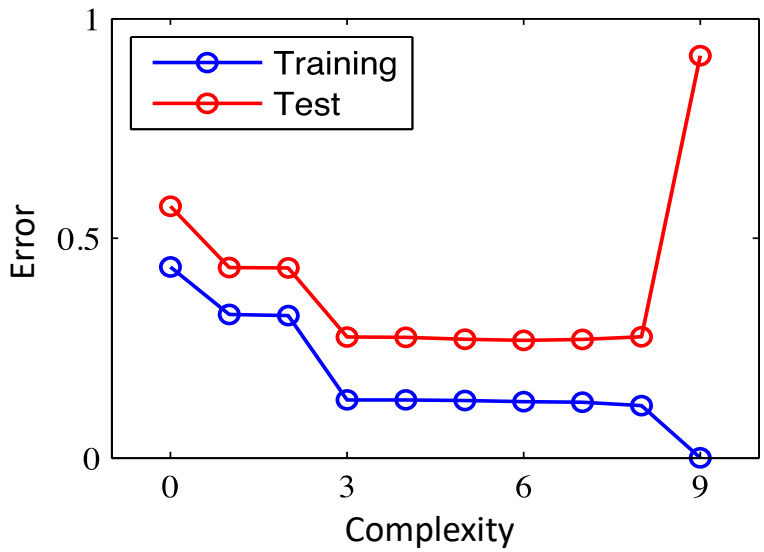
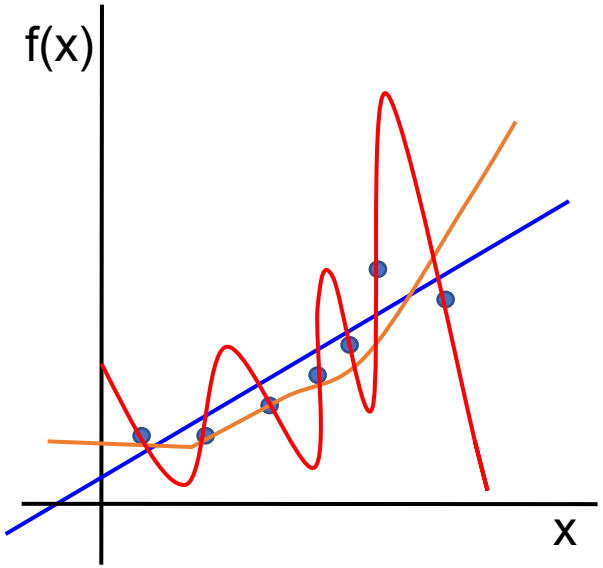
Contents

- Lecture 1: Introduction to Machine Learning
- Lecture 2: Linear regression
- Lecture 3+4: Clustering
- Lecture 5: Decision tree and Random forest
- Lecture 6: Neural networks
- Lecture 7: Support vector machines
- Lecture 8: Performance evaluation
- Lecture 9: Probabilistic models
- Lecture 10: Ensemble learning
- Lecture 11: Reinforcement learning
- **Lecture 12: Regularization**
- Lecture 13: Discussion on some advanced topics

Revisiting overfitting

- The complexity of the learned function: $y = \hat{f}(x; \boldsymbol{D})$
  - For a given training data **D**: *the more complicated $\hat{f}$, the more possibility that $\hat{f}$ fits **D** better.*
  - For a given **D**: there exist many functions that fit **D** perfectly (i.e., no error on **D**).
  - However, those functions might generalize badly.





The Bias-Variance Decomposition

- Consider $y(\boldsymbol{x}) = y^*(\boldsymbol{x}) + \epsilon$ as the (unknown) regression function
  - $\epsilon \sim Normal(0, \sigma^2)$ is a Gaussian noise with mean 0 and variance σ^2.
  - ϵ may represent the *noise* due to measurement or data collection.
- Let $\hat{f}(\boldsymbol{x}; \boldsymbol{D})$ be the regressor, learned by method $\mathcal{A}$ from a training set **D**
- Note:
  - We want that $\hat{f}$ well approximates the truth y^*.
  - $\hat{f}(\boldsymbol{x}; \boldsymbol{D})$ is random, according to the randomness when collecting **D**.
- For any **x**, the error made by $\hat{f}$ is $\left(y(\boldsymbol{x}) - \hat{f}(\boldsymbol{x}; \boldsymbol{D})\right)^2$
- *The error made by learning method* $\mathcal{A}$
  (Lỗi của thuật toán $\mathcal{A}$ khi phán đoán mẫu **x**)

$$err_A(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{D},\epsilon}\left(y(\boldsymbol{x}) - \hat{f}(\boldsymbol{x}; \boldsymbol{D})\right)^2$$

  - Why expectation? a different $\boldsymbol{D}$' will make $\mathcal{A}$ to return a different function $\hat{f}(\boldsymbol{x}; \boldsymbol{D}')$

The Bias-Variance Decomposition (2)

$$err_A(\boldsymbol{x}) = \sigma^2 + [Bias]^2 + Variance$$

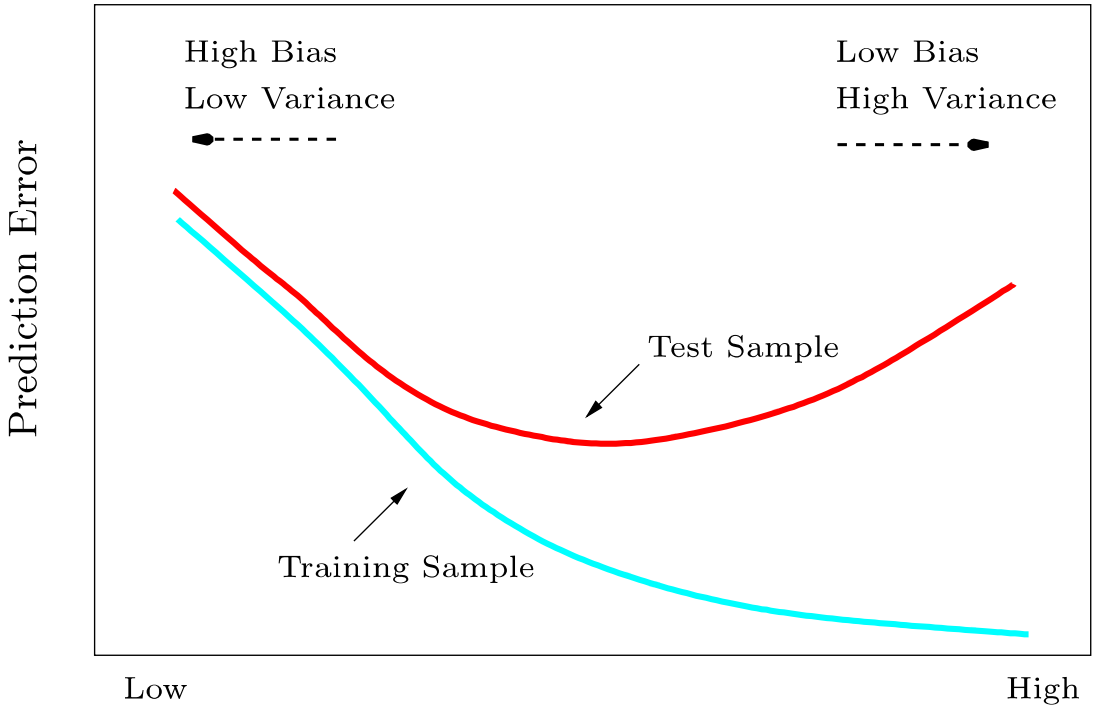
- $Bias = y^*(\boldsymbol{x}) - \mathbb{E}_{\boldsymbol{D}}\hat{f}(\boldsymbol{x}; \boldsymbol{D})$; $\quad Variance = \mathbb{E}_{\boldsymbol{D}}\left(\hat{f}(\boldsymbol{x}; \boldsymbol{D}) - \mathbb{E}_{\boldsymbol{D}'}\hat{f}(\boldsymbol{x}; \boldsymbol{D}')\right)^2$

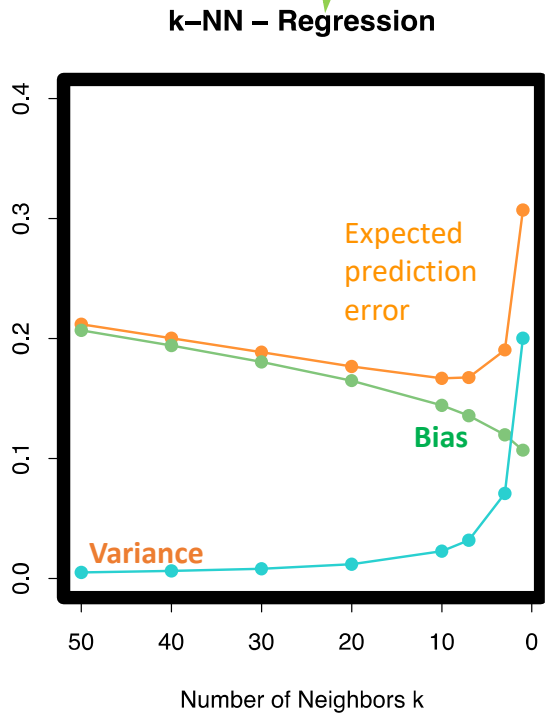
- This is known as **Bias-Variance Decomposition**
  - σ^2*:* cannot be avoided due to noises or uncontrolled factors
  - *Bias:* how far is the true value from the mean of predictions by method $\mathcal{A}$?
  - *Variance:* how much does each prediction by $\mathcal{A}$ vary around its mean?
- To obtain a small prediction error:
  - Small bias? Increase model complexity ➔ Variance tends to increase
  - Small variance? Decrease model complexity ➔ Bias tends to increase

Bias-Variance tradeoff: classical view

- The more complex the model $\hat{f}(x; \boldsymbol{D})$ is, the more data points it can capture, and the lower the bias can be.
  - However, higher complexity will make the model *"move" more* to capture the data points, and hence its variance will be larger.

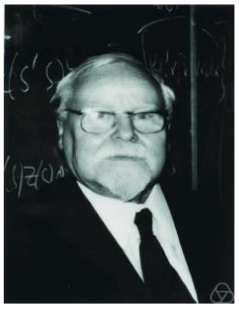
Classical view



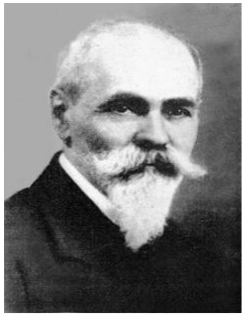


Regularization: introduction

- *Regularization* is now a popular and useful technique in ML.
- It is a technique to exploit further information to
  - Reduce overfitting in ML.
  - Solve ill-posed problems in Maths.
- The further information is often enclosed in a *penalty on the complexity* of $\hat{f}(x; \boldsymbol{D})$.
  - More penalty will be imposed on complex functions.
  - We prefer simpler functions among all that fit well the training data.



Tikhonov, smoothing an ill-posed problem



Zaremba, model complexity minimization

Bayes: priors over parameters

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

Regularization: the principle

- We need to learn a function $f(x, w)$ from the training set **D**
  - x is a data example and belongs to **input space**.
  - w is the parameter and often belongs to a ***parameter space*** **W**.
  - $\boldsymbol{F} = \{f(x, w): w \in \boldsymbol{W}\}$ is the **function space**, parameterized by w.
- For many ML models, the training problem is often reduced to an optimization problem:

$$w^* = \arg\min_{w \in \boldsymbol{W}} L(f(x, w), \boldsymbol{D}) \quad (1)$$

  - w sometimes tells the size/complexity of that function.
  - $L(f(x, w), \boldsymbol{D})$ is an *empirical loss/risk* which depends on **D**. This loss shows how well function *f* fits **D**.
- Another view:

$$f^* = \arg\min_{f \in \boldsymbol{F}} L(f, \boldsymbol{D})$$

Regularization: the principle

- Adding a penalty to (1), we consider

$$w^* = \arg\min_{w \in \boldsymbol{W}} L(f(x, w), \boldsymbol{D}) + \lambda g(w) \quad (2)$$

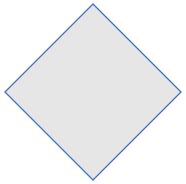
  - Where $\lambda > 0$ is called *the regularization/penalty constant*.
  - $g(w)$ measures the complexity of w. $(g(w) \geq 0)$

- $L(f, \boldsymbol{D})$ measures the goodness of function *f* on **D**.
- The penalty (regularization) term: $\lambda g(w)$
  - Allows to trade off the fitness on **D** and the generalization.
    (cho phép đánh đổi lỗi trên tập học với khả năng tổng quát hoá)
  - The greater λ, the heavier penalty, implying that $g(w)$ should be smaller.
  - In practice, λ should be neither too small nor too large.
    (λ không nên quá lớn hoặc quá bé trong thực tế)

Regularization: popular types

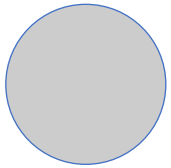
- $g(w)$ often relates to some norms when w is an n-dimensional vector.
  - L_0-norm: $\|w\|_0$ counts the number of non-zeros in w.
  - L_1-norm:

$$\|w\|_1 = \sum_{i=1}^{n} |w_i|$$



  - L_2-norm:

$$\|w\|_2^2 = \sum_{i=1}^{n} w_i^2$$



  - L_p-norm: $\|w\|_p = \sqrt[p]{|w_1|^p + \cdots + |w_n|^p}$

Regularization in Ridge regression

- Ridge regression can be derived from OLS by adding a penalty term into the objective function when learning.
- Learning a regressor in Ridge is reduced to

$$w^* = \arg\min_{\mathbf{w}} RSS(w, \boldsymbol{D}) + \lambda \|w\|_2^2$$

  - Where λ is a positive constant.
  - The term $\lambda \|w\|_2^2$ plays the role as regularization.
  - Large λ reduces the size of w.

Regularization in Lasso

- Lasso [Tibshirani, 1996] is a variant of OLS for linear regression by using L_1 to do regularization.
- Learning a linear regressor is reduced to

$$w^* = \arg\min_{\mathbf{w}} RSS(w, \boldsymbol{D}) + \lambda \|w\|_1$$

  - Where λ is a positive constant.
  - $\lambda \|w\|_1$ is the regularization term. Large λ reduces the size of w.
- Regularization here amounts to imposing a Laplace distribution (as prior) over each w_i, with density function:

$$p(w_i|\lambda) = \frac{\lambda}{2} e^{-\lambda|w_i|}$$

  - The larger λ, the more possibility that $w_i = 0$.

Regularization in SVM

- Learning a classifier in SVM is reduced to the following problem:
  - Minimize $\frac{\langle \mathbf{w} \cdot \mathbf{w} \rangle}{2}$
  - Conditioned on $y_i(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b) \geq 1, \quad \forall i = 1..r$
- In the cases of noises/errors, learning is reduced to
  - Minimize $\frac{\langle \mathbf{w} \cdot \mathbf{w} \rangle}{2} + C\sum_{i=1}^{r} \xi_i$
  - Conditioned on $\begin{cases} y_i(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b) \geq 1 - \xi_i, & \forall i = 1..r \\ \xi_i \geq 0, & \forall i = 1..r \end{cases}$
- $\xi_1 + \cdots + \xi_r$ measures the training error, $\frac{1}{2}\langle \boldsymbol{w} \cdot \boldsymbol{w} \rangle$ is *the regularization term*.

Some other regularization methods

- **Dropout:** (Hilton and his colleagues, 2012)
  - At each iteration of the training process, randomly drop out some parts and just update the other parts of our model.
- **Batch normalization** [Ioffe & Szegedy, 2015]
  - Normalize the inputs at each neuron of a neural network
  - Reduce input variance, easier training, faster convergence
- **Data augmentation**
  - Produce different versions of an example in the training set, by adding simple noises, translation, rotation, cropping, …
  - Those versions are added to the training data set
- **Early stopping**
  - Stop training early to avoid overtraining & reduce overfitting

Regularization: MAP role

- Under some conditions, we can view regularization as

$$w^* = \arg\min_{w \in \boldsymbol{W}} L(f(x,w), \boldsymbol{D}) + \lambda g(w)$$

Likelihood Prior

  - Where **D** is a sample from a probability distribution whose log likelihood is $-L(f(x,w), \boldsymbol{D})$.
  - w is a random variable and follows the prior with density

$$p(w) \propto \exp(-\lambda g(w))$$

- Then $w^* = \arg\max_{w \in \boldsymbol{W}} \{-L(f(x,w), \boldsymbol{D}) - \lambda g(w)\}$

$$w^* = \arg\max_{w \in \boldsymbol{W}} \log \Pr(\boldsymbol{D}|w) + \log \Pr(w) = \arg\max_{w \in \boldsymbol{W}} \log \Pr(w|\boldsymbol{D})$$

- As a result, regularization in fact helps us to learn an MAP solution w*.

Regularization: MAP in Ridge

- Consider the regression model: $\boldsymbol{x} \in \mathbb{R}^n$
  - *Pick* $\boldsymbol{w} \sim Normal(0, \sigma^2 \boldsymbol{I})$, *where* $\boldsymbol{I}$ *is the identity matrix*
  - *Generate sample* $\boldsymbol{x} \sim Normal(0, \frac{1}{n}\boldsymbol{I})$
  - *Let* $y = \boldsymbol{w}^T \boldsymbol{x}$

y thus follows a Normal distribution with mean 0 and variance 1

- Then the MAP estimation from the training data $\boldsymbol{D}$ is

$$\boldsymbol{w}^* = \arg\max_{\boldsymbol{w}} \log \Pr(\boldsymbol{w}|\boldsymbol{D}) = \arg\max_{\boldsymbol{w}} \log[\Pr(\boldsymbol{D}|\boldsymbol{w}) \Pr(\boldsymbol{w})]$$

$$= \arg\max_{\boldsymbol{w}} \sum_{(\boldsymbol{x},y)\in\boldsymbol{D}} \log \Pr(\boldsymbol{x}, y|\boldsymbol{w}) + \log \Pr(\boldsymbol{w})$$

$$= \arg\min_{\boldsymbol{w}} \sum_{(\boldsymbol{x},y)\in\boldsymbol{D}} \frac{1}{2}\left(y - \boldsymbol{w}^T\boldsymbol{x}\right)^2 + \frac{1}{2\sigma^2}\boldsymbol{w}^T\boldsymbol{w} + constant$$

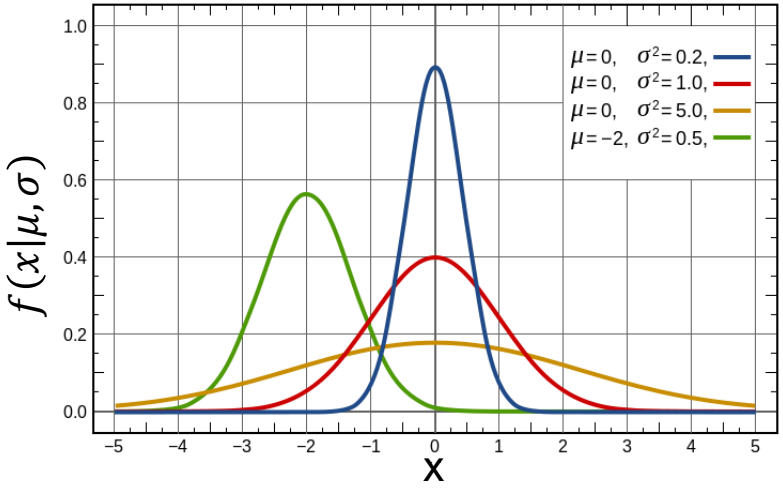
Ridge regression @@

- *Regularization using* L_2 *with penalty constant* $\lambda = \sigma^{-2}$.

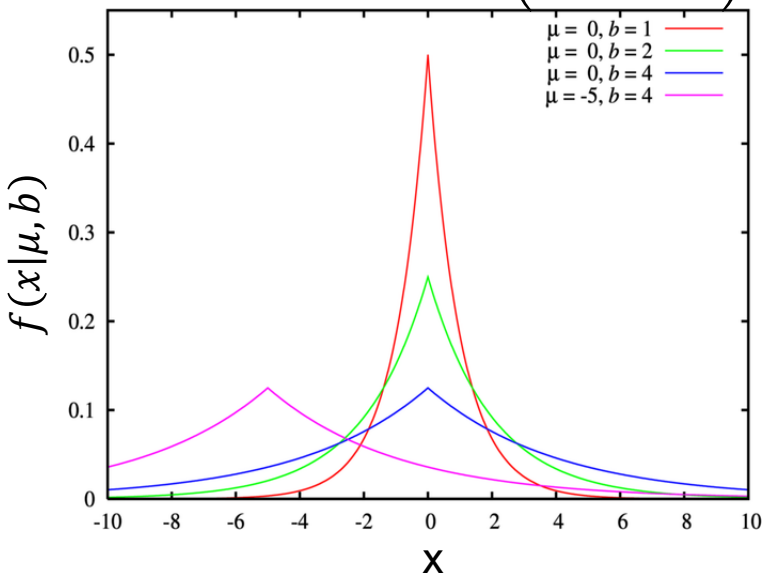
Regularization: MAP in Ridge & Lasso

- The regularization constant in Ridge: $\lambda = \sigma^{-2}$
- The regularization constant in Lasso: $\lambda = b^{-1}$
- Gaussian (left) and Laplace distribution (right)

$$f(x|\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$



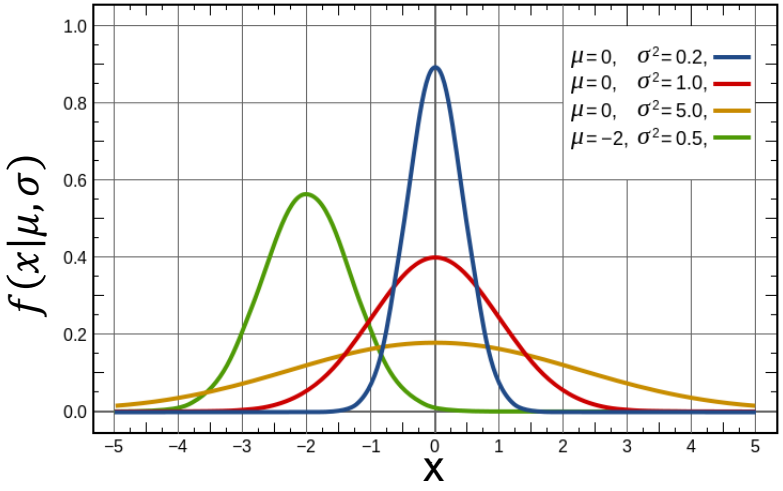
$$f(x|\mu,b) = \frac{1}{2b} \exp\left(-\frac{|x-\mu|}{b}\right)$$



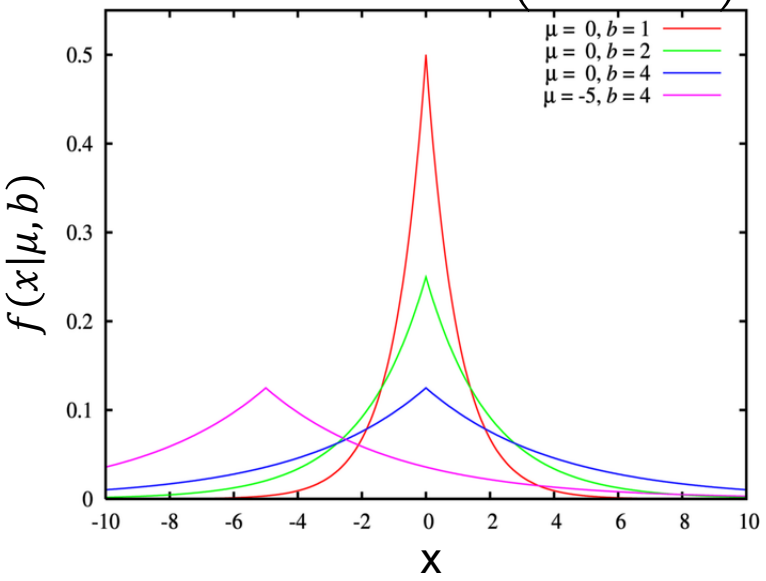
Regularization: limiting the search space

- The regularization constant in Ridge: $\lambda = \sigma^{-2}$
- The regularization constant in Lasso: $\lambda = b^{-1}$
- *The larger λ, the higher probability that x occurs around 0.*

$$f(x|\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$



$$f(x|\mu,b) = \frac{1}{2b} \exp\left(-\frac{|x-\mu|}{b}\right)$$



Regularization: limiting the search space

- The regularized problem:

$$w^* = \arg\min_{w \in \boldsymbol{W}} L(f(x, w), \boldsymbol{D}) + \lambda g(w) \quad (2)$$

- A result from the optimization literature shows that (2) is equivalent to the following:

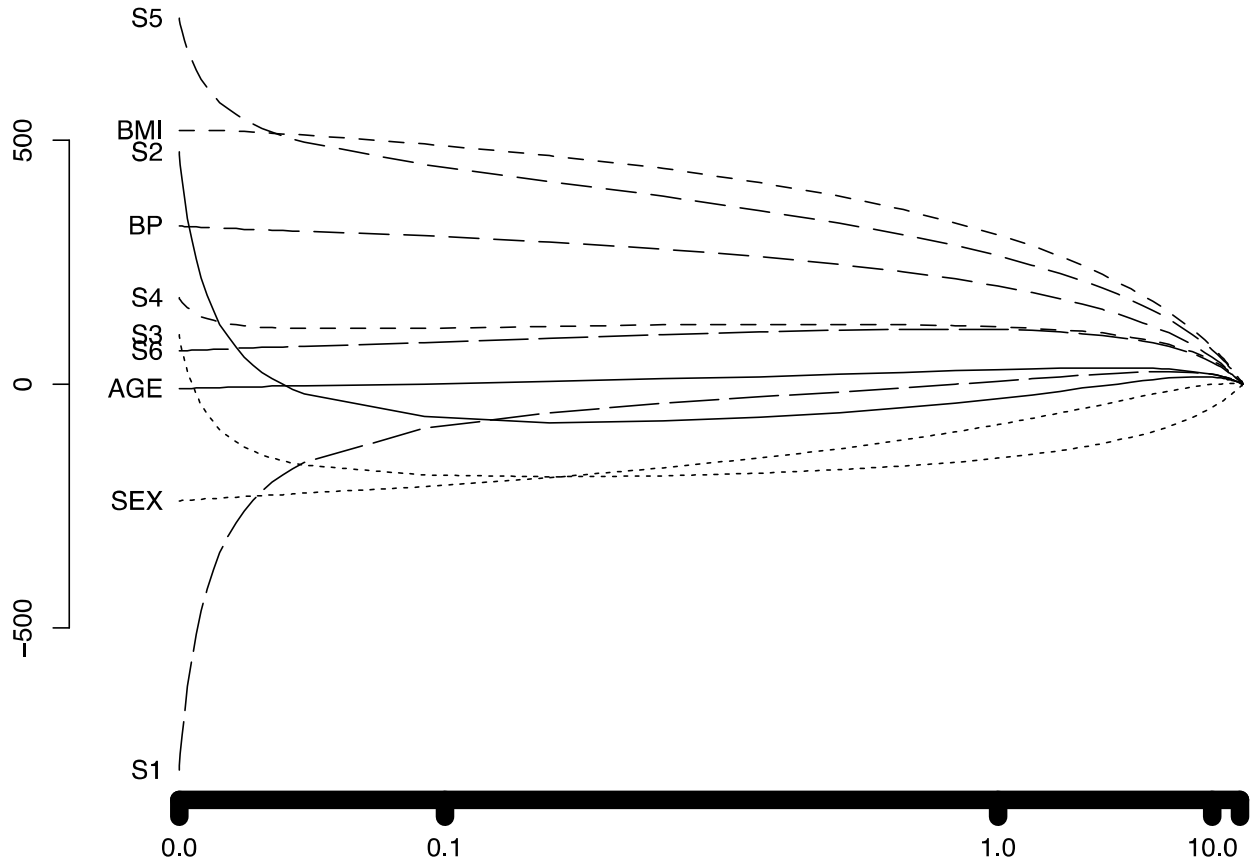
$$w^* = \arg\min_{w \in \boldsymbol{W}} L(f(x, w), \boldsymbol{D}) \quad \text{such that} \quad g(w) \leq s \quad (3)$$

  - For some constant s.

- *Note that the constraint of g(w) ≤ s plays the role as limiting the search space of w.*

Regularization: effects of λ

- Vector $\mathbf{w}^* = (w_0, s1, s2, s3, s4, s5, s6, Age, Sex, BMI, BP)$ changes when λ changes in Ridge regression.
  - $\mathbf{w}^*$ goes to 0 as λ increases.



Regularization: practical effectiveness

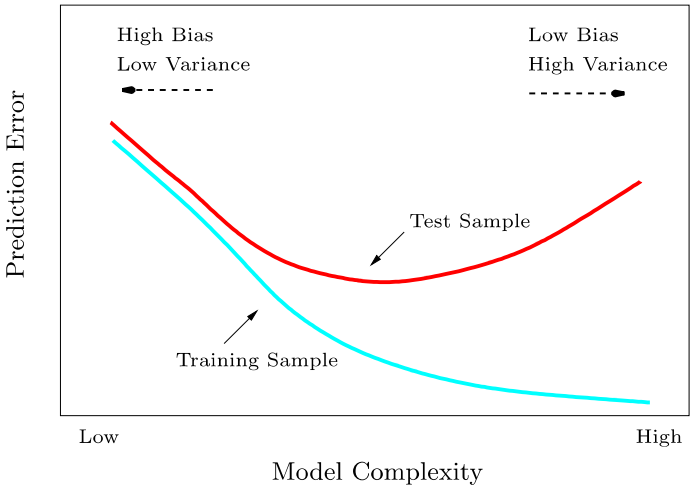
- Ridge regression was under investigation on a prostate dataset with 67 observations.
  - Performance was measured by RMSE (root mean square errors) and Correlation coefficient.

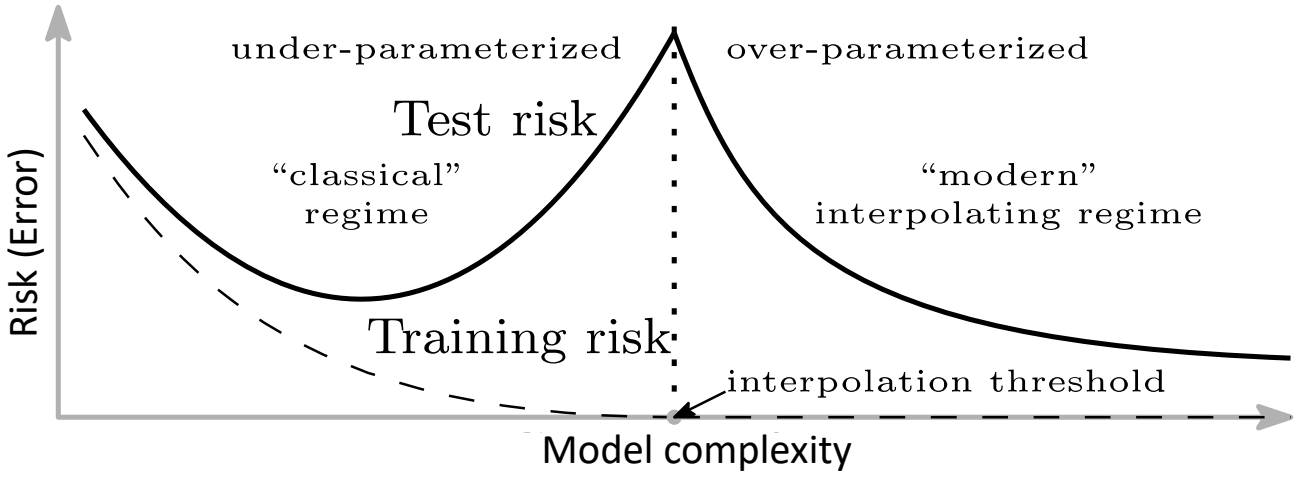
λ	0.1	1	10	100	1000	10000
RMSE	**0.74**	**0.74**	**0.74**	0.84	1.08	1.16
Correlation coeficient	0.77	0.77	**0.78**	0.76	0.74	0.73

  - Why??

Bias-Variance tradeoff: revisit

- Classical view:
  More complex model $\hat{f}(x; \boldsymbol{D})$
  - Lower bias, higher variance
- Modern phenomenon:
  - *Very rich models such as neural networks are trained to **exactly fit** the data, but often obtain **high accuracy** on test data*
    [Belkin et al., 2019; Zhang et al., 2021]
  - $Bias \cong 0$
  - GPT-4, ResNets, StyleGAN, DALLE-3, …
- **Why???**





Regularization: summary

- Advantages:
  - Avoid overfitting.
  - Limit the search space of the function to be learned.
  - Reduce bad effects from noises or errors in observations.
  - Might model data better. As an example, L_1 often work well with data/model which are inherently sparse.
- Limitations:
  - Consume time to select a good regularization constant.
  - Might pose some difficulties to design an efficient algorithm.

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