Learning From Data
Lecture 11: 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

Start on your project early!

Empirical error & Generalization error

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

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

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

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

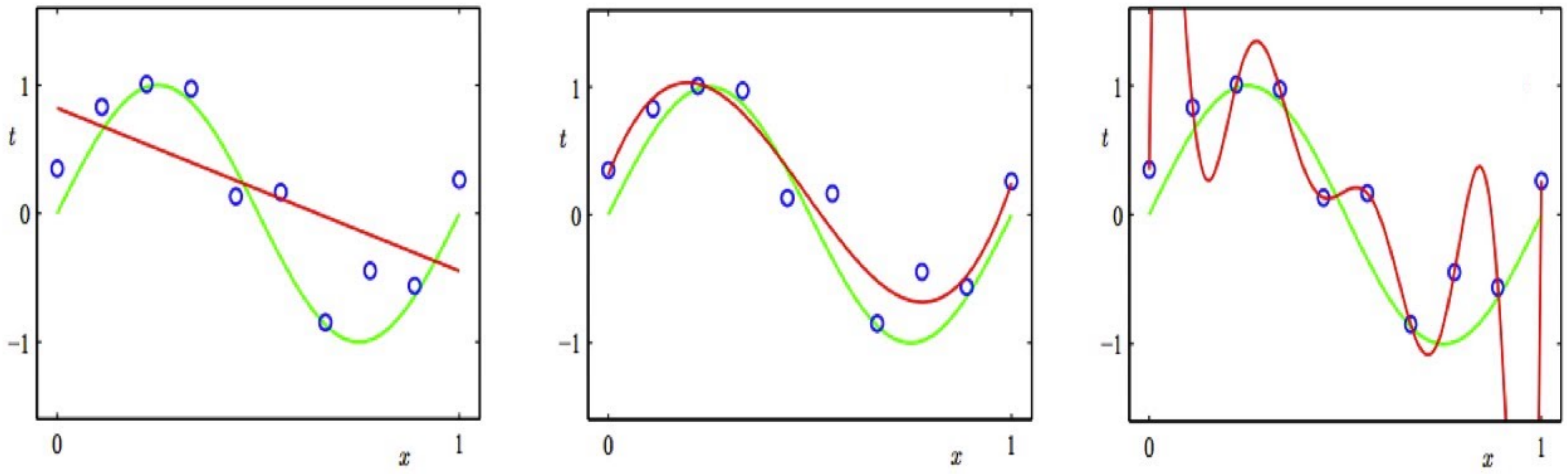
Goal of machine learning

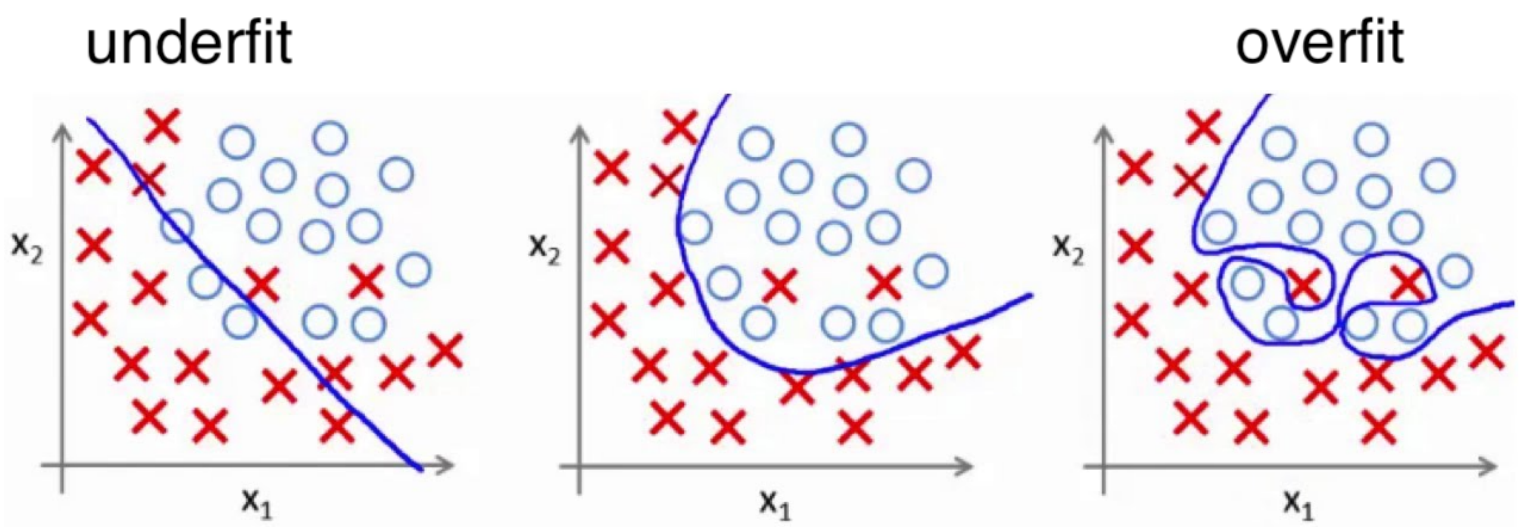
- make training error small (optimization)
- make the gap between empirical and generalization error small

Overfit & Underfit

Underfit Both training error and testing error are large

Overfit Training error is small, testing error is large



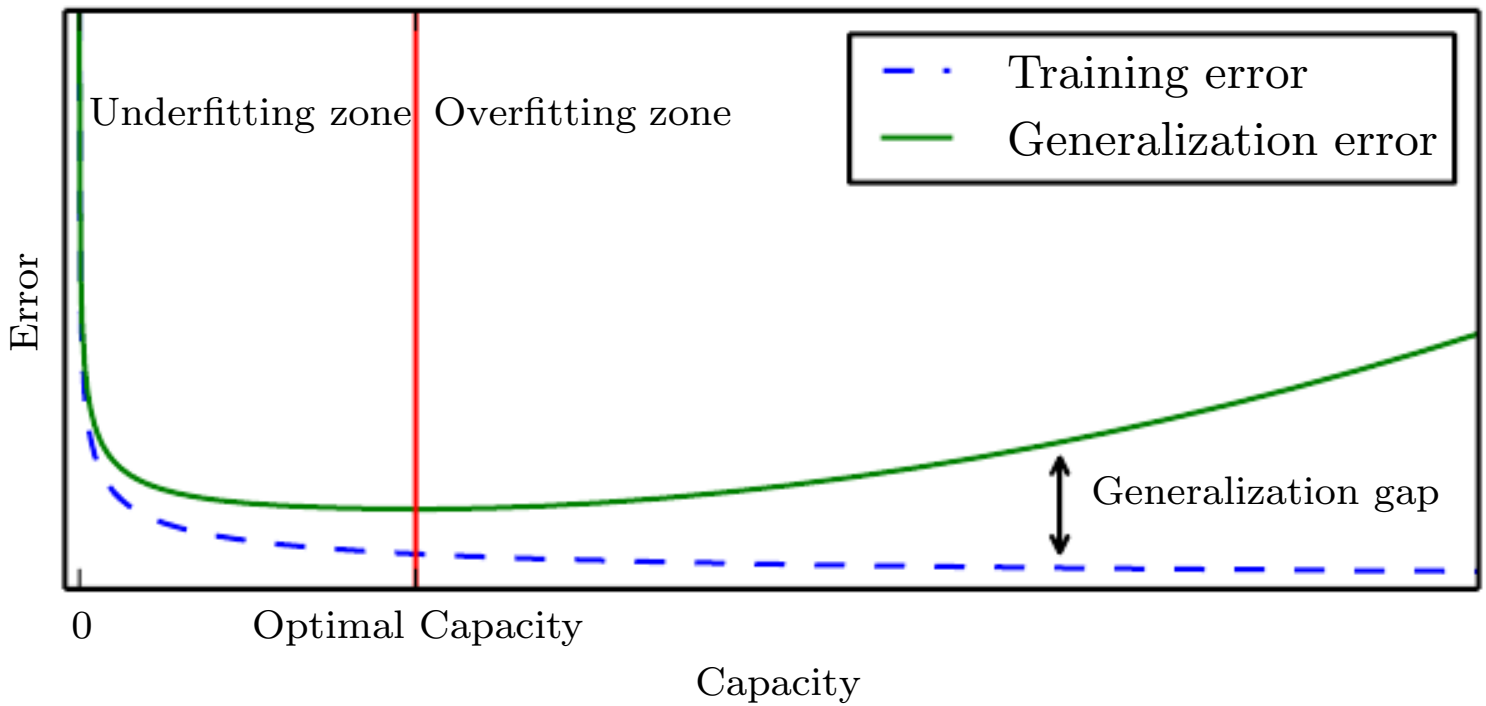


Model capacity: the ability to fit a wide variety of functions

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

$\hat{h}(x)$: estimated hypothesis function of a model. $h(x)$: true hypothesis function

Bias of a model: the expected generalization error if we were to fit it to an infinitely large training set.

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

- When we make wrong assumptions in the model, such as too few paramters, it has large bias (underfit)

Variance of a model:

$$Var(\hat{h}) = \mathbb{E}[\hat{h}(x)^2] - \mathbb{E}[\hat{h}(x)]^2$$

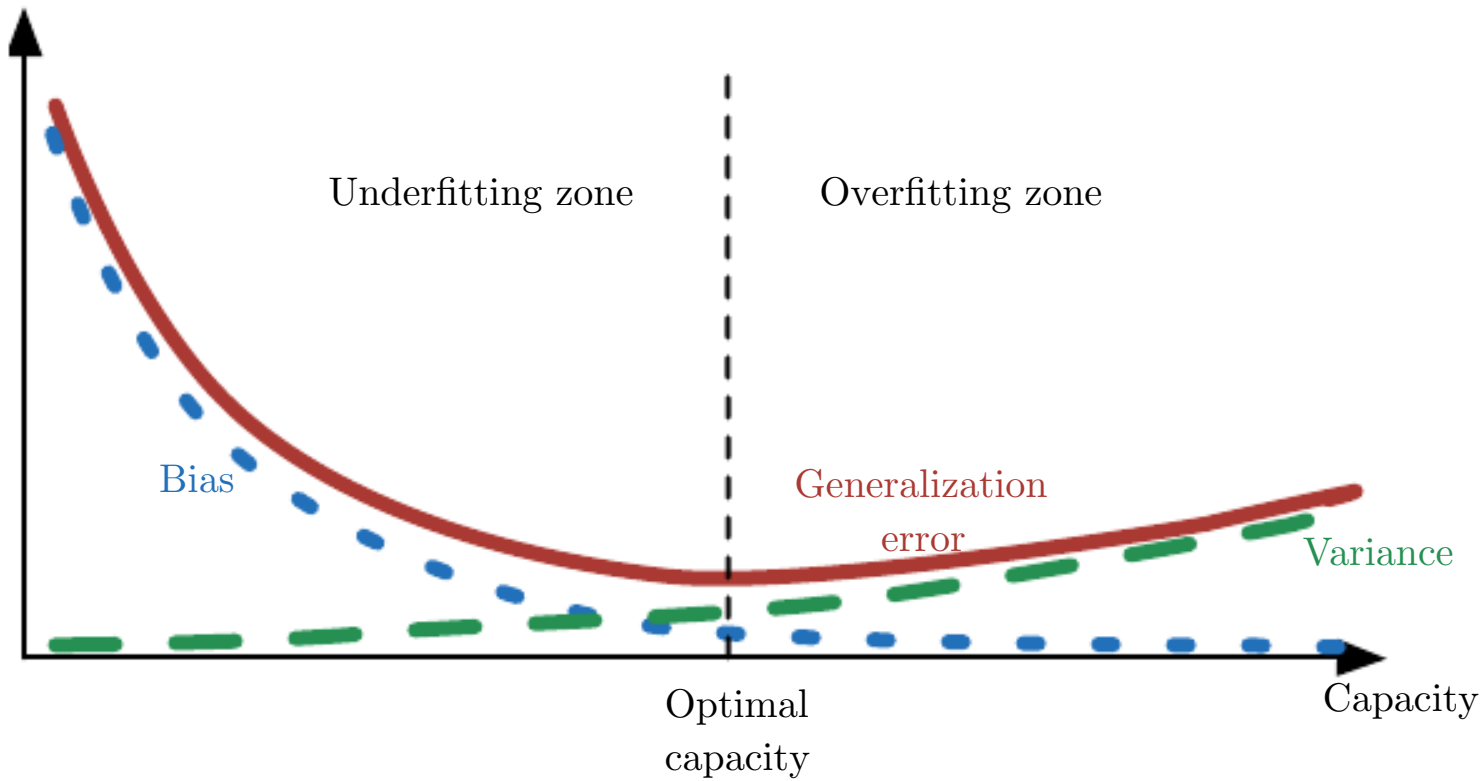
- When the model overfits "spurious" patterns, it has large variance (overfit).

Bias - Variance Tradeoff

If we measure generalization error by MSE

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

- 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 $M_1,\ldots,M_n$:

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}

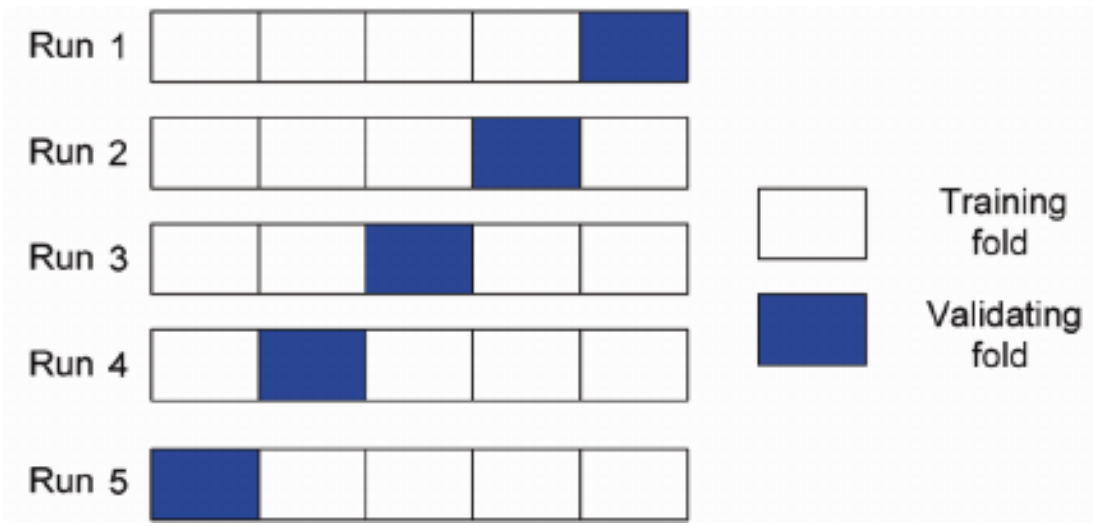
Disavantages of hold-out cross validation

- "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 (usually $k = 10$)
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)

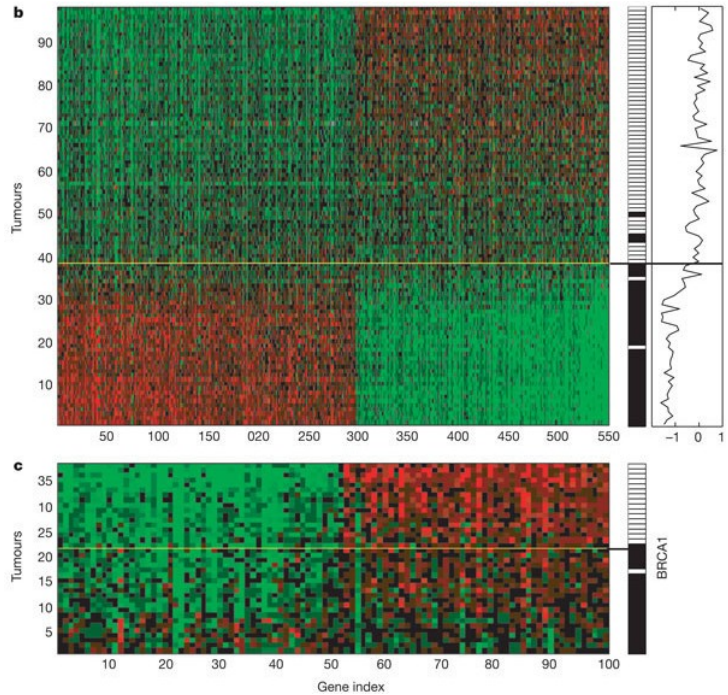
Cross validation can also be used to evaluate a single model.

Feature selection

Some supervised learning tasks involve a large number of features.

Example: microarray data analysis

- Each training example (tumor cases) contains thousands of features (gene expressions) , i.e. ($m \ll n$)
- Many gene expressions are correlated
- Many are not related to the disease



Expression data matrix of the 98 sporadic tumours across 550 optimal ER reporter genes. [van 't Veer et al, Nature 2002]

Feature selection methods

Feature selection: removes redundant and irrelevant features to improve learning accuracy and efficiency.

- **Wrapper model approach**: repeatedly make calls to the learning algorithm and evaluate on different subsets. good selection result, but computationally expensive
- **Filter approach**: select features based on a simple heuristic score function. computationally cheaper

Wrapper model

Forward Search

1. Initialize feature set $F = \{\}$
2. Repeat $\{$ $\leftarrow$ *terminate after finding the desired num. of features*
   - For each $i = 1, \ldots, n$ if $i \notin F$, use cross validation on feature subset $F_i = F \bigcup \{i\}$
   - Set F to be the best feature subset

   $\}$
3. Output feature subset F

Backward search starts with all features $F = 1, 2, \ldots, n$, repeatedly delete features one at a time.

Feature selection: Filter approach

Select k features based on a simple heuristic score function $S(i)$.

Example: Correlation Criteria

Rank features x_i by their correlations with $\vec{y}$:

$$S(i) = \frac{cov(x_i, y)}{\sqrt{var(x_i)var(y)}}$$

Example: Mutual information Criteria

Rank features x_i by their mutual information with $\vec{y}$:

$$MI(x_i, y) = \sum_{x_i \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x_i, y) \log \frac{p(x_i, y)}{p(x_i), p(y)}$$

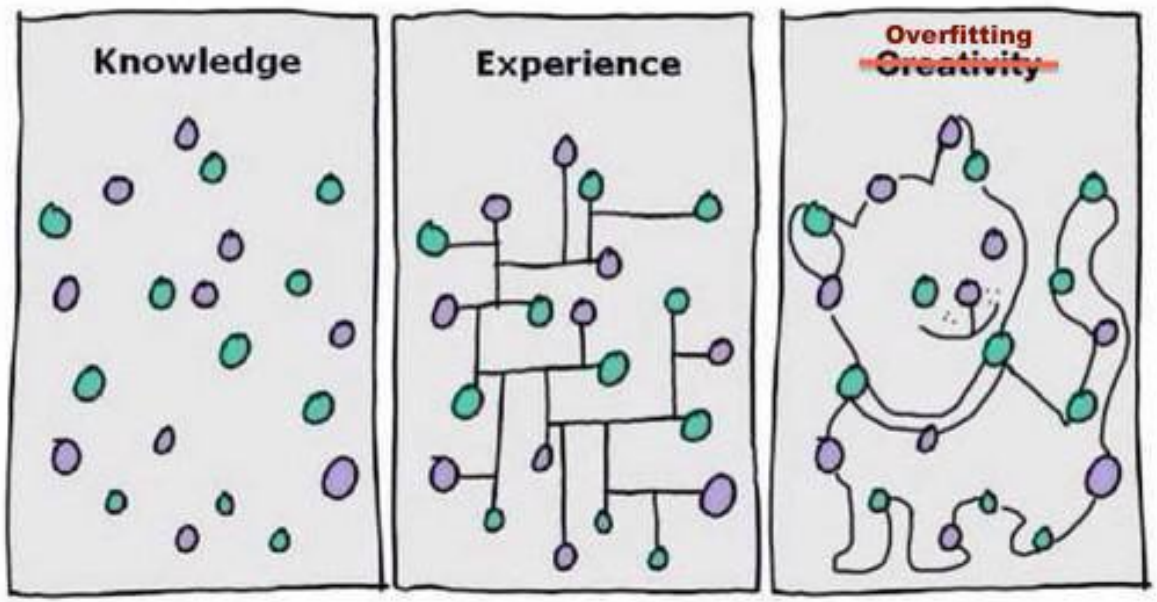
Assume x_i and y are both discrete valued.

How to chose k? use cross validation

Model Selection Summary

- Cross validation
  - Estimate how well the model runs on test data
  - Prevents over fitting
- Feature selection
  - A special case of model selection
  - Difference from feature extraction: feature selection do not change the representation of the original features

More on generalization error and hypothesis testing: statistical learning theory (next lecture)


Knowledge
Experience
Overfitting
Creativity

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

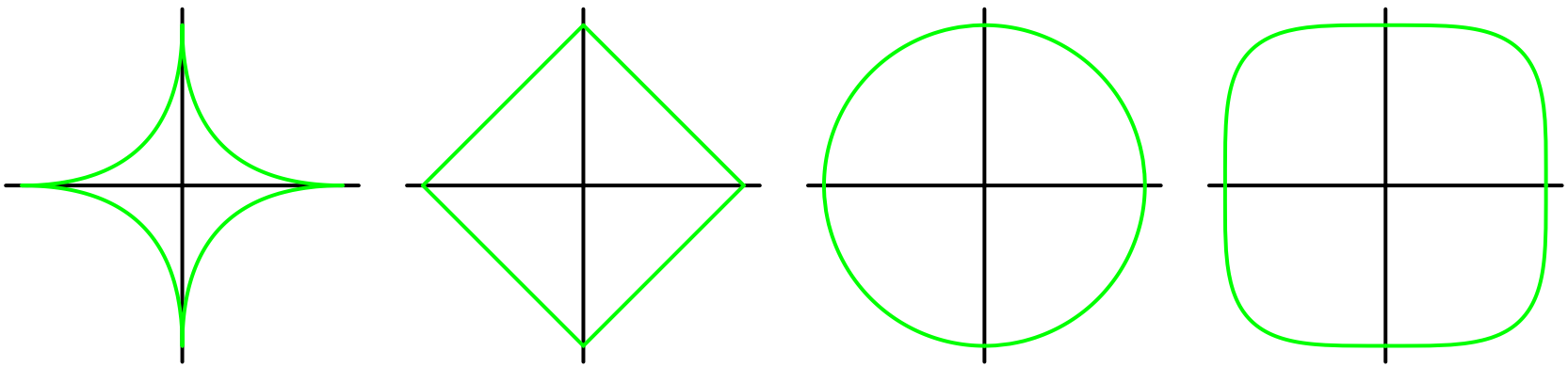
Parameter Norm Penalty

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

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



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), $\tilde{\theta}_{OLS} = (X^TX + \lambda I)^{-1}(X^TY)$

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

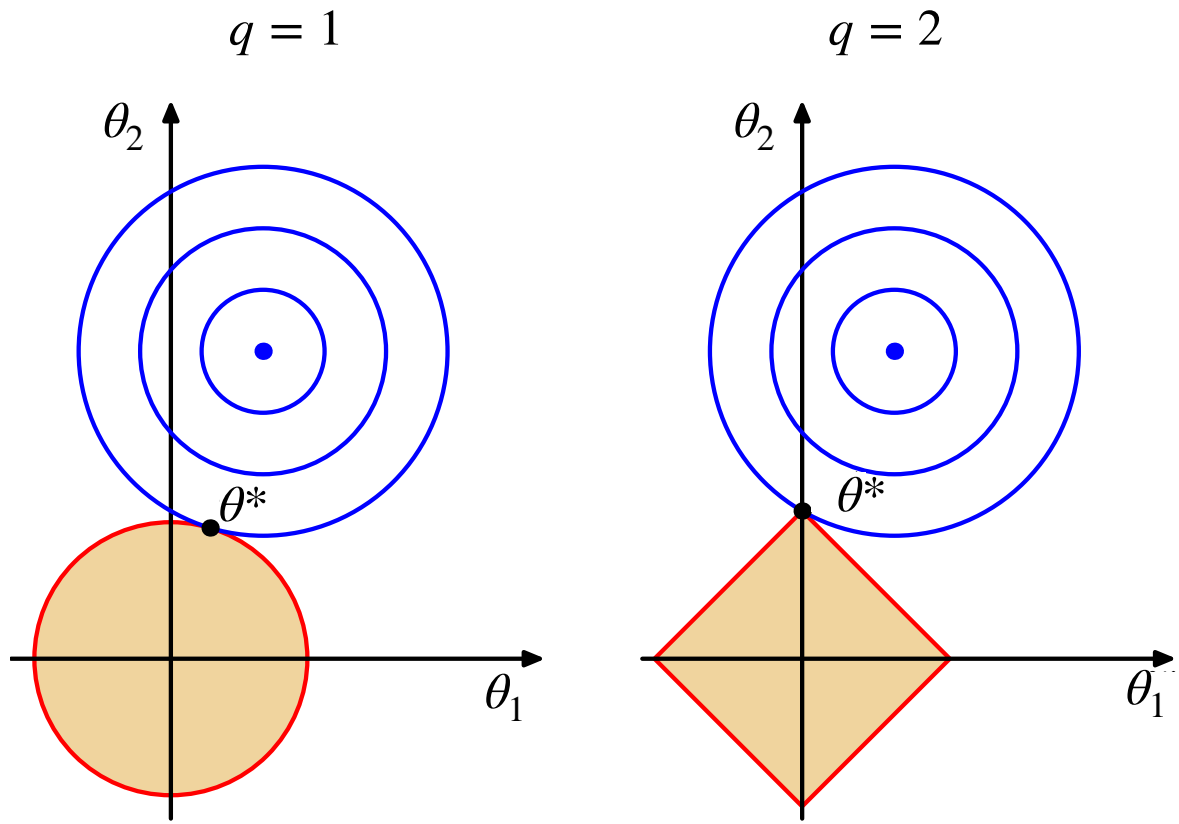
Solving $\min_\theta \tilde{J}(X, Y; \theta) = J(X, Y; \theta) + \frac{\lambda}{2}\sum_{j=1}^{n} |\theta_j|^q$ *is equivalent to*

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

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

L1 vs L2 parameter penalty

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

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

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

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

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

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

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

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

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}

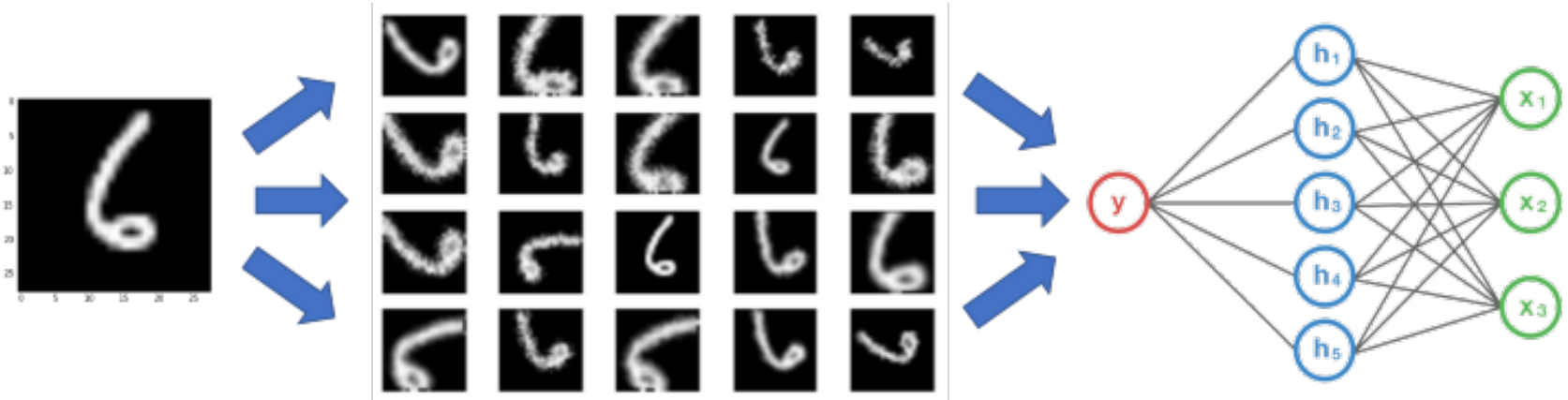
Regularization for neural networks

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.)



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

Generate images of different styles using GAN

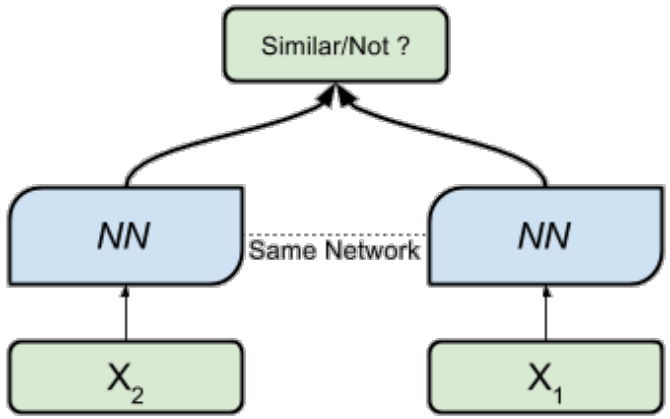
Shorten et. al. A survey on Image Data Augmentation for Deep Learning, 2019

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)

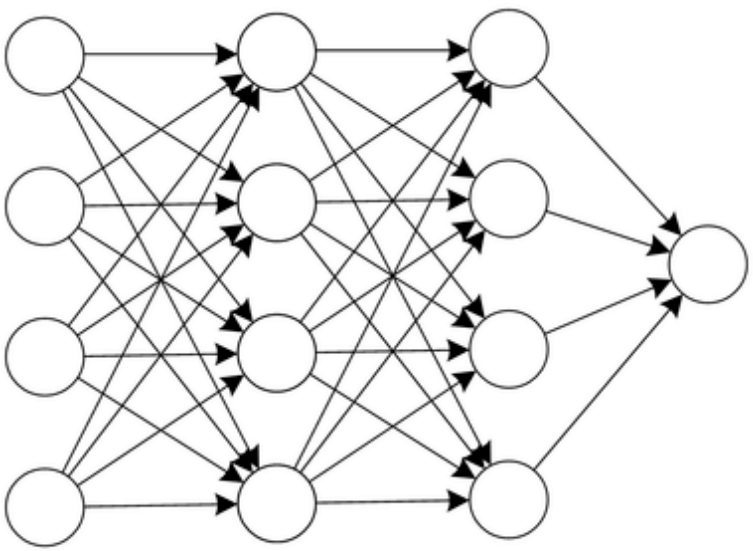
- Image features should be invariant to translation
- CNN shares parameters across multiple image locations.

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

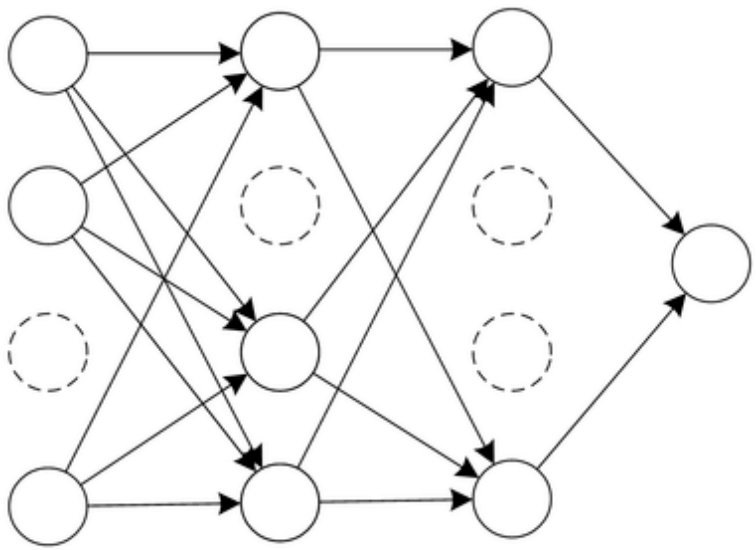
$$\Omega(\theta^A, \theta^B) = ||\theta^A - \theta^B||_2^2$$

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



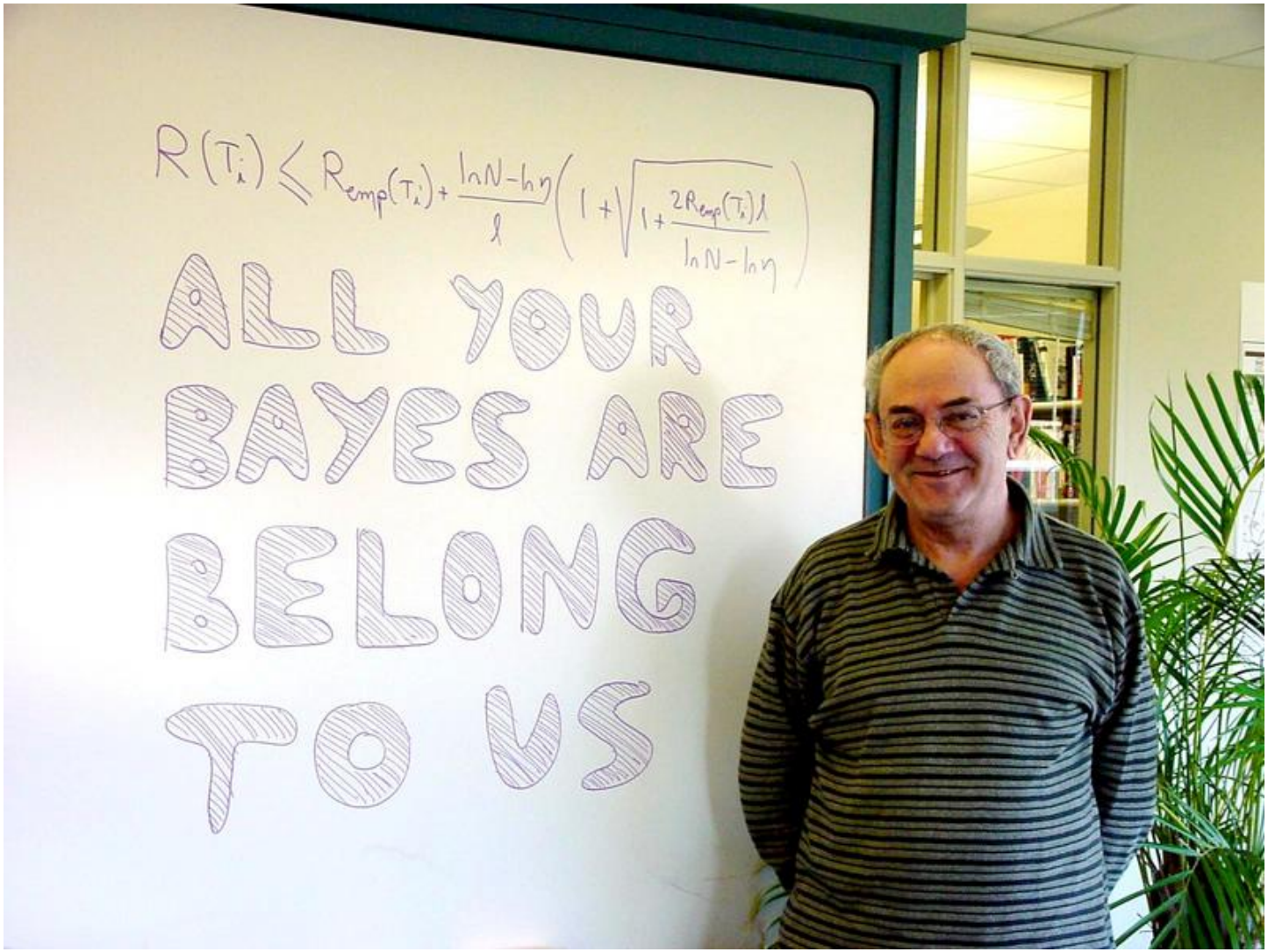
(a) Standard Neural Network



(b) Network after Dropout

Next lecture: learning theory

How to quantify generalization error?



Prof. Vladimir Vapnik in front of his famous theorem