Learning From Data
Lecture 7: Model Selection & Regularization

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Today's Lecture

Practical tools to improve machine learning performance:

- Bias and variance trade off
- Model selection and feature selection
- Regularization
  - Generic techniques
  - Neural network regularization tricks
- Midterm information

Empirical error & Generalization error

Consider a learning task, the **empirical (training) error** of hypothesis h is the expected loss over m training samples

$$\hat{\epsilon}_{0,1}(h) = \frac{1}{m}\sum_{i=1}^{m} 1\{h(x^{(i)}) \neq y^{(i)}\} \quad \text{(classification, 0-1 loss)}$$

$$\hat{\epsilon}_{LS}(h) = \frac{1}{m}\sum_{i=1}^{m} ||h(x^{(i)}) - y^{(i)}||_2^2 \quad \text{(regression, least-square loss)}$$

The **generalization (testing) error** of h is the expected error on examples not necessarily in the training set.

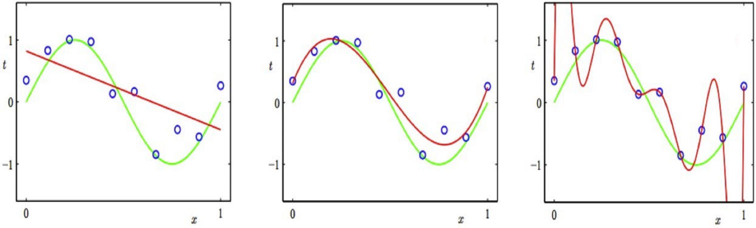
Goal of machine learning

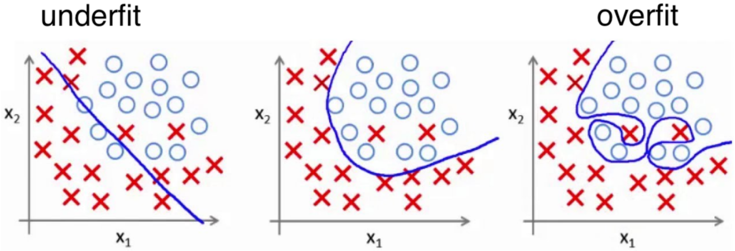
- make training error small (optimization)
- make the gap between empirical and generalization error small

Overfit & Underfit

Underfit Both training error and testing error are large

Overfit Training error is small, testing error is large



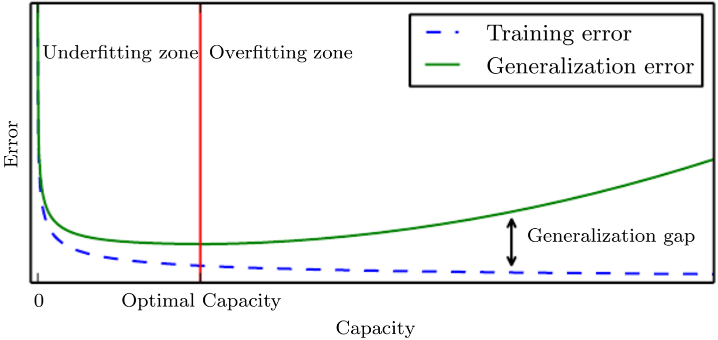


Model capacity: the ability to fit a wide variety of functions

Model Capacity

Changing a model's **capacity** controls whether it is more likely to overfit or underfit

- Choose a model's hypothesis space: e.g. increase # of features (adding parameters)
- Find the best among a family of hypothesis functions



How to formalize this idea?

Bias & Variance

Suppose data is generated by the following model:

$$y = h(x) + \epsilon$$

with $\mathbb{E}[\epsilon] = 0, Var(\epsilon) = \sigma^2$

- $h(x)$: true hypothesis function $\rightarrow$ *fixed value*
- D: training data $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\}$ sampled from P_{XY}
- $\hat{h}(x; D)$: estimated hypothesis function based on D, sometimes written as $\hat{h}(x)$ for short $\rightarrow$ *random variable*

Bias & Variance

Bias of a model: The expected estimation error of $\hat{h}$ over all choices of training data D sampled from P_{XY},

$$Bias(\hat{h}) = \mathbb{E}_D[\hat{h}(x) - h(x)] = \mathbb{E}_D[\hat{h}(x)] - h(x)$$

When we make wrong assumptions about the model, $\hat{h}$ will have large bias (underfit)

Variance of a model: How much $\hat{h}$ move around its mean

$$\begin{aligned} Var(\hat{h}) &= \mathbb{E}_D[(\hat{h}(x) - \mathbb{E}_D(\hat{h}(x))^2] \\ &= \mathbb{E}_D[\hat{h}(x)^2] - \mathbb{E}_D[\hat{h}(x)]^2 \end{aligned}$$

When the model overfits "spurious" patterns, it has large variance (overfit).

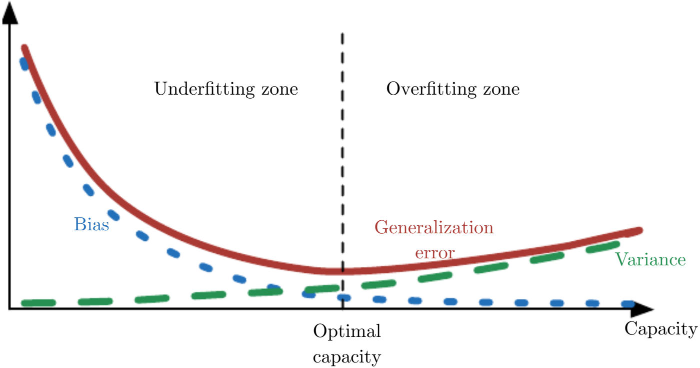
Bias - Variance Tradeoff

MSE Decomposition

We can decompose the expected error of MSE on a new sample (x,y):

$$MSE = \mathbb{E}_{D,\epsilon}[(\hat{h}(x) - y)^2] = Bias(\hat{h})^2 + Var(\hat{h}) + \sigma^2,$$

- σ^2 represents irreducible error
- in practice, increasing capacity tends to increase variance and decrease bias.



Model Selection

For a given task, how do we select which model to use?

- Different learning models
  - e.g. SVM vs. logistic regression for binary classification
- Same learning models with different **hyperparameters**
  - e.g. # of clusters in k-means clustering

Cross validation is a class of methods for selecting models using a *validation set*.

Hold-out cross validation

Given training set S and candidate models M_1,...,M_n:

1. Randomly split S into S_{train} and S_{cv} (e.g. 70% S_{train})
2. Training each M_i on S_{train},
3. Select the model with smallest empirical error on S_{cv}

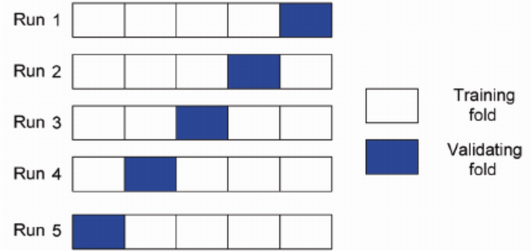
Disavantages of hold-out cross validation

- "wastes" about 30% data
- chances of an unfortunate split

K-Fold Cross Validation

Goal: ensure each sample is equally likely to be selected for validation.

1. Randomly split S into k disjoint subsets $S_1, \ldots, S_k$ of m/k training examples (e.g. $k = 5$)
2. For $j = 1 \ldots k$:
   Train each model on $S \backslash S_j$, then validate on S_j,



3. Select the model with the smallest **average** empirical error among all k trails.

Leave-One-Out Cross Validation

A special case of k-fold cross validation, when $k = m$.

1. For each training example x_i
   Train each model on $S \backslash \{x_i\}$, then evaluate on x_i,
2. Select the model with the smallest average empirical error among all m trails.

Often used when training data is scarce.

Other Cross Validation Methods

- Random subsampling
- Bootstrapping: sample with replacement from training examples (used for small training set)
- Information criteria based methods: e.g. Bayesian information criterion (BIC), Akaike information criterion (AIC)

Cross validation can also be used to evaluate a single model.

Regularization

Regularization is any modification we make to a learning algorithm to reduce its generalization error, but not the training error

Common regularization techniques:

- Penalize parameter size
  e.g. linear regression with **weight decay**:

$$J(\theta) = \sum_{i=1}^{m} \log p(y^{(i)}|x^{(i)};\theta) + \lambda||\theta||_2^2$$

- Use prior probability: max-a-posteriori estimation

Parameter Norm Penalty

Adding a regularization term to the loss (error) function:

$$\tilde{J}(X, Y; \theta) = \underbrace{J(X, Y; \theta)}_{\text{data-dependent loss}} + \lambda \underbrace{\Omega(\theta)}_{\text{regularizer}}$$

where

$$\Omega(\theta) = \frac{1}{2} \sum_{j=1}^{n} |\theta_j|^q = \frac{1}{2} ||\theta||_q^q$$

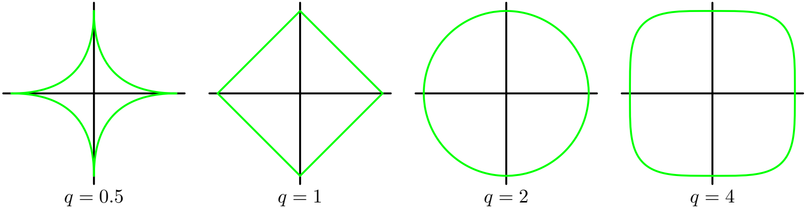


Figure: Contours of the regularizer ($||\theta||^q = 1$) for different q

L2 parameter penalty

When $q = 2$, it's also known as **Tokhonov regularization** or **ridge regression**

$$\tilde{J}(X, Y; \theta) = J(X, Y; \theta) + \frac{\lambda}{2}\theta^T\theta$$

Gradient descent update:

$$\begin{aligned}\theta &\leftarrow \theta - \alpha \nabla_\theta \tilde{J}(X, Y; \theta) \\ &= \theta - \alpha(\nabla_\theta J(X, Y; \theta) + \lambda\theta) \\ &= (1 - \alpha\lambda)\theta - \alpha\nabla_\theta J(X, Y; \theta)\end{aligned}$$

L2 penalty multiplicatively shrinks parameter θ by a constant

Example: regularized least square

When $J(X, Y; \theta) = \frac{1}{2}\sum_{i=1}^{m}(y^{(i)} - \theta^T x^{(i)})^2$ (ordinary least squares),
$\tilde{\theta}_{OLS} = (X^T X + \lambda I)^{-1}(X^T Y)$

L1 parameter penalty

When $q = 1$, $\Omega(\theta) = \frac{1}{2}\sum_{j=1}^{n}|\theta_j|$ is also known as **LASSO regression**.

- If λ is sufficiently large, some coefficients θ_j are driven to 0.
- It will lead to a *sparse* model

Proposition 1

Solving $\min_\theta \tilde{J}(X, Y; \theta) = J(X, Y; \theta) + \frac{\lambda}{2}\sum_{j=1}^{n}|\theta_j|^q$ *is equivalent to*

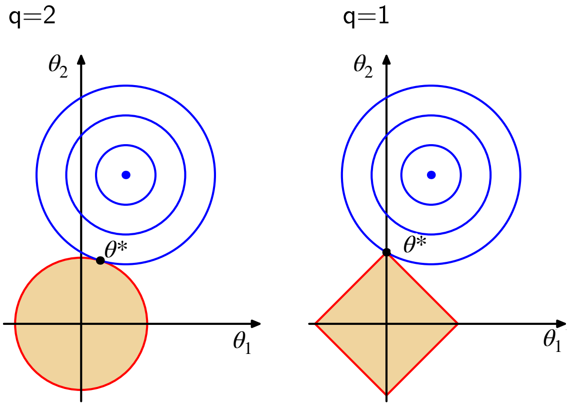
$$\begin{gathered}\min_\theta J(X, Y; \theta) \\ s.t. \sum_{j=1}^{n}|\theta_j|^q \leq \eta\end{gathered}$$

for some constant $\eta > 0$ *(*$\star$*). Furthermore,* $\eta = \sum_{j=1}^{n}|\theta_j^*(\lambda)|^q$ *where* $\theta^*(\lambda) = \operatorname{argmin}_\theta \tilde{J}(X, Y; \theta, \lambda)$

- $(\star)$ assumes constraints are satisfiable (e.g. with slater's condition)
- Choosing λ is equivalent to choosing η and vice versa
- Smaller $\lambda \rightarrow$ larger constraint region

L1 vs L2 parameter penalty

Figure: Contour plot of unregularized error $J(X, Y; \theta)$ and the constraint region $\sum_{j=1}^{n} |\theta|^q \leq \eta$



The lasso (l1 regularizer) gives a sparse solution with $\theta_1^* = 0$.

Bayesian Statistics

Maximum likelihood estimation: θ is an unknown constant

$$\theta_{MLE} = \operatorname*{argmax}_{\theta} \prod_{i=1}^{m} p(y^{(i)}|x^{(i)};\theta)$$

Bayesian view: θ is a random variable

$$\theta \sim p(\theta)$$

Given training set $S = \{x^{(i)}, y^{(i)}\}$, posterior distribution of θ

$$p(\theta|S) = \frac{p(S|\theta)p(\theta)}{p(S)}$$

Fully Bayesian statistics

$$p(\theta|S) = \frac{p(S|\theta)p(\theta)}{p(S)} = \frac{\prod_{i=1}^{m} p(y^{(i)}|x^{(i)}, \theta)p(\theta)}{\int_\theta (\prod_{i=1}^{m} p(y^{(i)}|x^{(i)}, \theta)p(\theta))d\theta}$$

To predict the label for new sample x, compute the posterior distribution over training set S:

$$p(y|x, S) = \int_\theta p(y|x, \theta)p(\theta|S)d\theta$$

The label is

$$\mathbb{E}[y|x, S] = \int_y y \; p(y|x, S)dy$$

Fully bayesian estimate of θ is difficult to compute, has no close-form solution.

Bayesian Statistics

Posterior distribution on class label y using $p(\theta|S)$

$$p(y|x,S) = \int_\theta p(y|x,\theta)p(\theta|S)d\theta$$

We can approximate $p(y|x,\theta)$ as follows:

MAP approximation

The **MAP (maximum a posteriori) estimate** of θ is

$$\theta_{MAP} = \underset{\theta}{\text{argmax}} \prod_{i=1}^{m} p(y^{(i)}|x^{(i)},\theta)p(\theta)$$

$p(y^{(i)}|x^{(i)},\theta)$ is not the same as $p(y^{(i)}|x^{(i)};\theta)$

MAP estimation and regularized least square

Recall ordinary least square is equivalent to maximum likelihood estimation when $p(y^{(i)}|x^{(i)}) \sim \mathcal{N}(\theta^T x^{(i)}, \sigma^2)$:

$$\begin{aligned}\theta_{MLE} &= \underset{\theta}{\operatorname{argmax}} \prod_{i=1}^{m} p(y^i|x^i;\theta) \\ &= (X^T X)^{-1} X^T Y = \theta_{OLS}\end{aligned}$$

The MAP estimation when $\theta \sim N(0, \tau^2 I)$ is

$$\begin{aligned}\theta_{MAP} &= \underset{\theta}{\operatorname{argmax}} \left(\prod_{i=1}^{m} p(y^i|x^i;\theta)\right) p(\theta) \\ &= \underset{\theta}{\operatorname{argmin}} \left(\frac{\sigma^2}{\tau^2}\theta^T\theta + (Y - X\theta)^T (Y - X\theta)\right) \\ &= (X^T X + \frac{\sigma^2}{\tau} I)^{-1} X^T Y = \tilde{\theta}_{OLS} \text{ when } \lambda = \frac{\sigma^2}{\tau}\end{aligned}$$

Discussion on MAP Estimation

General remarks on MAP:

- When θ is uniform, $\theta_{MAP} = \theta_{MLE}$
- A common choice for $p(\theta)$ is $\theta \sim \mathcal{N}(0, \tau^2 I)$, and θ_{MAP} corresponds to weight decay (L2-regularization)
- When θ is an isotropic Laplace distribution, θ_{MAP} corresponds to LASSO (L1-regularization).
- θ_{MAP} often have smaller norm than θ_{MLE}

Regularization for neural networks

Common regularization techniques:

- Data augmentation
- Parameter sharing
- Drop out

Data augmentation

Create fake data and add it to the training set. (Useful in certain tasks such as object classification.)

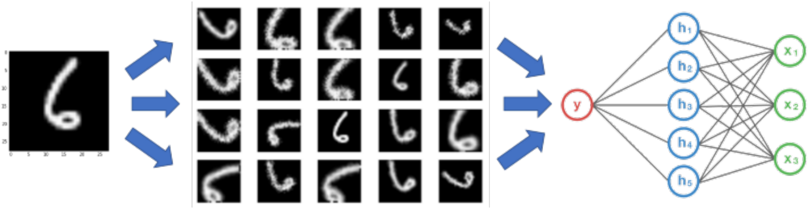


Figure: Generate fake digits via geometric transformation, e.g. scale, rotation etc

Figure: Generate images of different styles using GAN

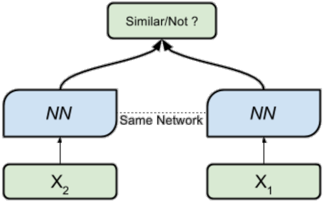
Shorten et. al. A survey on Image Data Augmentation for Deep Learning, 2019

Parameter Sharing

Force sets of parameters to be equal based on prior knowledge.

Siamese Network

- Given input X, learns a discriminative feature $f(X)$
- For every pair of samples (X_1, X_2) in the same class, minimize their distance in feature space $||f(X_1) - f(X_2)||^2$



Convolutional Neural Network (CNN)

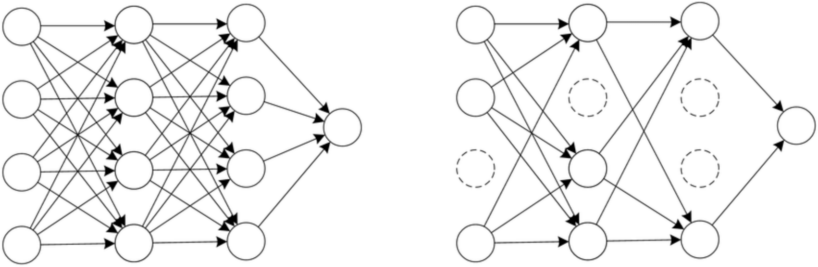
- Image features should be invariant to translation
- CNN shares parameters across multiple image locations.

Soft parameter sharing: add a norm penalty between sets of parameters:

$$\Omega(\theta^A, \theta^B) = ||\theta^A - \theta^B||_2^2$$

Drop Out

- Randomly remove a non-output unit from network by multiplying its output by zero (with probability p)
- In each mini-batch, randomly sample binary masks to apply to all inputs and hidden units
- Dropout trains an ensemble of different sub-networks to prevent the "co-adaptation" of neurons



(a) Standard Neural Network   (b) Network after Dropout

Midterm Information

- Time: Next Friday, November 1, 10:00am (Arrive at 9:50am)
- Location: TBA
- What to bring: Pen + One A4 size notesheet (can be written on both sides)
- Covers everything up to today.
- Midterm review session this weekend (Time & Location TBA)

Stop by my office hour if you have questions!