

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

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

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

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

$$x, y \sim P_{x,y}$$

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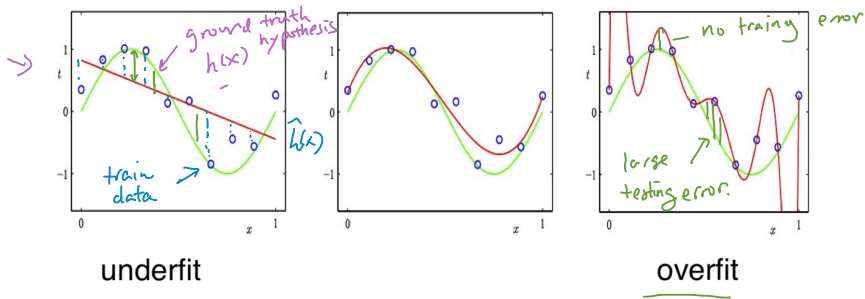
Goal of machine learning

- ▶ 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

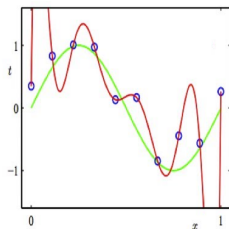
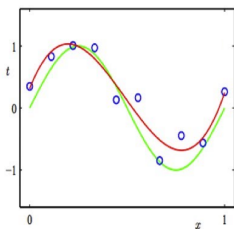
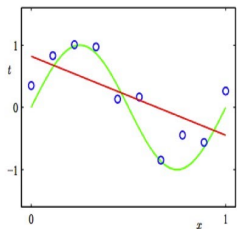
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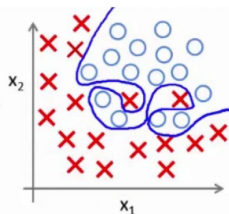
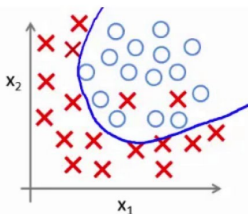
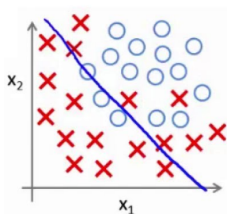
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underfit

overfit



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) $h(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2$.
- ▶ Find the best among a family of hypothesis functions

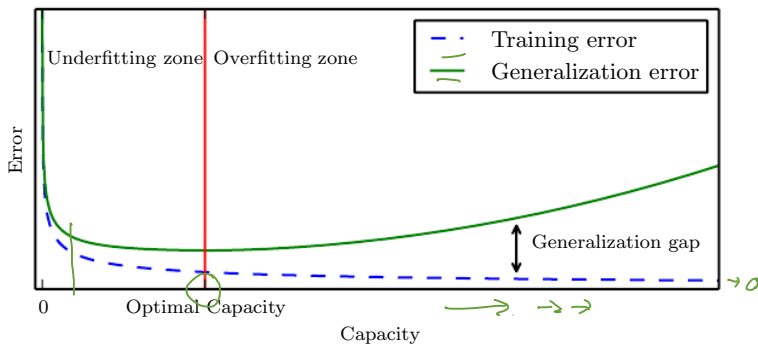
$$\{h(x) \mid \theta_0, \theta_1, \theta_2 \in \mathbb{R}^n\}$$

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix}$$

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How to formalize this idea?

Bias & Variance

Suppose data is generated by the following model:

$$y = \underbrace{h(x)}_{\text{true hypothesis}} + \underbrace{\epsilon}_{\text{noise}}$$

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

$h(x)$: true hypothesis function \rightarrow *fixed value*

D : training data $\{(x^{(1)}, y^{(1)}), \dots, (x^{(m)}, y^{(m)})\}$ 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*

$$\min_{h \in \mathcal{H}} \ell(h(x), y) \\ (x, y) \in D$$

Bias & Variance

Bias of a model: The expected estimation error of \hat{h} over all choices of training data D sampled from P_{XY} , *true hypothesis (label) function*

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

Annotations: $\mathbb{E}_D[\hat{h}(x)] \rightarrow \mathbb{E}_P[\hat{h}(x)]$, $h(x) \rightarrow \mathbb{E}_P(h(x))$

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

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

*Annotations: $\mathbb{E}_D(\hat{h}(x))$ is circled in green. *average hypothesis function**

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) :

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

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

proof. $Bias(\hat{h}(x)) = \mathbb{E}_D[\hat{h}(x) - h(x)] = \mathbb{E}_D[\hat{h}(x)] - h(x) \checkmark$ $\epsilon \sim \mathcal{N}(0, \sigma^2)$
 $Var(\hat{h}(x)) = \mathbb{E}_D[\hat{h}(x)^2] - \mathbb{E}_D[\hat{h}(x)]^2$ (*) $y = h(x) + \epsilon$

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

$$\mathbb{E}_{D,\epsilon}[y^2] = \mathbb{E}_{D,\epsilon}[(h(x) + \epsilon)^2] = \mathbb{E}_{D,\epsilon}[h(x)^2] + \mathbb{E}_{D,\epsilon}[\epsilon^2] + 2\mathbb{E}_{D,\epsilon}[h(x)\epsilon]$$

$h(x)$ and ϵ are independent

$$\mathbb{E}_{D,\epsilon}[\hat{h}(x)y] = \mathbb{E}_{D,\epsilon}[\hat{h}(x)h(x)] + \mathbb{E}_{D,\epsilon}[\hat{h}(x)\epsilon] = h(x)\mathbb{E}_{D,\epsilon}[\hat{h}(x)] + \mathbb{E}_{D,\epsilon}[\hat{h}(x)]\mathbb{E}_{D,\epsilon}[\epsilon] = h(x)\mathbb{E}_{D,\epsilon}[\hat{h}(x)]$$

$$\mathbb{E}_{D,\epsilon}[\hat{h}(x)^2] = \underbrace{Var(\hat{h}(x))}_{\text{Variance}} + \mathbb{E}_{D,\epsilon}[\hat{h}(x)]^2 \text{ by (*)}$$

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

Bias - Variance Tradeoff

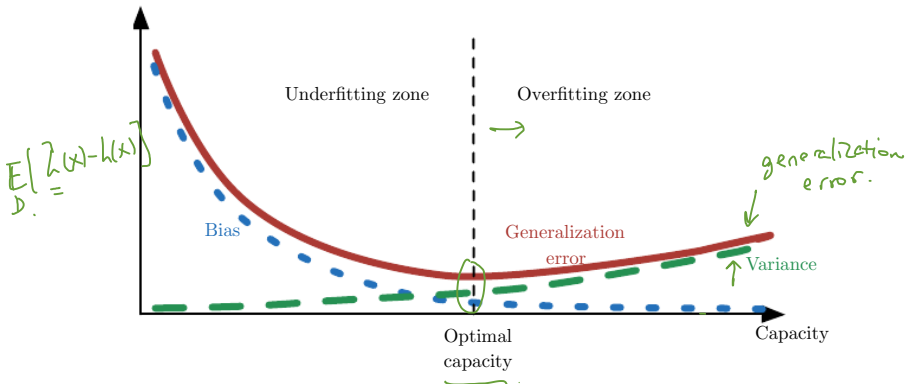
$$= \text{Var}(\hat{h}(x)) + (\underbrace{\mathbb{E}[\hat{h}(x)] - h(x)}_{\text{Bias}})^2 + \sigma^2$$
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Cross validation

Model selection

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

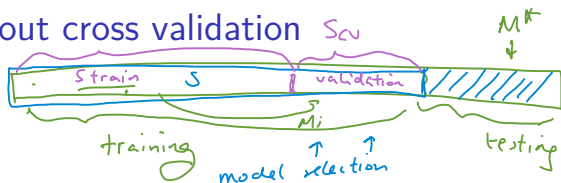
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Cross validation is a class of methods for selecting models using a *validation set*.

Hold-out cross validation S_{cv}



Given training set S and candidate models M_1, \dots, 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}

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Disadvantages of hold-out cross validation

- ▶ "wastes" about 30% data S_{cv}
- ▶ 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, \dots, S_k of m/k training examples (e.g. $k = 5$)

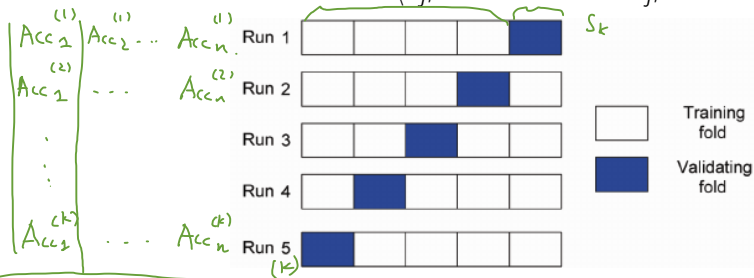
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M_1, \dots, M_n

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2. For $j = 1 \dots k$:

Train each model on $S \setminus S_j$, then validate on S_j ,



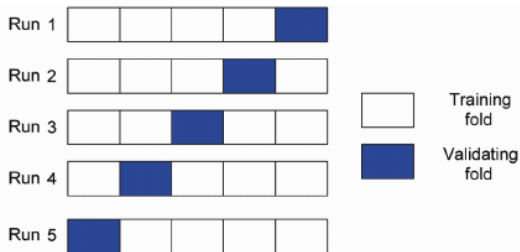
$\bar{Acc}(M_1)$ $\bar{Acc}(M_2)$

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

Leave-One-Out Cross Validation

$$\begin{array}{ccc} x_1, & \dots & x_m \\ \underbrace{\hspace{1.5cm}} & & \boxed{x_m} \\ S_1 & \dots & \downarrow \\ & & S_{k=m} \end{array}$$

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

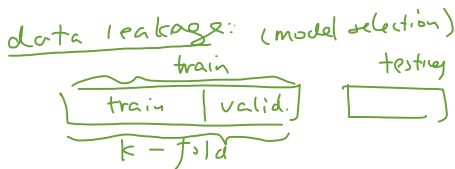
1. For each training example x_i
Train each model on $S \setminus \{x_i\}$, then evaluate on x_i ,
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Often used when training data is scarce.

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)

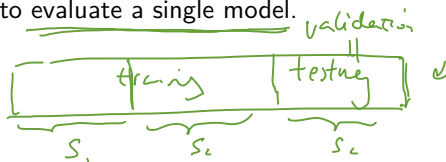
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Cross validation can also be used to evaluate a single model.

$k=3$.



report $\text{Arg}(\text{Acc}_i)$ no. picking involved!
 $i=1, \dots, k$

Regularization

Parameter Norm Penalty

MAP estimation

Regularization for neural networks

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

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Common regularization techniques:

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

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

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- ▶ Use prior probability: max-a-posteriori estimation

Parameter Norm Penalty

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

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

where

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

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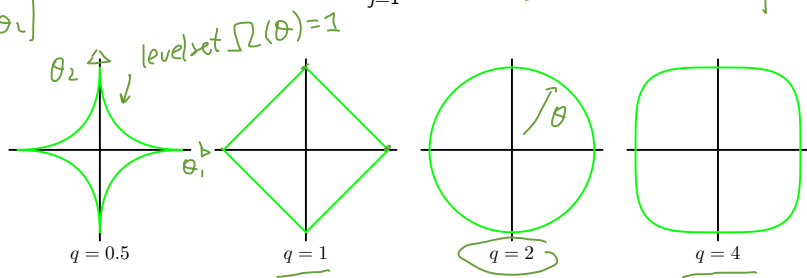
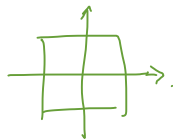


Figure: Contours of the regularizer ($\|\theta\|_q^q = 1$) for different q

L2 parameter penalty

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

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

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Gradient descent update:

weight decay

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

$$\begin{aligned} &\nabla_{\theta} (J(X, Y; \theta) + \frac{\lambda}{2} \theta^T \theta) \\ &= \nabla_{\theta} J(X, Y; \theta) + \frac{\lambda}{2} \nabla_{\theta} \theta^T \theta \\ & \qquad \qquad \qquad \underbrace{\qquad \qquad \qquad}_{2\theta} \end{aligned}$$

L2 penalty multiplicatively shrinks parameter θ by a constant

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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

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Proposition 1 θ^*, λ . (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

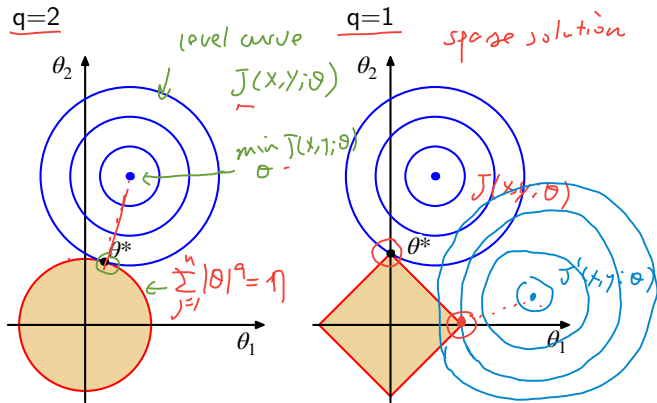
$$\begin{cases} \min_{\theta} J(X, Y; \theta) & (2) \quad \underline{0, \eta} \\ \text{s.t. } \sum_{j=1}^n |\theta_j|^q \leq \eta \end{cases}$$

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

- ▶ (*) assumes constraints are satisfiable (e.g. with Slater's condition)
- ▶ Choosing $\underline{\lambda}$ is equivalent to choosing $\underline{\eta}$ and vice versa
- ▶ Smaller $\lambda \rightarrow$ larger constraint region
larger η

L1 vs L2 parameter penalty

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



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

Bayesian Statistics

Maximum likelihood estimation: θ is an unknown constant

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

Bayesian view: θ is a random variable

$$\theta \sim p(\theta) \quad \text{prior distribution} \quad \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}$$

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

parameter

data

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

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

NLE

$$p(y|x; \theta)$$

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

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 $p(\theta|S)$

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

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

MAP approximation

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

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

Bayesian Statistics

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$p(y^{(i)}|x^{(i)}, \theta)$ 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 $p(y^{(i)}|x^{(i)}) \sim \mathcal{N}(\theta^T x^{(i)}, \sigma^2)$:

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

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The MAP estimation when $\theta \sim \mathcal{N}(0, \tau^2 I)$ is $\begin{bmatrix} \tau^2 & & \\ & \tau^2 & \\ & & \ddots \\ & & & \tau^2 \end{bmatrix}$

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

variance $p(y|x)$
prior variance

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.)

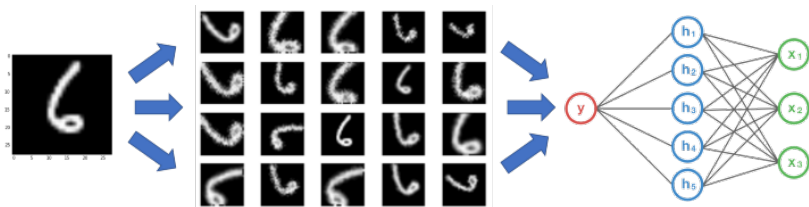


Figure: Generate fake digits via geometric transformation, e.g. scale, rotation etc



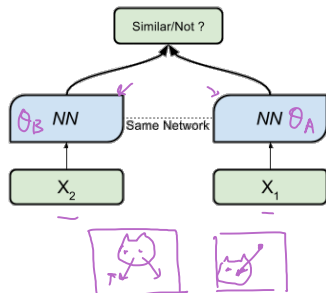
Figure: Generate images of different styles using GAN

Parameter Sharing

Force sets of parameters to be equal based on prior knowledge. $y_1 = y_2$

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)

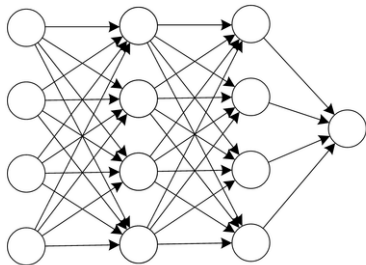
- ▶ Image features should be invariant to translation
- ▶ CNN shares parameters across multiple image locations.

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

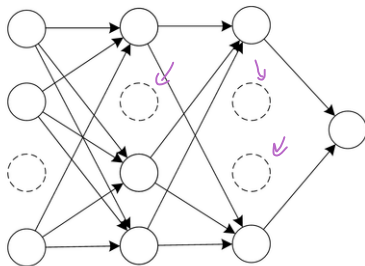
$$\Omega(\theta^A, \theta^B) = \|\theta^A - \theta^B\|_2^2$$

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, April 19, 10:00am (Arrive at 9:50am)
- ▶ Location: A307
- ▶ What to bring: One double-sided A4 notesheet
- ▶ Covers everything up to today (neural networks and model selection will only be short questions.)
- ▶ Midterm review session @ C401, April 14th 9:50am
- ▶ No late submission for WA2 13th

My office hour will be moved to tomorrow afternoon 2pm

Next lecture: learning theory

How to quantify generalization error?

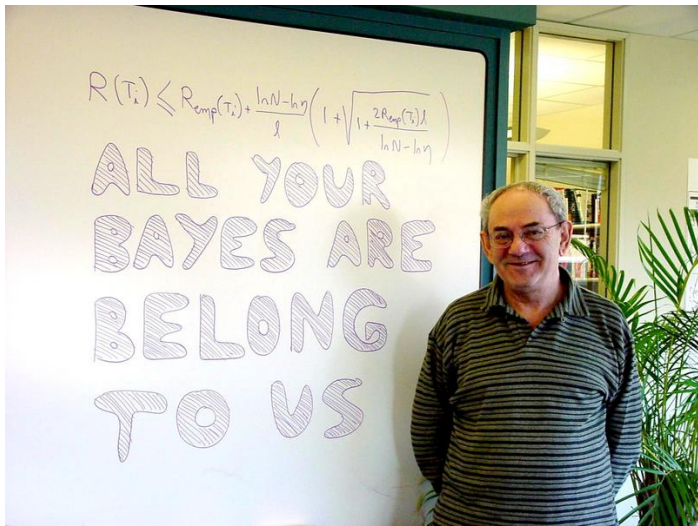


Figure: Prof. Vladimir Vapnik in front of his famous theorem