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**PATTERN RECOGNITION  
AND MACHINE LEARNING  
CHAPTER  $\infty$ : SUMMARY**

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# Teaching Objectives

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- Fundamental knowledge about machine learning and pattern recognition, from Bayesian approaches to deep learning frameworks through lectures, quizzes and assignments
  - Machine learning system development methods with Python through labs and projects
  - Model-based and data-driven machine learning system design and integration skills through the final project, literature surveys and reports
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# Lecture Schedule

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Section 0	Course Introduction	
Section 1	Preliminary	(HW1)
Section 2	Probability Distributions	(HW2)
Section 3	Linear Regression and Classification	(HW3, HW4)
Section 4	Neural Networks	(HW5)
Section 5	Sparse Kernel Machine	(HW6)
<i>--Midterm Exam--</i>		
Section 6	Mixture Models and EM learning	(HW7)
Section 8	Sequential Data (Hidden Markov Model)	(HW8)
Section 9	Bayesian Networks	
Section 10	Markov Decision Process	
Section 11	Reinforcement Learning	
<i>--Final Exam--</i>		

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# Lab Schedule

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Section 0      Lab Introduction

Section 1      Preliminary

Section 2      Bayes

Section 3      Regression

*--Final Project Proposal--*

Section 4      Decision Tree

Section 5      Support Vector Machine

Section 6      Convolution Neural Network

Section 7      K-Mean Clustering

Section 8      Gaussian Mixture Model

Section 9      Markov Decision Process

Section 10     Reinforcement Learning

*--Final Project Report--*

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# Final Projects

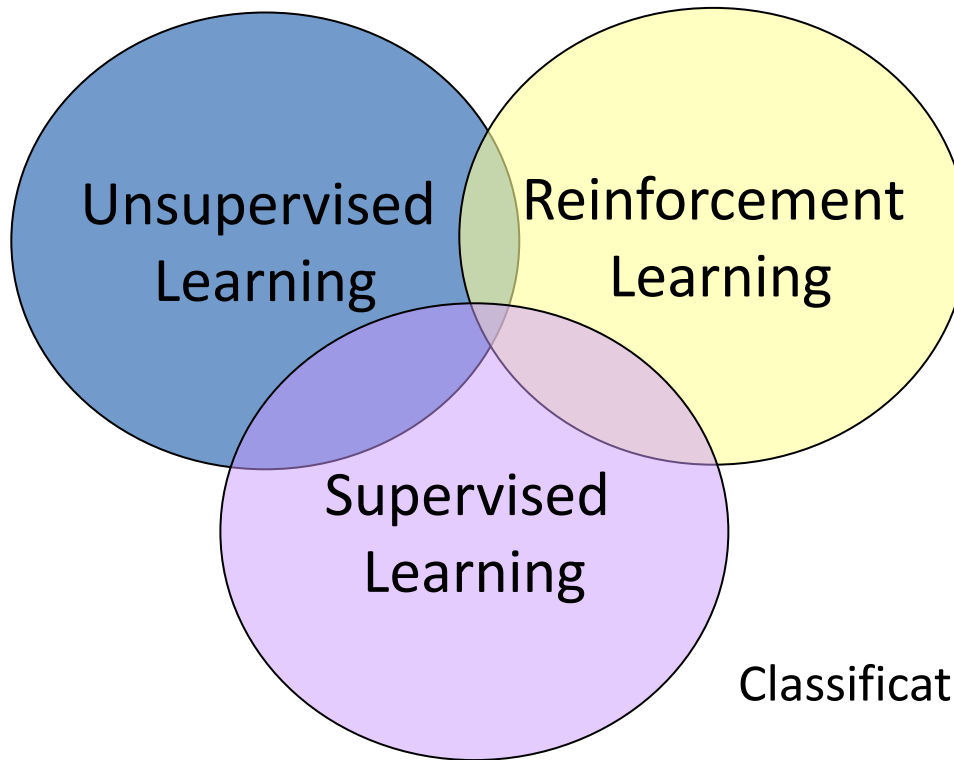
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- [1] Reinforcement learning based planning using a self-driving car simulator
  - [2] Segmentation of 2D/3D measurements for self-driving applications
  - [3] Detection and recognition of traffic signs for self-driving applications
  - [4] Detection and tracking of 2D/3D objects for self-driving applications
  - [5] Generation of annotated self-driving datasets with the CARLA simulator
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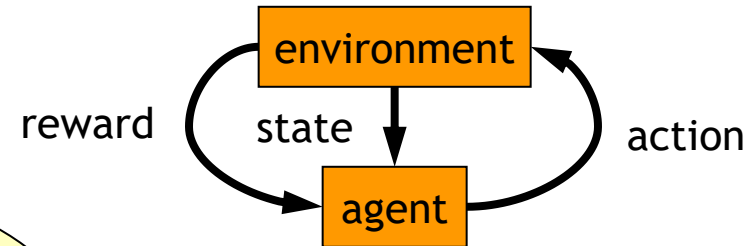
# Machine Learning

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Clustering  
Dimension reduction

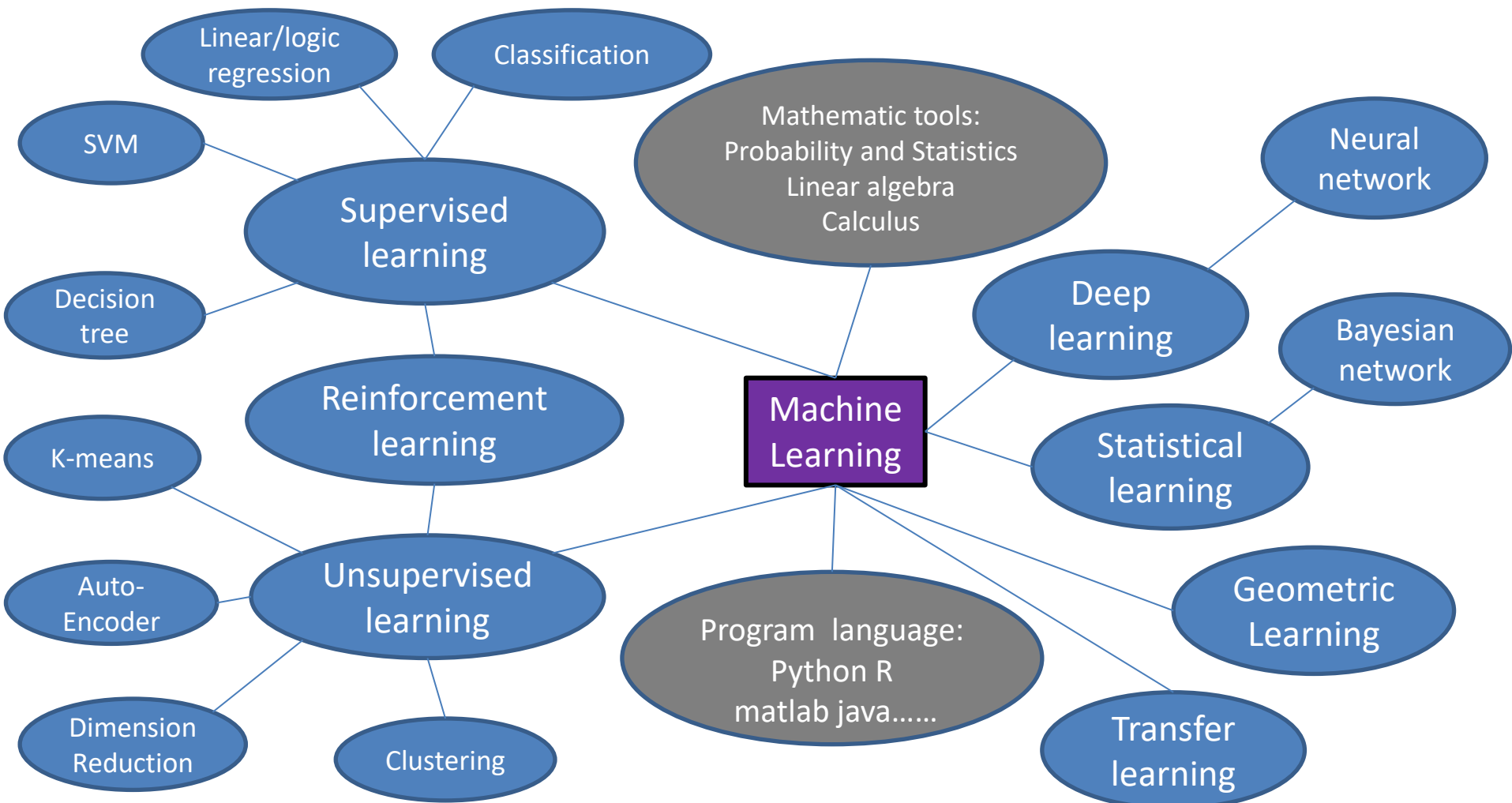


Classification, Regression



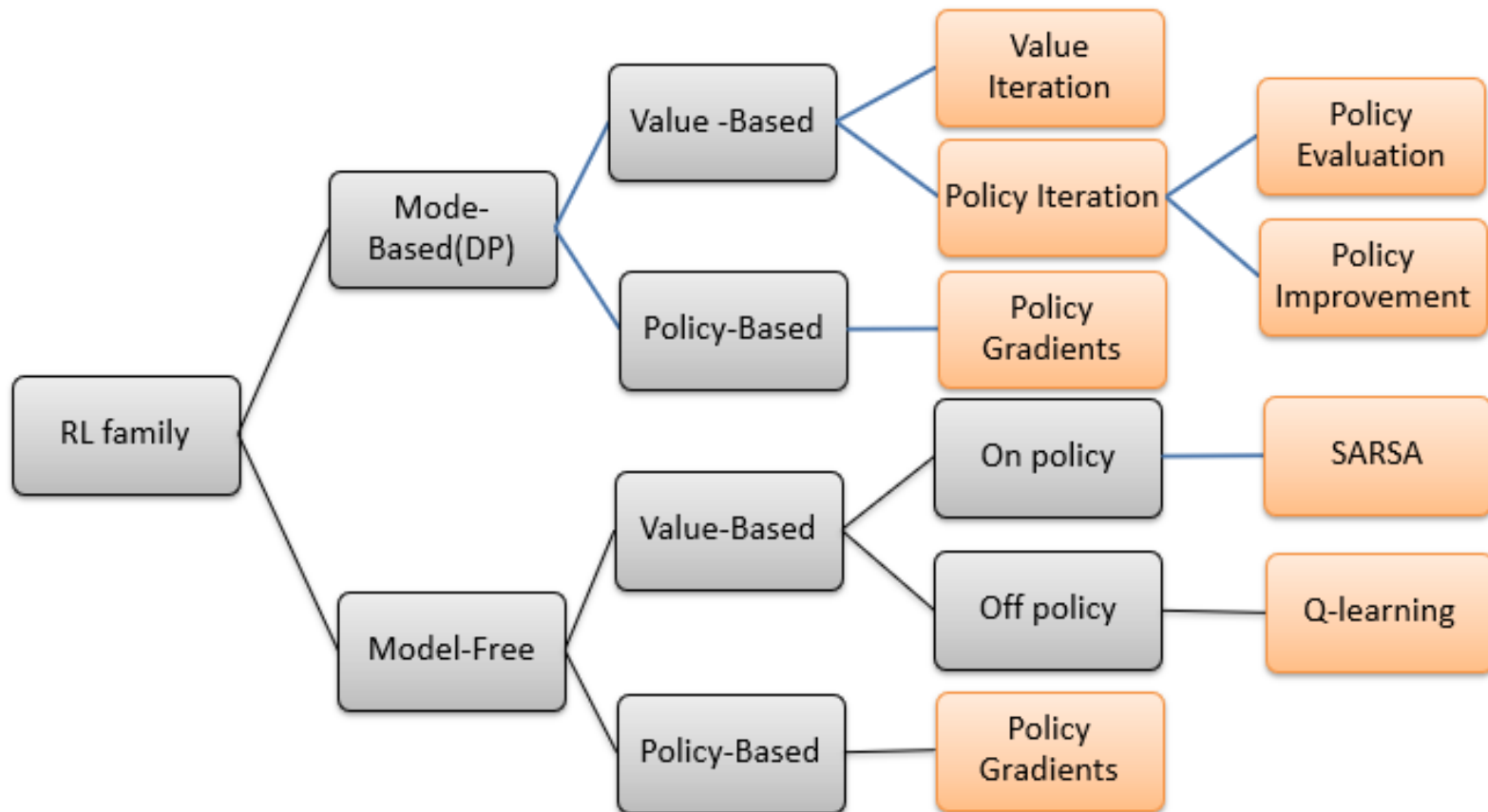
# Framework

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# Reinforcement Learning

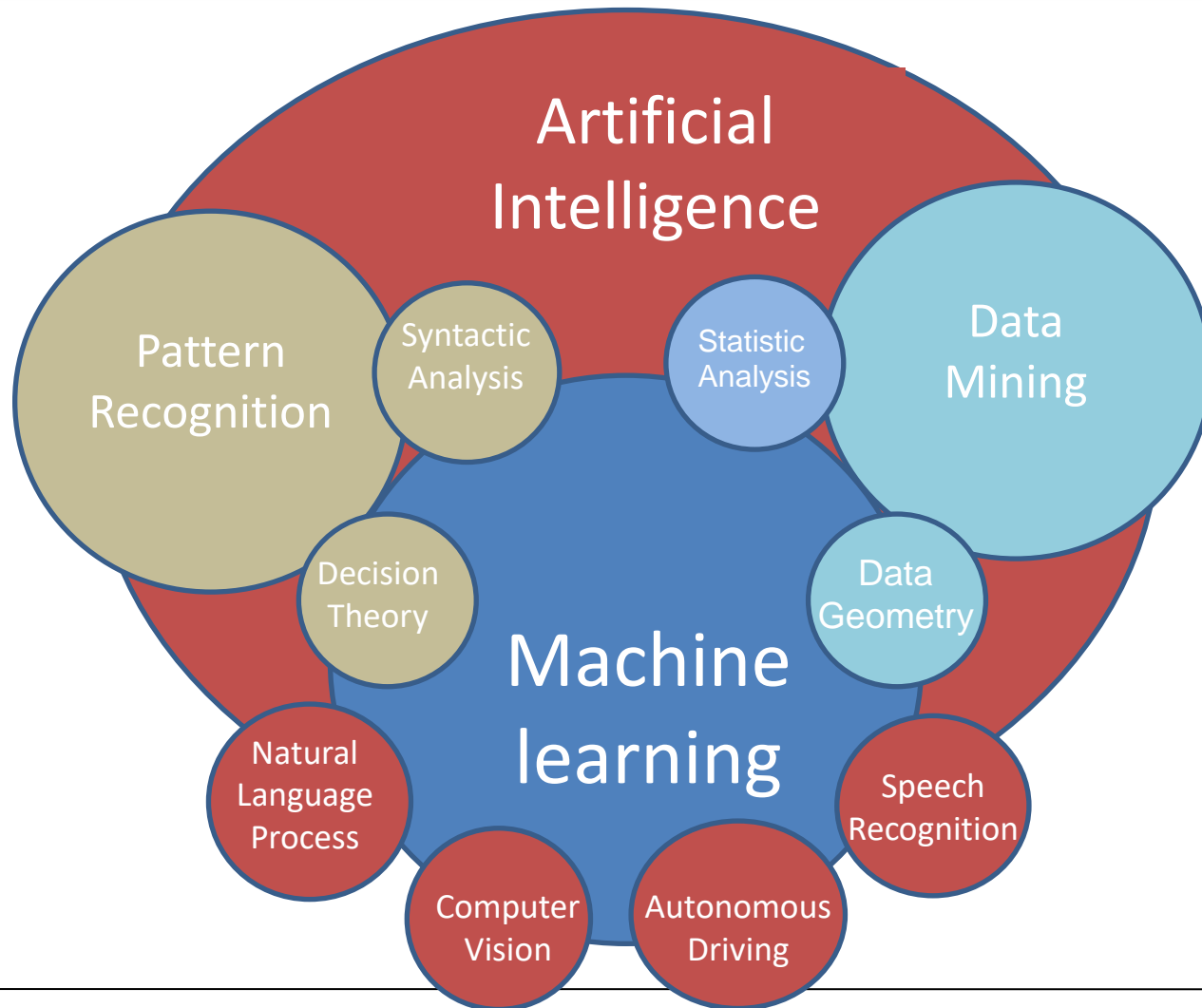
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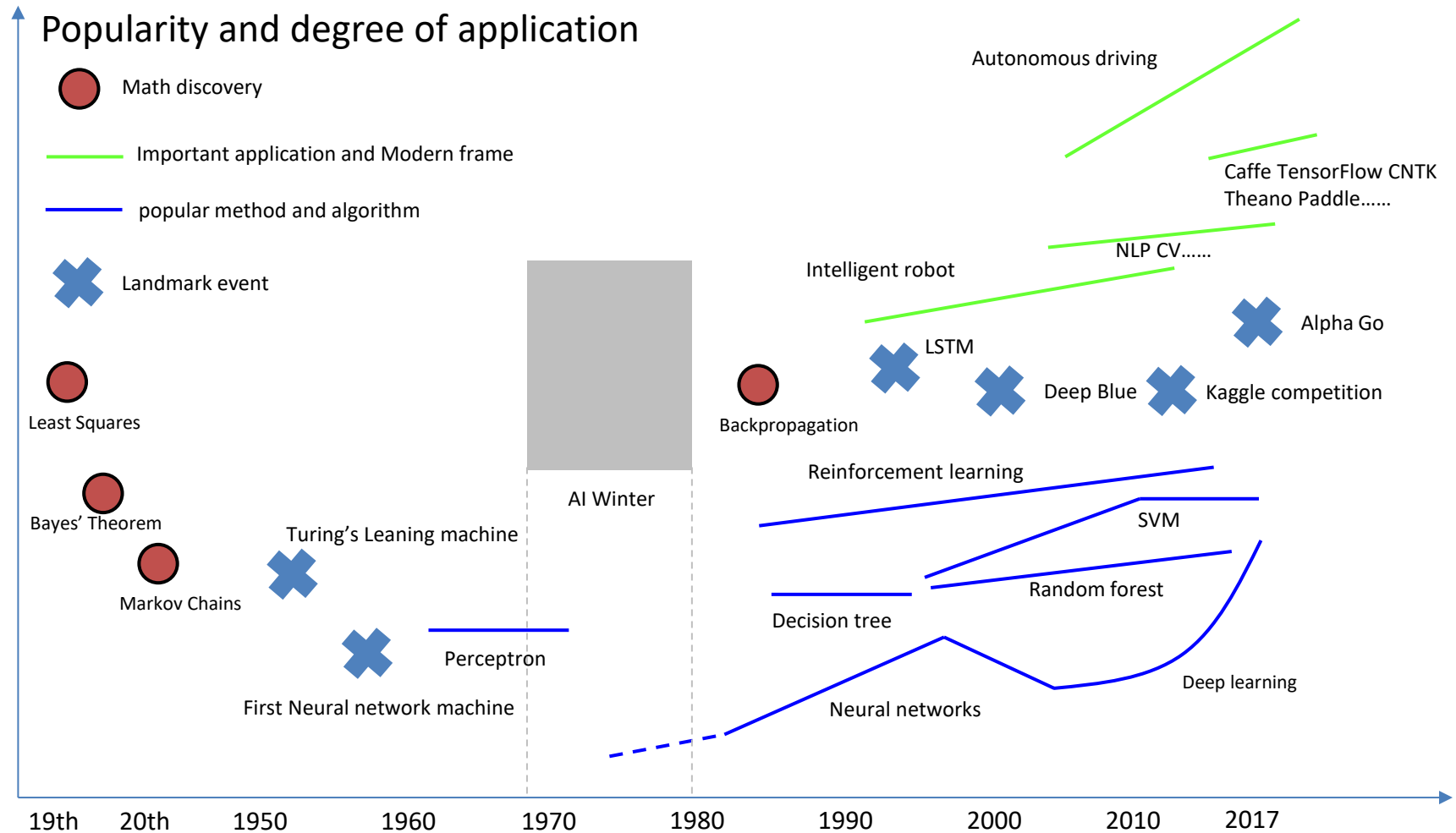


# The Whole Picture

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# History



# Machine learning

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- **Machine Learning**—minimization of some loss function for generalizing data sets with models.
  - **Datasets** —annotated, indexed, organized
  - **Models** —tree, distance, probabilistic, graph, bio-inspired
  - **Optimization** —algorithms can minimize the loss.
-

# Datasets

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- Collection
  - Storage
  - Annotation
  - Indexing
  - Organization
  - Access
-

# Simulators

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- Data visualization
  - Generate training data
  - Algorithm evaluation
-

# Benchmark Metrics

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- System functionalities
  - System scalability
  - System robustness
  - System efficiency
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# Models

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- Tree Models
  - Distance-based Models
  - Probabilistic Models
  - Neural Network Models
  - Graph-based Models
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# Models

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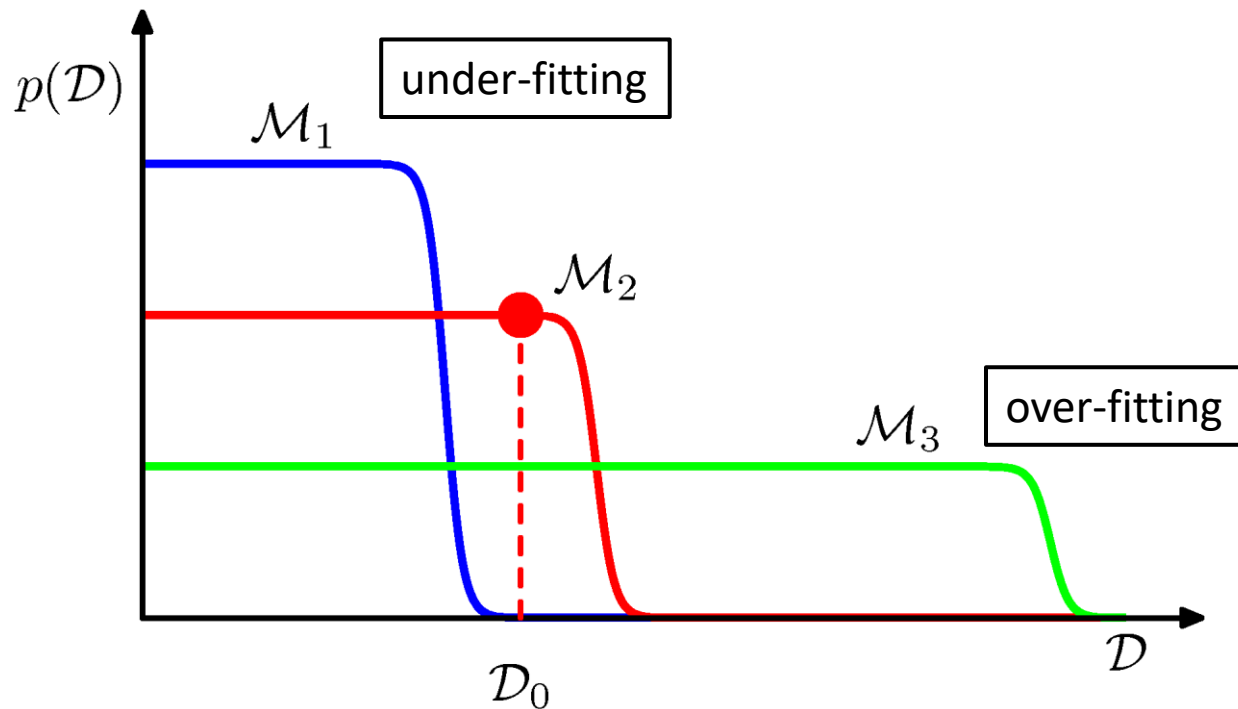
- Boosting
- Ensemble Learning



# Model Comparison

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- ❑ Matching data and model complexity



# Machine learning and Optimization

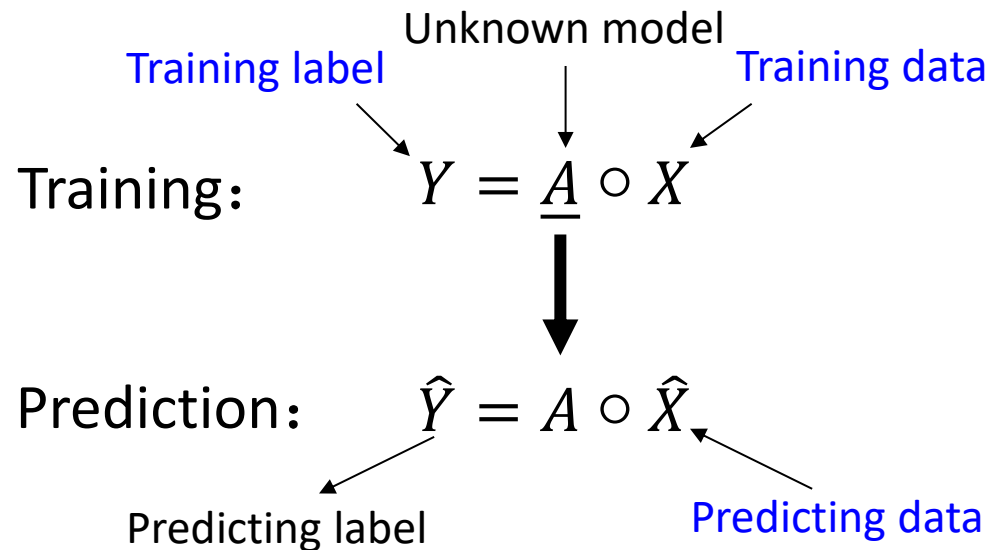
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- **Machine Learning**—minimization of some loss function for generalizing data sets with models.
  - **Datasets** —annotated, indexed, organized
  - **Models** —tree, distance, probabilistic, graph, bio-inspired
  - **Optimization** —algorithms can minimize the loss.
-

# Problem Statement

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- **Problem:** Predict the label  $\hat{Y}$  and data  $\hat{X}$  with training set  $(X, Y)$  ?



$\left\{ \begin{array}{l} Y \text{ and } X \text{ is known: supervised learning} \\ Y \text{ or } X \text{ is unknown: unsupervised learning} \end{array} \right. \quad \left\{ \begin{array}{l} Y, \hat{Y} \text{ are continuous: Regression} \\ Y, \hat{Y} \text{ are discrete: classification} \end{array} \right.$

$Y \text{ is known and } \text{Dim}(Y) > \text{Dim}(X) : \text{ dimensionality reduction}$

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# Optimization

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- Finding (one or more) minimizer of a function subject to constraints

$$\arg \min_x f_0(x)$$

$$s.t. f_i(x) \leq 0, i = \{1, \dots, k\}$$

$$s.t. h_j(x) = 0, j = \{1, \dots, l\}$$

- Most of the machine learning problems are, in the end, optimization problems
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# Lagrange Method

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- Minimize an object function s. t. constraints of inequality

$$\min_x f(x) \quad \text{s.t.} \quad g(x) \geq 0$$

- By Introducing a Lagrange multiplier  $\lambda \geq 0$ , then we will have

$$\min_x \max_{\lambda \geq 0} \{\mathcal{L}(x, \lambda) = f(x) - \lambda g(x)\}$$

- When certain conditions are satisfied, its dual problem is

$$\max_{\lambda \geq 0} \min_x \{\mathcal{L}(x, \lambda) = f(x) - \lambda g(x)\}$$

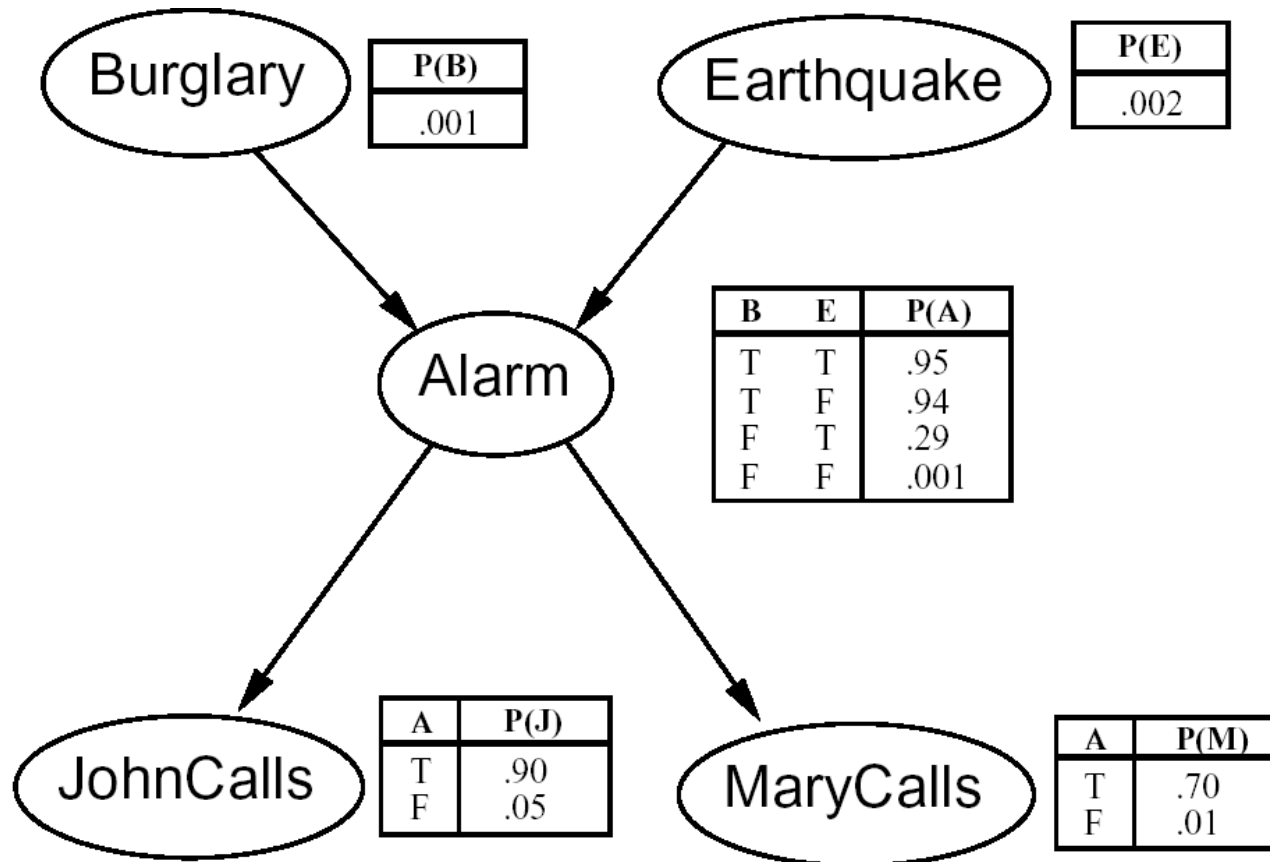
- By setting derivatives of  $\mathcal{L}$  w.r.t.  $x$  equal to 0, we will have

$$x = h(\lambda), \text{ and then the problem becomes } \lambda^* = \max_{\lambda \geq 0} Q(\lambda)$$

- Finally,  $x^* = h(\lambda^*)$  is the solution
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# Bayes

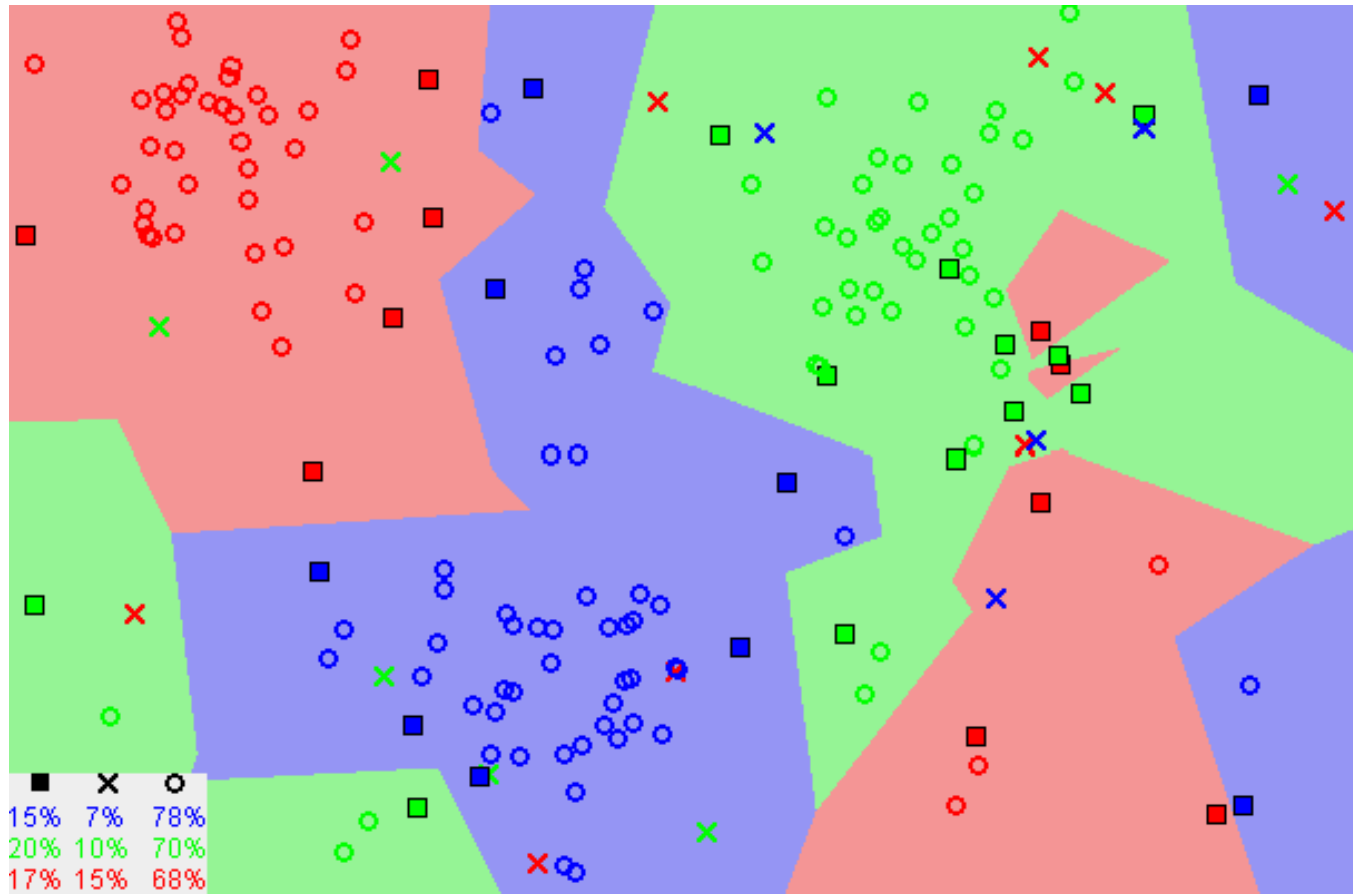
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# K-Nearest Neighbors

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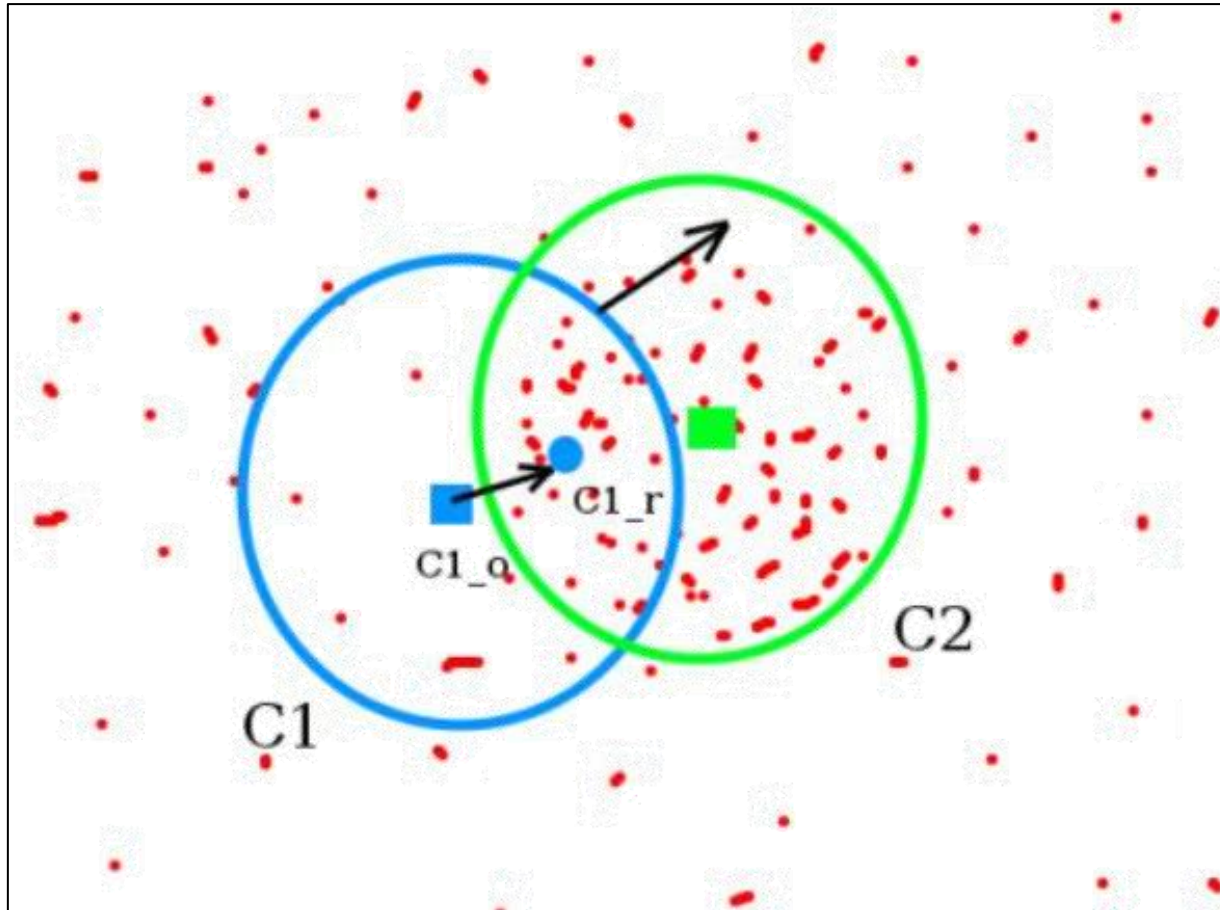
- Use training data for classification



# K-Means

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## □ Mean-shift

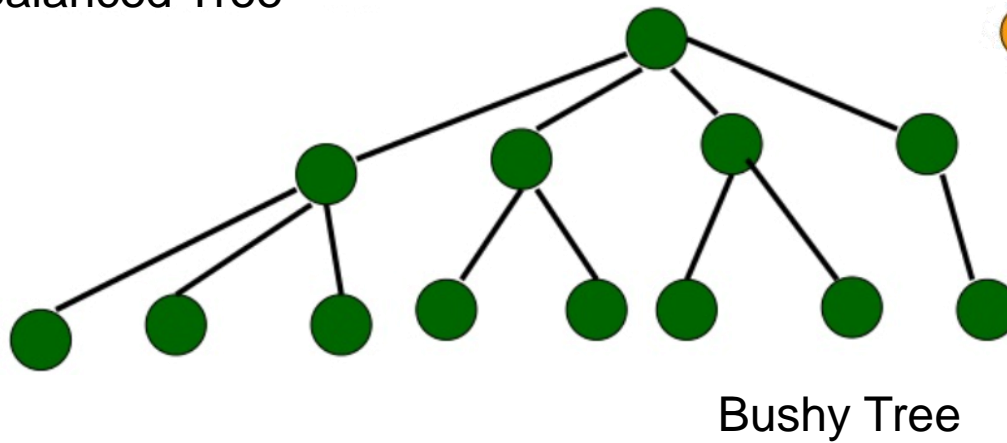
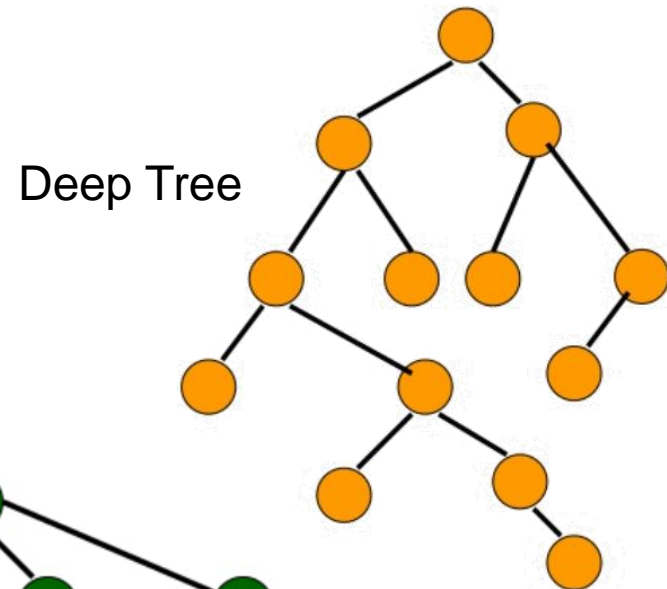
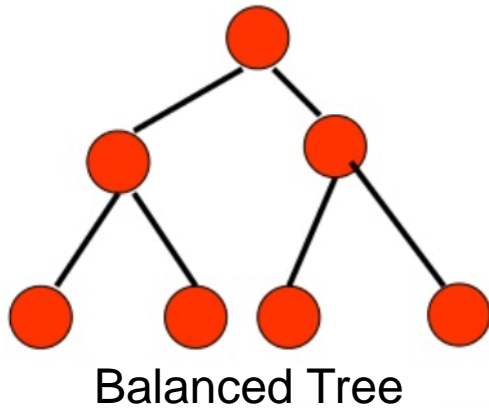




# Decision Tree

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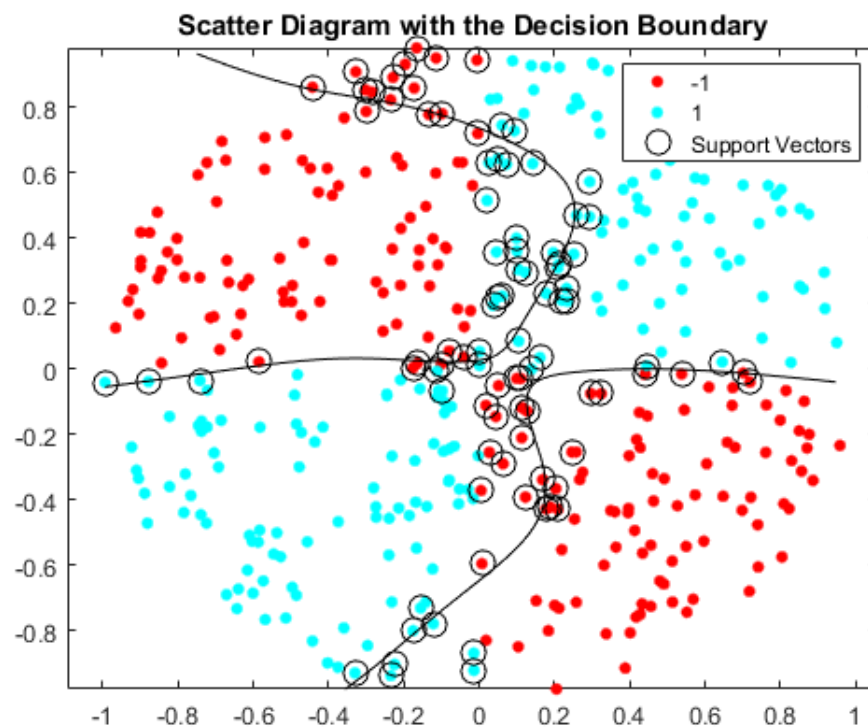
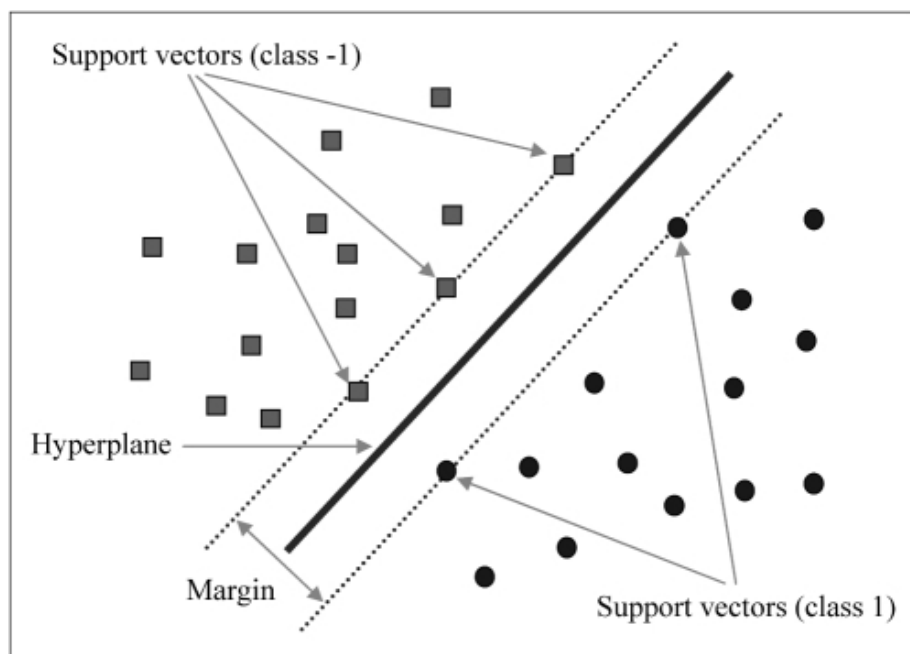
## ▣ Types of Decision Tree:



# SVM

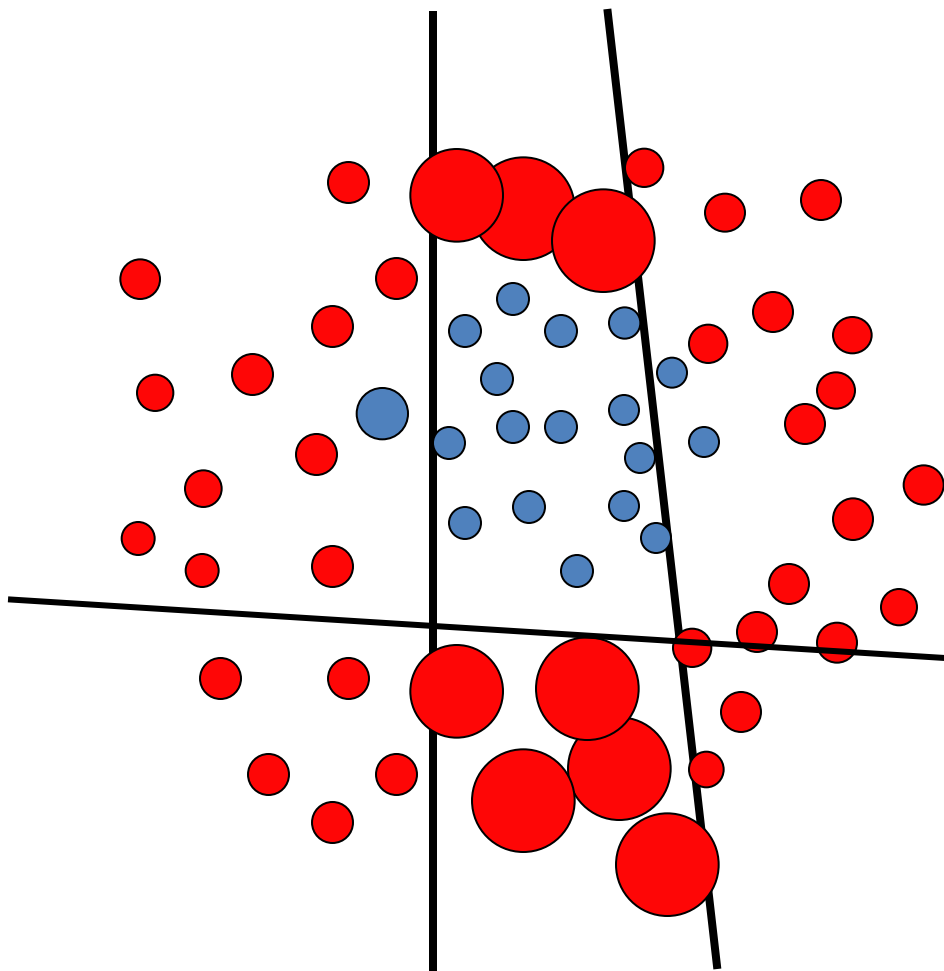
□ Linear SVM:

$$\arg \min_w \sum_{i=1}^n \|w\|^2 + C \sum_{i=1}^n \xi_i$$
$$\text{s.t. } 1 - y_i x_i^T w \leq \xi_i$$
$$\xi_i \geq 0$$



# Boosting

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Each data point has  
a class label:

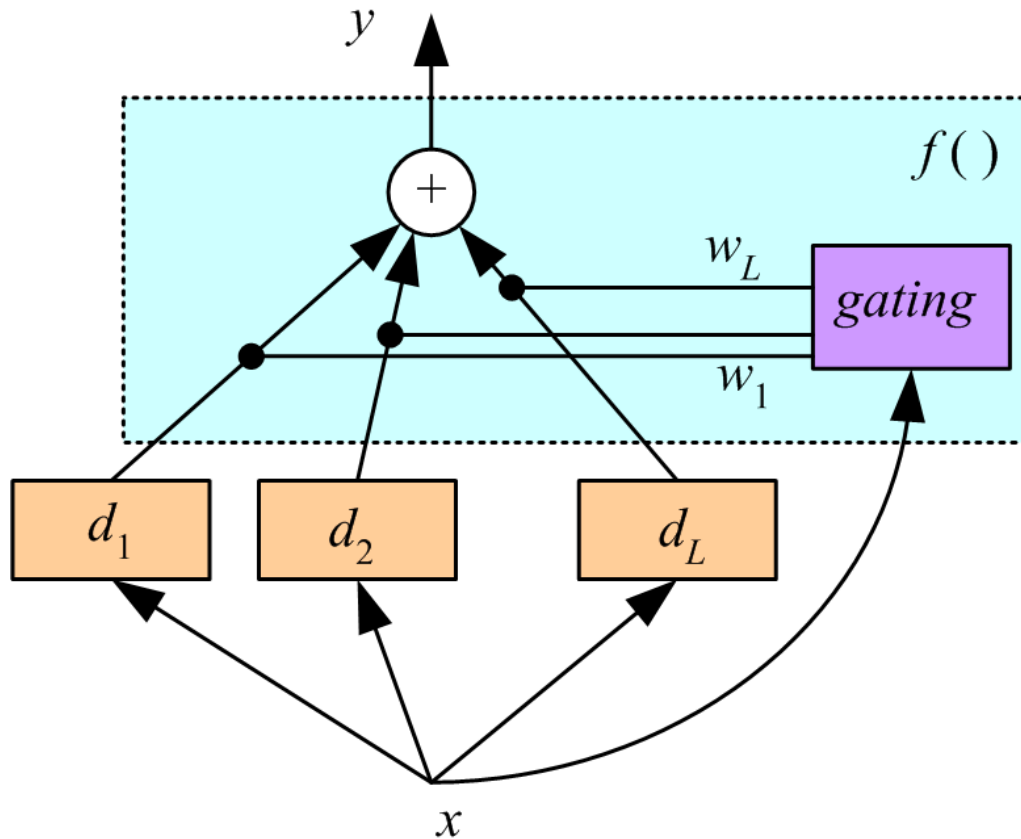
$$y_t = \begin{cases} +1 & (\text{red circle}) \\ -1 & (\text{blue circle}) \end{cases}$$

**We update the weights:**

$$w_t \leftarrow w_t \exp\{-y_t H_t\}$$

# Ensemble Learning

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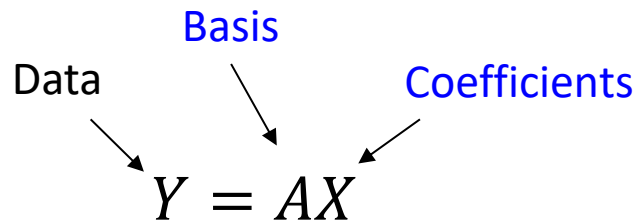


$$y = \sum_{j=1}^L w_j d_j$$

# Linear Statistical Learning

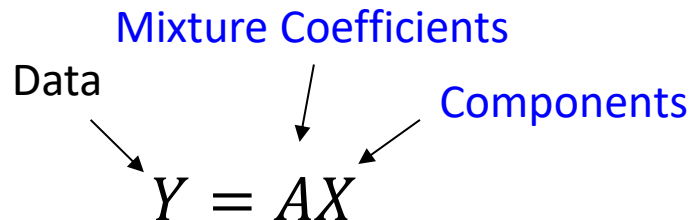
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## ■ PCA



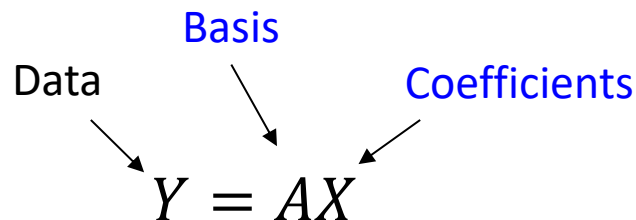
$$A_i \perp A_j$$

## ■ ICA



$$\max I(X)$$

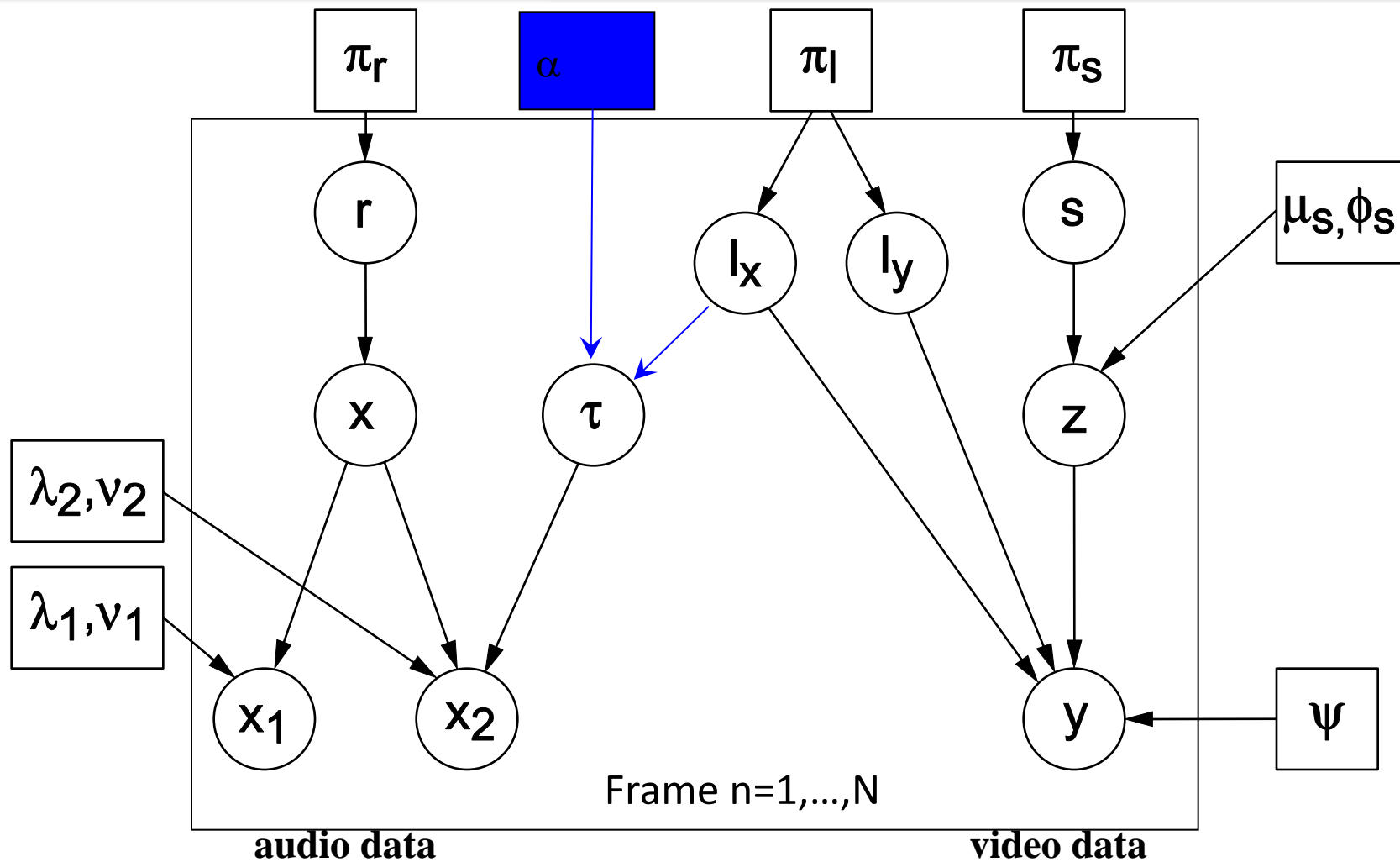
## ■ NMF



$$A, X > 0$$

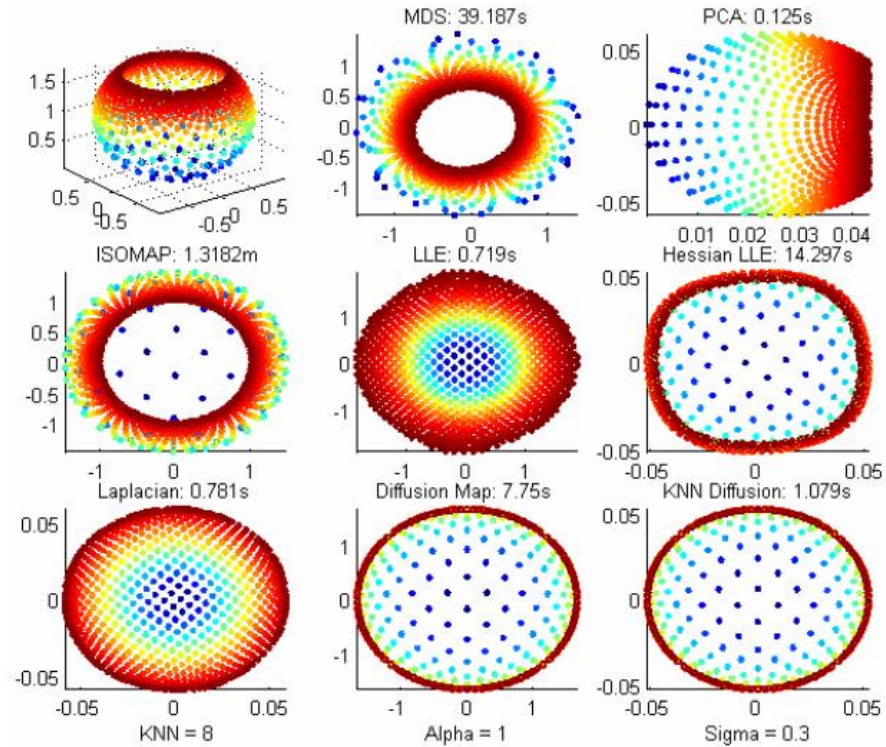
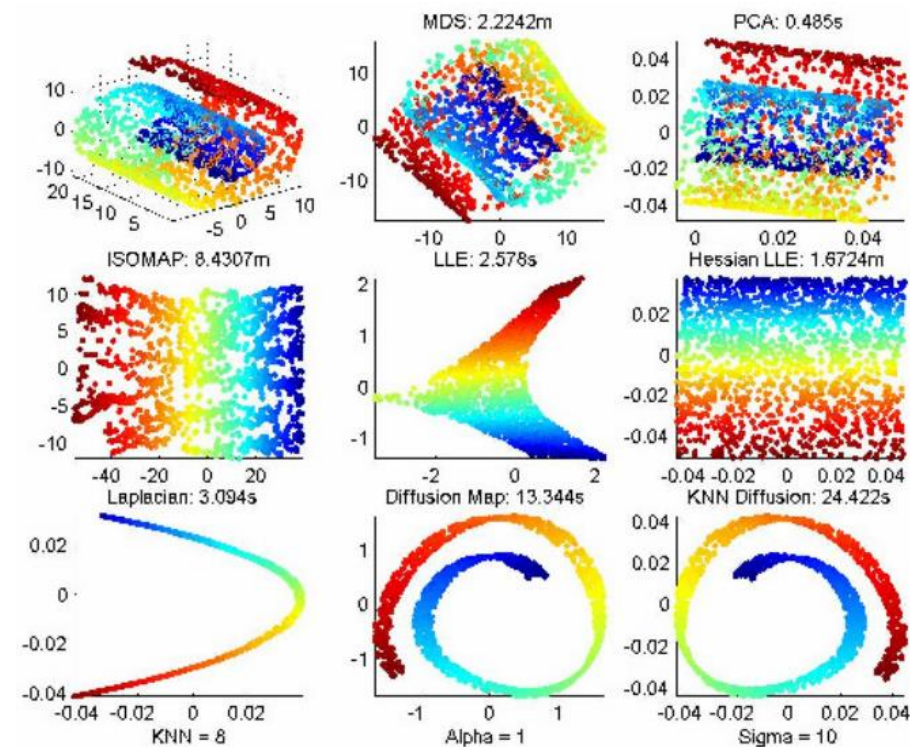
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# Bayesian Networks

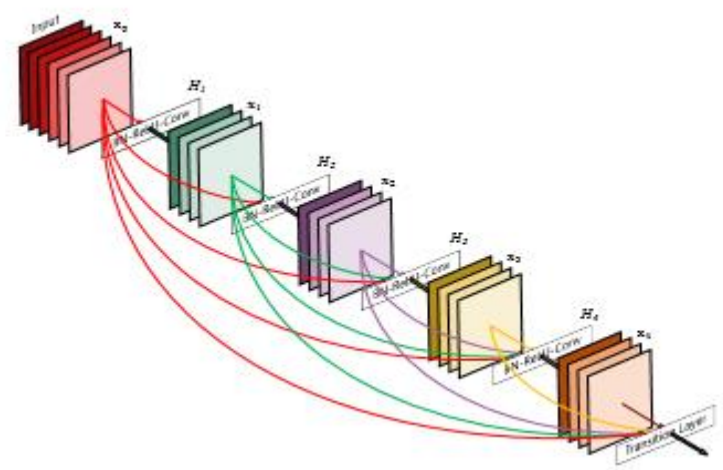
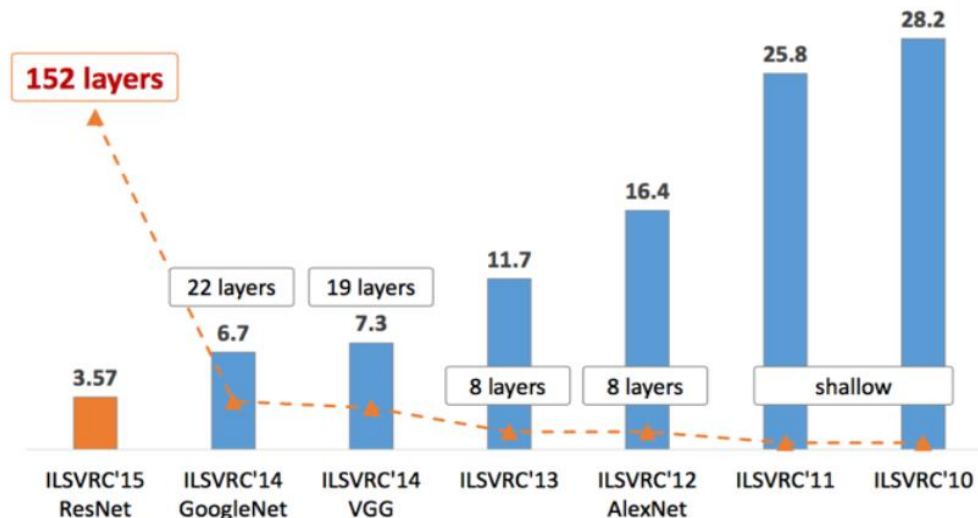


# Nonlinear Statistical Learning

## ■ Manifold learning



# Deep Neural Networks

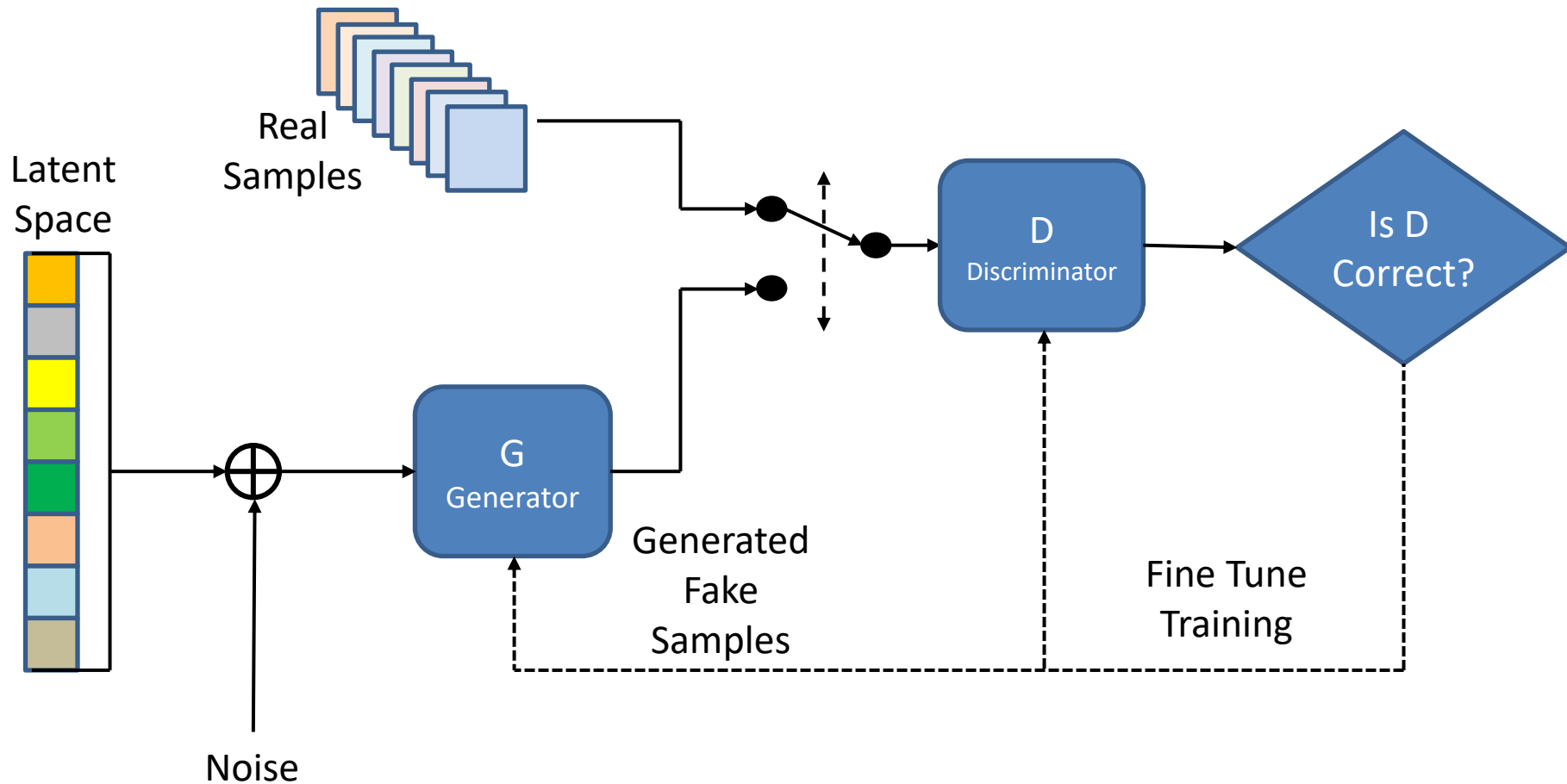


- Task: recognition
- Dataset: ILSVRC
- Huang G, Liu Z, Weinberger K Q, et al. Densely connected convolutional networks[J]. arXiv preprint arXiv:1608.06993, 2016.

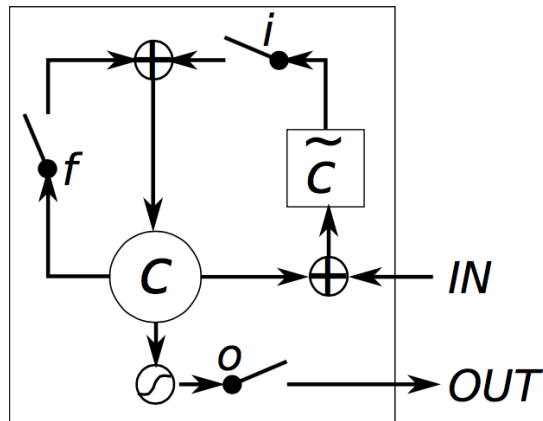
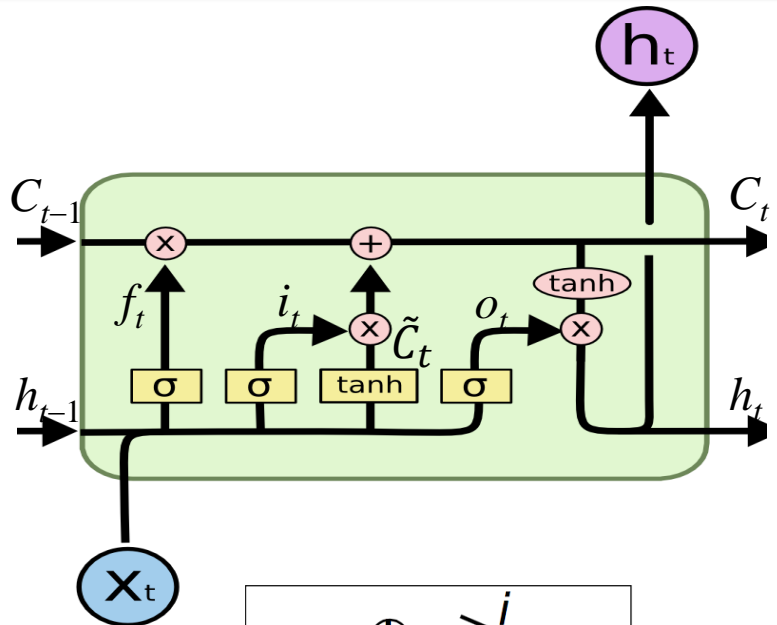


# Generative Adversarial Networks

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# Long Short Term Memory



$$f_t = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f)$$

$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i)$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$$

$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

$$o_t = \sigma(W_o \cdot [h_{t-1}, x_t] + b_o)$$

$$h_t = o_t * \tanh(C_t)$$

$C_t$ : cell state

$\tilde{C}_t$ : cell state prediction

$f_t$ : forget gate

$i_t$ : input gate

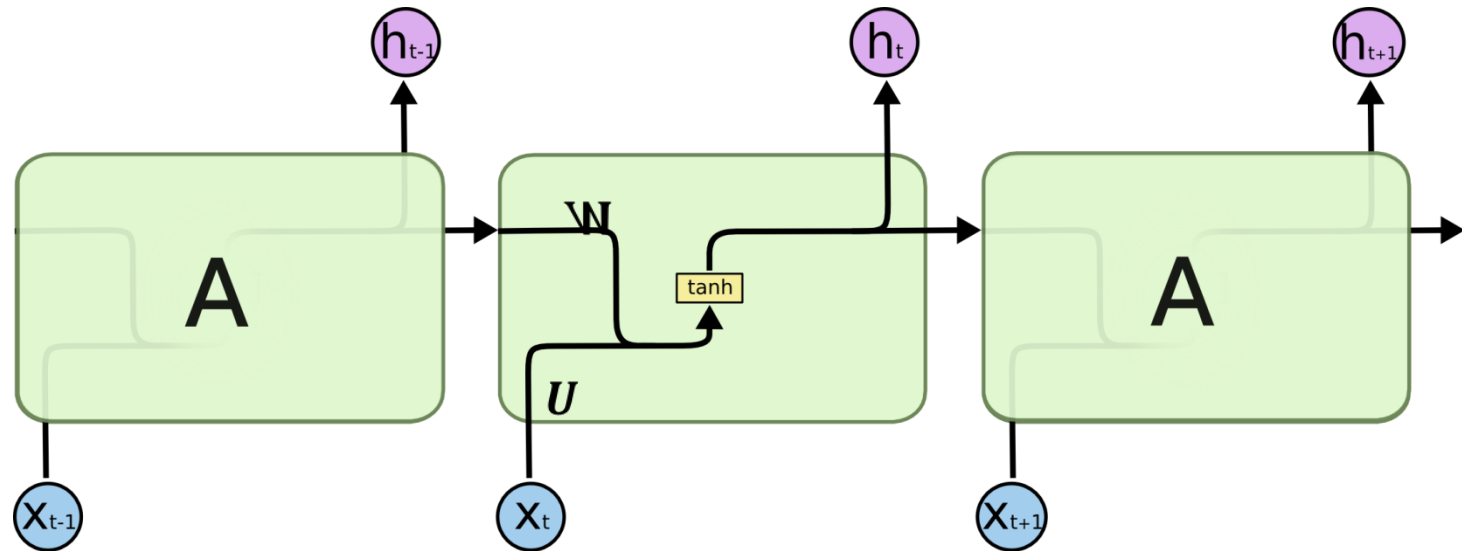
$o_t$ : output gate

$h_t$ : output

$x_t$ : input

# Recurrent Neural Networks

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$$h_t = f(Ux_t + Wh_{t-1} + b)$$

$h_t$ : output

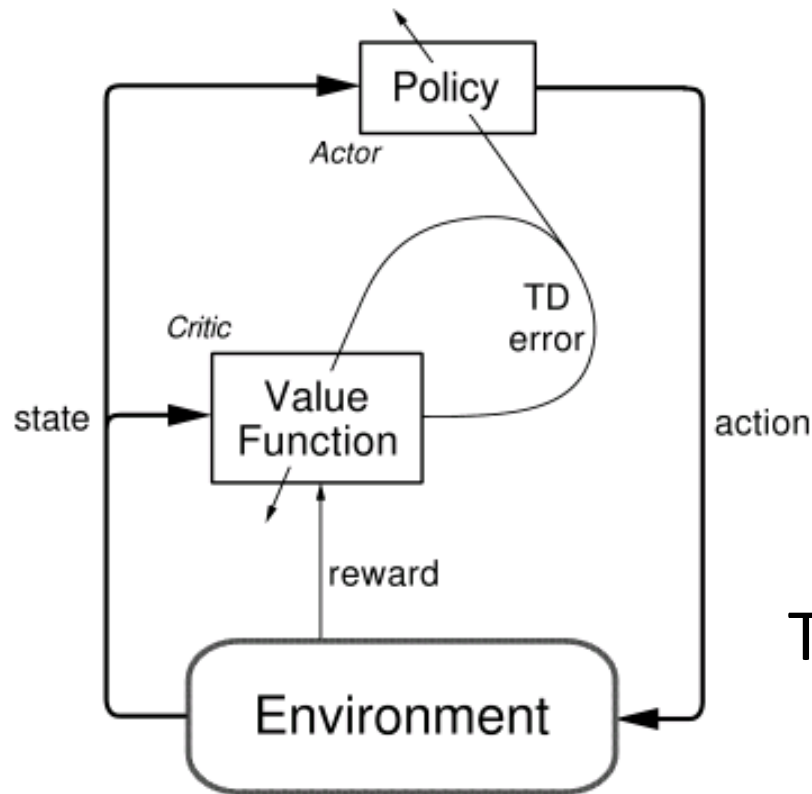
$x_t$ : input

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# Reinforcement Learning

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- State, action, and Reward

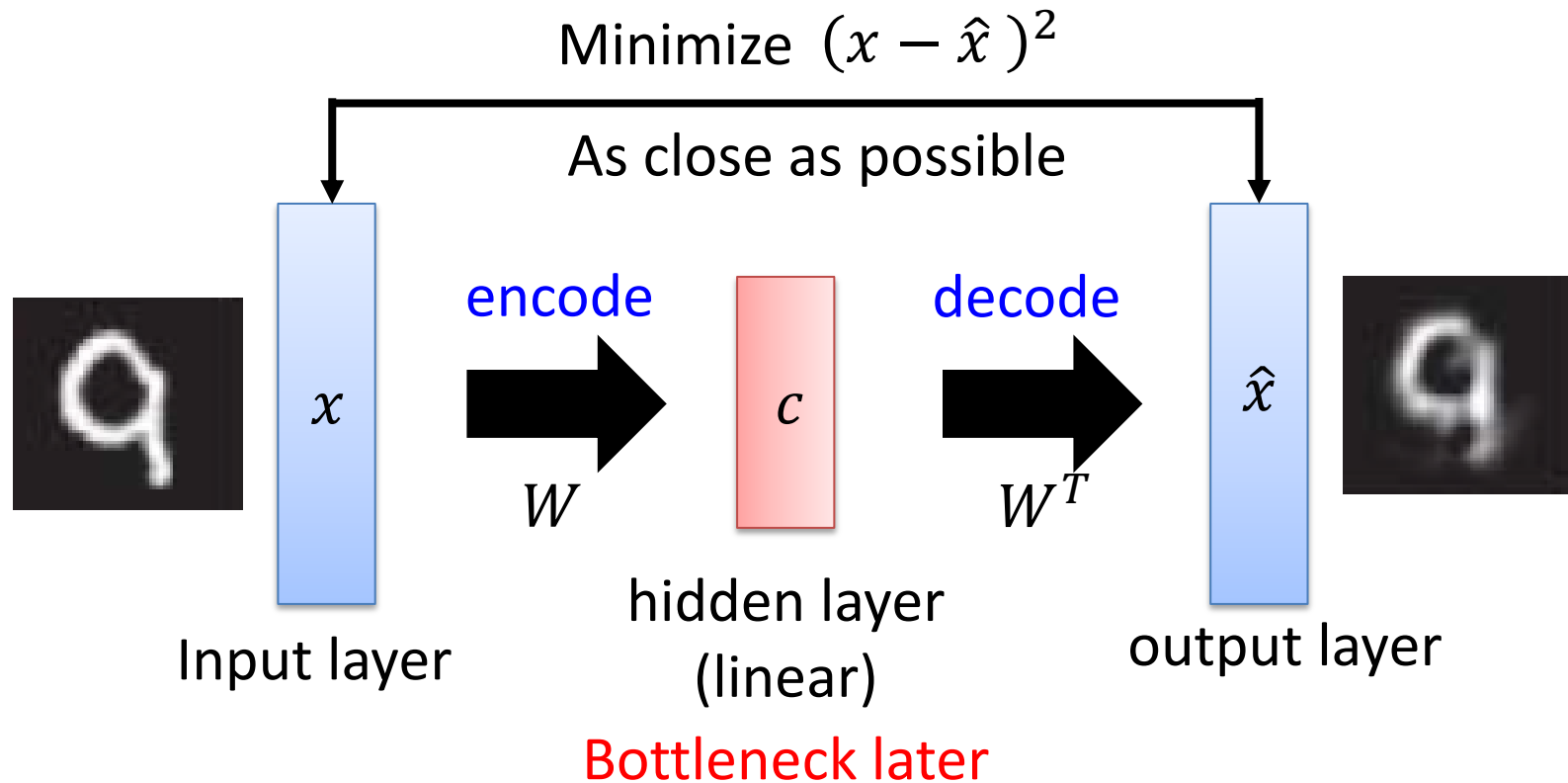


Update: Policy Function  
Value Function

TD Error: Temporal Difference  
between Real Reward  
and Estimated Reward

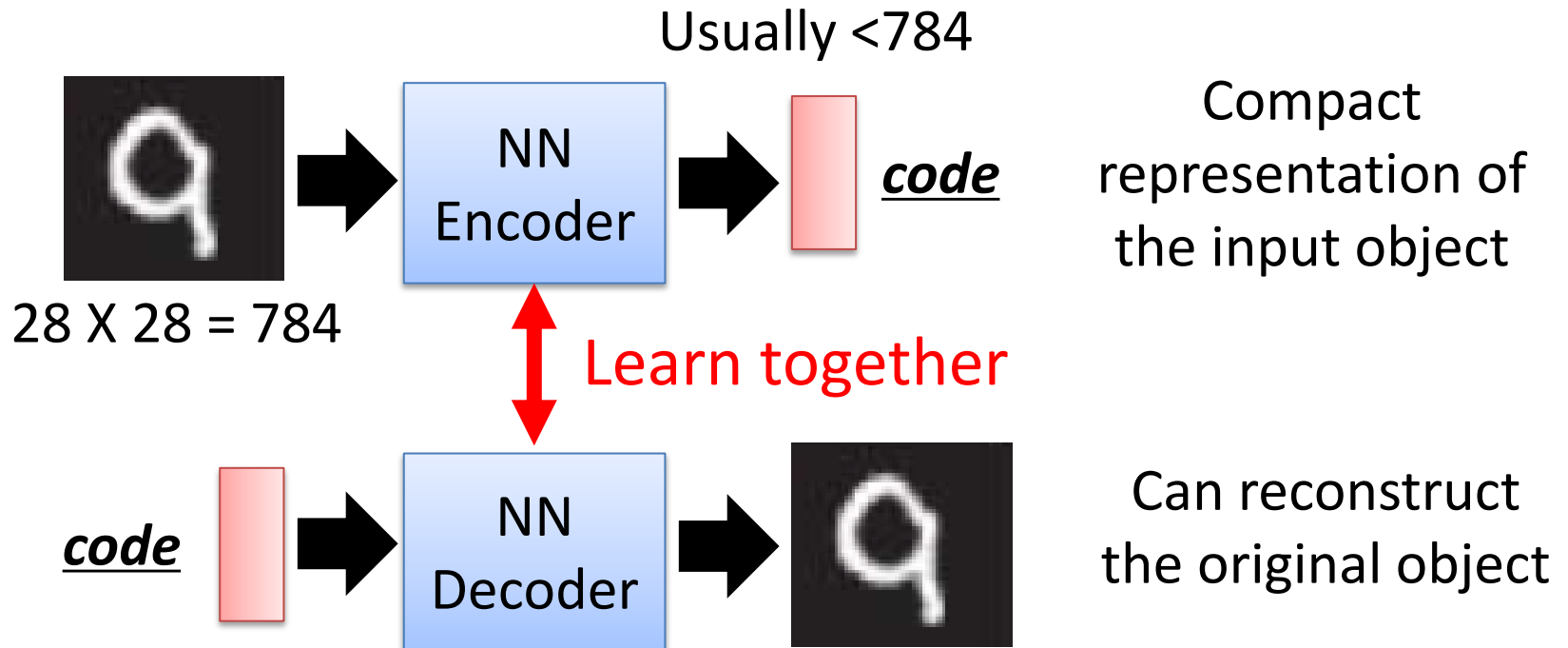
# PCA-Encoder

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# Auto-Encoder

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# Gaussian Models

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## ■ Joint and Marginal Models

- ✓ Joint probability
- ✓ Marginal probability

## ■ Conditional Models

- ✓ Conditional probability
- ✓ Posterior probability

## ■ Predictive Models

- ✓ Prior predictive
- ✓ Posterior predictive

## ■ Conjugate Prior Model

- ✓ Gaussian
  - ✓ Gaussian-Gamma
  - ✓ Gaussian-Washart
-

# Bernoulli and 1-out-of-K Models

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## ■ Probability Models

- ✓ Bernoulli
- ✓ 1-out-of-K

## ■ Conjugate Prior Model

- ✓ Beta
  - ✓ Dirichlet
-



# Bayesian Machine Learning

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## ■ Maximum Likelihood

- ✓ Dataset
- ✓ Error square cost function (model parameters)

## ■ Maximum A Posterior

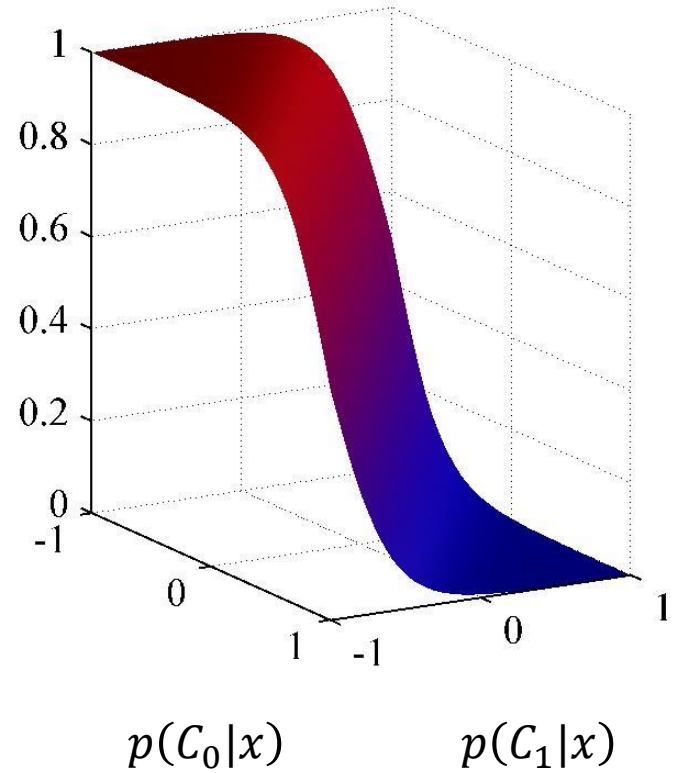
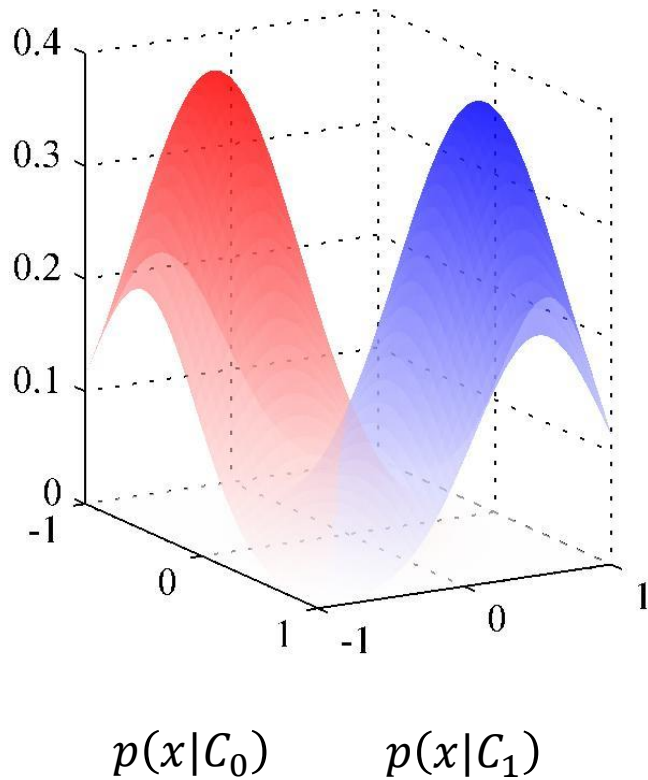
- ✓ Dataset
- ✓ Cost function and regularization (model parameters)

## ■ Expectation and Maximization

- ✓ Expectation (hidden variables)
  - ✓ Maximization (model parameters)
-

# Gaussian Mixture

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# ML Solution to Gaussian Mixtures

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$$p(x, C_1) = p(C_1)p(x|C_1) = \pi N(x|\mu_1, \Sigma)$$

$$p(x, C_2) = p(C_2)p(x|C_2) = (1 - \pi)N(x|\mu_2, \Sigma)$$

Likelihood

$$p(\mathbf{t}, \mathbf{X}|\pi, \mu_1, \mu_2, \Sigma) = \prod_{n=1}^N [\pi N(x_n|\mu_1, \Sigma)]^{t_n} [(1 - \pi)N(x_n|\mu_2, \Sigma)]^{1-t_n}$$

$$\Rightarrow \quad \pi = \frac{1}{N} \sum_{n=1}^N t_n = \frac{N_1}{N} \quad \mu_1 = \frac{1}{N_1} \sum_{n=1}^N t_n x_n \quad \mu_2 = \frac{1}{N_2} \sum_{n=1}^N (1 - t_n) x_n$$

$$\Sigma = \pi \Sigma_1 + (1 - \pi) \Sigma_2 \quad \Sigma_i = \frac{1}{N_i} \sum_{x_n \in C_i} (x_n - \mu_i)(x_n - \mu_i)^T \quad i=1,2$$

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# Generative: MAP Gaussian Mixtures

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$$\pi_0 = \frac{N_{10}}{N_{10} + N_{20}} \quad x \in \mathcal{C}_i \sim \mathcal{N}(x | \mu_{i0}, \Sigma_{i0})$$

$$\pi_{MAP} = \frac{N_1 + N_{10}}{N + N_0} = \frac{N_1 + N_{10}}{N_1 + N_2 + N_{10} + N_{20}}$$

$$\begin{cases} \Sigma_{iMAP}^{-1} &= \Sigma_{iML}^{-1} + \Sigma_{i0}^{-1} \\ \Sigma_{iMAP}^{-1} \mu_{iMAP} &= \Sigma_{iML}^{-1} \mu_{iML} + \Sigma_{i0}^{-1} \mu_{i0} \end{cases}$$

$$\Sigma = \pi \Sigma_1 + (1 - \pi) \Sigma_2$$

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# Logistic Regression

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- When there are only two classes we can model the conditional probability of the positive class as

$$p(C_1 | \mathbf{x}) = \sigma(\mathbf{w}^T \mathbf{x} + w_0) \quad \text{where} \quad \sigma(z) = \frac{1}{1 + \exp(-z)}$$

- If we use the right error function, something nice happens: The gradient of the logistic and the gradient of the error function cancel each other:

$$E(\mathbf{w}) = -\ln p(\mathbf{t} | \mathbf{w}), \quad \nabla E(\mathbf{w}) = \sum_{n=1}^N (y_n - t_n) \mathbf{x}_n$$

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# ML Solution to Logistic Regression

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$$p(C_0|\phi) = y(\phi) = \sigma(w^T\phi) \quad p(C_1|\phi) = 1 - p(C_0|\phi)$$

where  $\frac{d\sigma(a)}{da} = \sigma(1 - \sigma)$

$$p(t|w) = \prod_{n=1}^N y_n^{t_n} (1 - y_n)^{1-t_n}$$

$$E(w) = -\ln p(t|w) = -\sum_{n=1}^N [t_n \ln y_n + (1 - y_n) \ln(1 - y_n)] \quad \text{Likelihood}$$

$$\nabla E(w) = \sum_{n=1}^N (y_n - t_n) \phi_n \quad H = \nabla \nabla E(w) = \sum_{n=1}^N y_n (1 - y_n) \phi_n \phi_n^T$$

$$w_{ML} \longleftarrow w^{new} = w^{old} - H^{-1} \nabla E(w) \quad q(w) = N(w|w_{ML}, H^{-1})$$

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# MAP Solution to Logistic Regression

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$$p(w) = N(w|m_0, S_0) \quad p(w|t) \propto p(w)p(t|w)$$

$$E(w) = -\ln p(w|t) = \frac{1}{2}(w - m_0)^T S_0^{-1} (w - m_0) - \sum_{n=1}^N [t_n \ln y_n + (1 - y_n) \ln(1 - y_n)]$$

$$\nabla E(w) = S_0^{-1}(w - m_0) + \sum_{n=1}^N (y_n - t_n)\phi_n$$

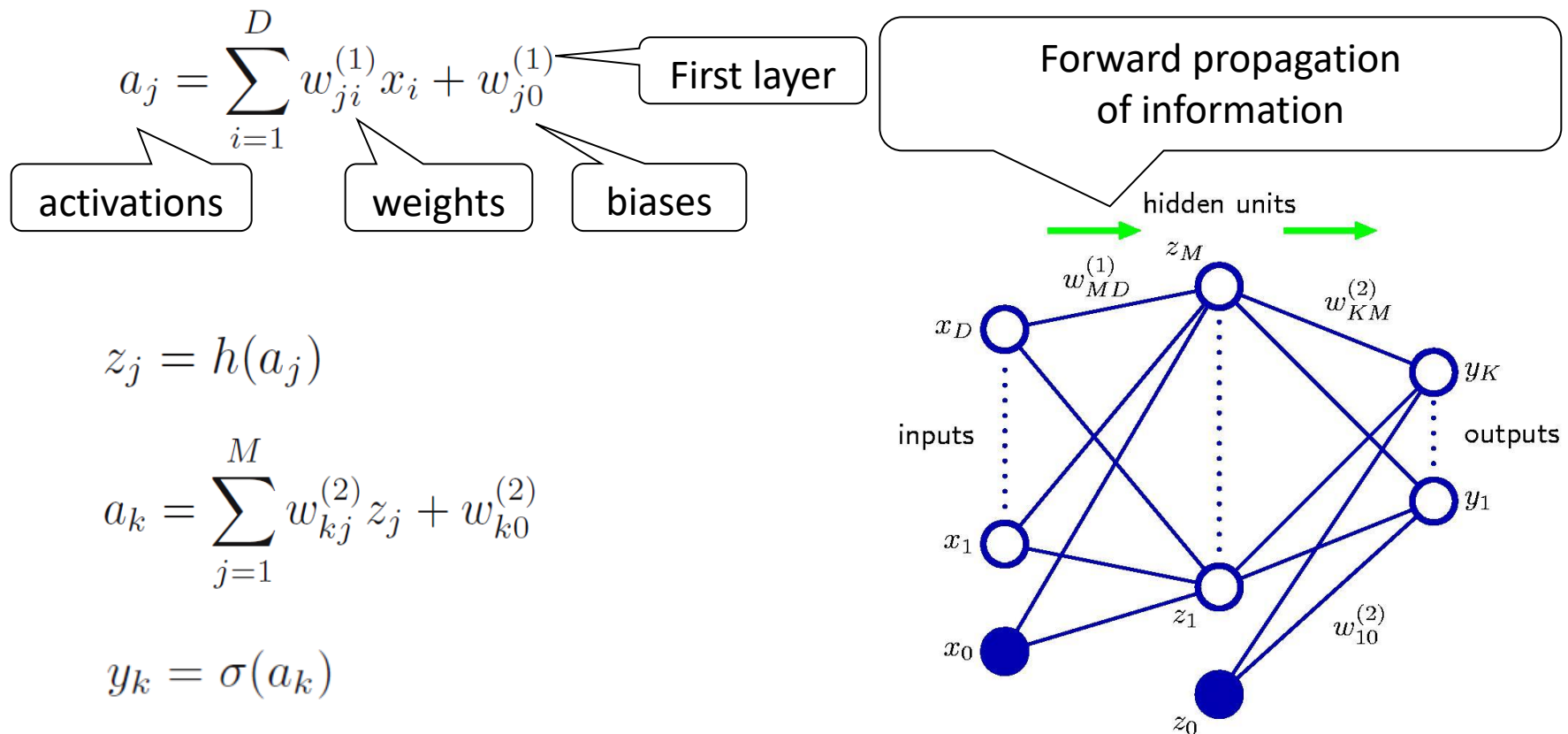
$$H = \nabla \nabla E(w) = S_0^{-1} + \sum_{n=1}^N y_n(1 - y_n)\phi_n\phi_n^T$$

$$w_{MAP} \longleftarrow w^{new} = w^{old} - H^{-1} \nabla E(w) \quad q(w) = N(w|w_{MAP}, H^{-1})$$

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# Feed-forward Network Functions

- Goal: to extend linear model by making the basis functions depend on parameters, allow these parameters to be adjusted.





# Feed-forward Network Functions

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- The overall network function, comprising two stage processing, becomes a linear regression model with adaptive basis functions

$$y_k(\mathbf{x}, \mathbf{w}) = \sigma \left( \sum_{j=1}^M w_{kj}^{(2)} h \left( \underbrace{\sum_{i=1}^D w_{ji}^{(1)} x_i + w_{j0}^{(1)}}_{\text{Adaptive basis functions}} \right) + w_{k0}^{(2)} \right)$$

# Bayesian Neural Networks I

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$$p(t|\mathbf{x}, \mathbf{w}, \beta) = N(t|y(\mathbf{x}, \mathbf{w}), \beta^{-1}) \quad p(\mathbf{w}) = N(\mathbf{w}|0, \alpha^{-1}I) \quad p(\mathbf{w}|t) \propto p(\mathbf{w})p(t|\mathbf{x}, \mathbf{w}, \beta)$$

$$E(\mathbf{w}) = -\ln p(\mathbf{w}|\mathbf{t}) = \frac{\alpha}{2} \mathbf{w}^T \mathbf{w} + \frac{\beta}{2} \sum_{n=1}^N [y_n(\mathbf{x}, \mathbf{w}) - y_n]^2 + Constant$$

$$\nabla E(\mathbf{w}) = \alpha \mathbf{w} + \beta \sum_{n=1}^N (y_n - t_n) \mathbf{g}_n \quad \mathbf{g} = \nabla_{\mathbf{w}} y(\mathbf{x}, \mathbf{w})$$

$$\mathbf{A} = \nabla \nabla E(\mathbf{w}) = \alpha \mathbf{I} + \beta \mathbf{H}$$

$$\mathbf{w}_{MAP} \longleftarrow \mathbf{w}^{new} = \mathbf{w}^{old} - \mathbf{A}^{-1} \nabla E(\mathbf{w}) \quad q(\mathbf{w}) = N(\mathbf{w}|\mathbf{w}_{MAP}, \mathbf{A}^{-1})$$

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# Bayesian Neural Networks I

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$$y(\mathbf{x}, \mathbf{w}) \simeq y(\mathbf{x}, \mathbf{w}_{MAP}) + \mathbf{g}_{MAP}^T (\mathbf{w} - \mathbf{w}_{MAP})$$

$$p(t|\mathbf{x}, \mathbf{w}, \beta) = N(t|y(\mathbf{x}, \mathbf{w}_{MAP}) + \mathbf{g}_{MAP}^T (\mathbf{w} - \mathbf{w}_{MAP}), \beta^{-1})$$

$$q(\mathbf{w}) = N(\mathbf{w}|\mathbf{w}_{MAP}, \mathbf{A}^{-1})$$

$$p(t|\mathbf{x}, D, \alpha, \beta) = \int p(t|\mathbf{x}, \mathbf{w}, \beta) q(\mathbf{w}) d\mathbf{w}$$

$$p(t|\mathbf{x}, D, \alpha, \beta) = N(t|y(\mathbf{x}, \mathbf{w}_{MAP}), \mathbf{g}_{MAP}^T \mathbf{A}^{-1} \mathbf{g}_{MAP} + \beta^{-1})$$

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# Bayesian Neural Networks II

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$$p(\mathbf{w}) = N(\mathbf{w}|0, \alpha^{-1}I) \quad p(\mathbf{w}|t) \propto p(\mathbf{w})p(t|\mathbf{w})$$

$$E(\mathbf{w}) = -\ln p(\mathbf{w}|t) = \frac{\alpha}{2} \mathbf{w}^T \mathbf{w} - \sum_{n=1}^N [t_n \ln y_n + (1 - t_n) \ln(1 - y_n)]$$

$$\nabla E(\mathbf{w}) = \alpha \mathbf{w} + \sum_{n=1}^N (y_n - t_n) \mathbf{g}_n$$

$$\mathbf{A} = \nabla \nabla E(\mathbf{w}) = \alpha \mathbf{I} + \mathbf{H} \quad \mathbf{H} = \sum_{n=1}^N y_n(1 - y_n) \mathbf{g}_n \mathbf{g}_n^T$$

$$\mathbf{w}_{MAP} \longleftarrow \mathbf{w}^{new} = \mathbf{w}^{old} - \mathbf{A}^{-1} \nabla E(\mathbf{w}) \quad q(\mathbf{w}) = N(\mathbf{w}|\mathbf{w}_{MAP}, \mathbf{A}^{-1})$$

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# The Kullback-Leibler Divergence

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$$\begin{aligned} \text{KL}(p\|q) &= \overset{\boxed{\text{Cross Entropy } C(p\|q)}}{-\int p(\mathbf{x}) \ln q(\mathbf{x}) d\mathbf{x}} - \overset{\boxed{\text{Entropy } H(p)}}{\left(-\int p(\mathbf{x}) \ln p(\mathbf{x}) d\mathbf{x}\right)} \\ &= -\int p(\mathbf{x}) \ln \left\{ \frac{q(\mathbf{x})}{p(\mathbf{x})} \right\} d\mathbf{x} \end{aligned}$$

$$\text{KL}(p\|q) \simeq \frac{1}{N} \sum_{n=1}^N \left\{ \overset{\boxed{\text{Cross Entropy}}}{-\ln q(\mathbf{x}_n|\boldsymbol{\theta})} + \overset{\boxed{\text{Negative Entropy}}}{\ln p(\mathbf{x}_n)} \right\}$$

$$\text{KL}(p\|q) \geq 0 \qquad \text{KL}(p\|q) \neq \text{KL}(q\|p)$$

KL divergence describes a distance between model  $p$  and model  $q$

---

# Cross Entropy for Machine Learning

---

Goal of Machine Learning:  $p(\text{real data}) \approx p(\text{model} | \theta)$

we assume:  $p(\text{training data}) \approx p(\text{real data})$

Operation of Machine Learning:  $p(\text{training data}) \approx p(\text{model} | \theta)$

$$\begin{aligned} & \min_{\theta} \text{KL}(p(\text{training data}) || p(\text{model} | \theta)) \\ \Leftrightarrow & \min_{\theta} C(p(\text{training data}) || p(\text{model} | \theta)) \quad \text{as } H(p(\text{training data})) \text{ is fixed} \end{aligned}$$

---

# Cross Entropy for Machine Learning

---

$$C(p(\text{training data}) \parallel p(\text{model} | \theta))$$

Bernoulli model:  $p(\text{model} / \theta) = \rho^t (1 - \rho)^{1-t}$   $t_n$ : training data

Cross entropy :  $C = -\frac{1}{N} \sum_n t_n \ln \rho + (1 - t_n) \ln(1 - \rho)$   $\rho$ : model parameter

Gaussian model:  $p(\text{model} / \theta) \propto e^{-0.5(t-\mu)^2}$   $t_n$ : training data

Cross entropy :  $C \propto \frac{1}{N} \sum_n (t_n - \mu)^2$   $\mu$ : model parameter

---

# SVM v.s. Logistic Regression I

---

For data points on the correct side,  $\xi = 0$

For the remaining points,  $\xi = 1 - y_n t_n$

$$C \sum_{n=1}^N \xi_n + \frac{1}{2} \|\mathbf{w}\|^2 \Leftrightarrow \sum_{n=1}^N E_{SV}(y_n, t_n) + \lambda \|\mathbf{w}\|^2$$

where  $\lambda = (2C)^{-1}$

$E_{SV}(y_n, t_n) = [1 - y_n t_n]_+$  : hinge error function

where  $[\cdot]_+$  denotes the positive part

---



# SVM v.s. Logistic Regression II

---

□ From maximum likelihood logistic regression

$$p(t = 1 | y) = \sigma(y)$$

$$p(t = -1 | y) = 1 - \sigma(y) = \sigma(-y)$$

$$\Rightarrow p(t | y) = \sigma(yt)$$

□ Error function with quadratic regularization

$$\sum_{n=1}^N E_{LR}(y_n t_n) + \lambda \|\mathbf{w}\|^2$$

$$\text{where } E_{LR}(yt) = \ln(1 + \exp(-yt))$$

---

# SVM v.s. Logistic Regression III

---

## □ Cross-Entropy

$y$ : Bernoulli parameter  
 $a$ : natural parameter

$$-\ln p(t|y) = -t \ln y - (1 - t) \ln(1 - y)$$

$$-\ln p(t|a) = -\ln \sigma(at) = \ln(1 + e^{-at}) \quad y = \sigma(a)$$

## □ Cross-Entropy with prior

$$-\ln p(t|y) + \alpha^{-1} \mathbf{w}^T \mathbf{w} = -t \ln y - (1 - t) \ln(1 - y) + \alpha^{-1} \mathbf{w}^T \mathbf{w}$$

$$-\ln p(t|a) + \alpha^{-1} \mathbf{w}^T \mathbf{w} = \ln(1 + e^{-at}) + \alpha^{-1} \mathbf{w}^T \mathbf{w}$$

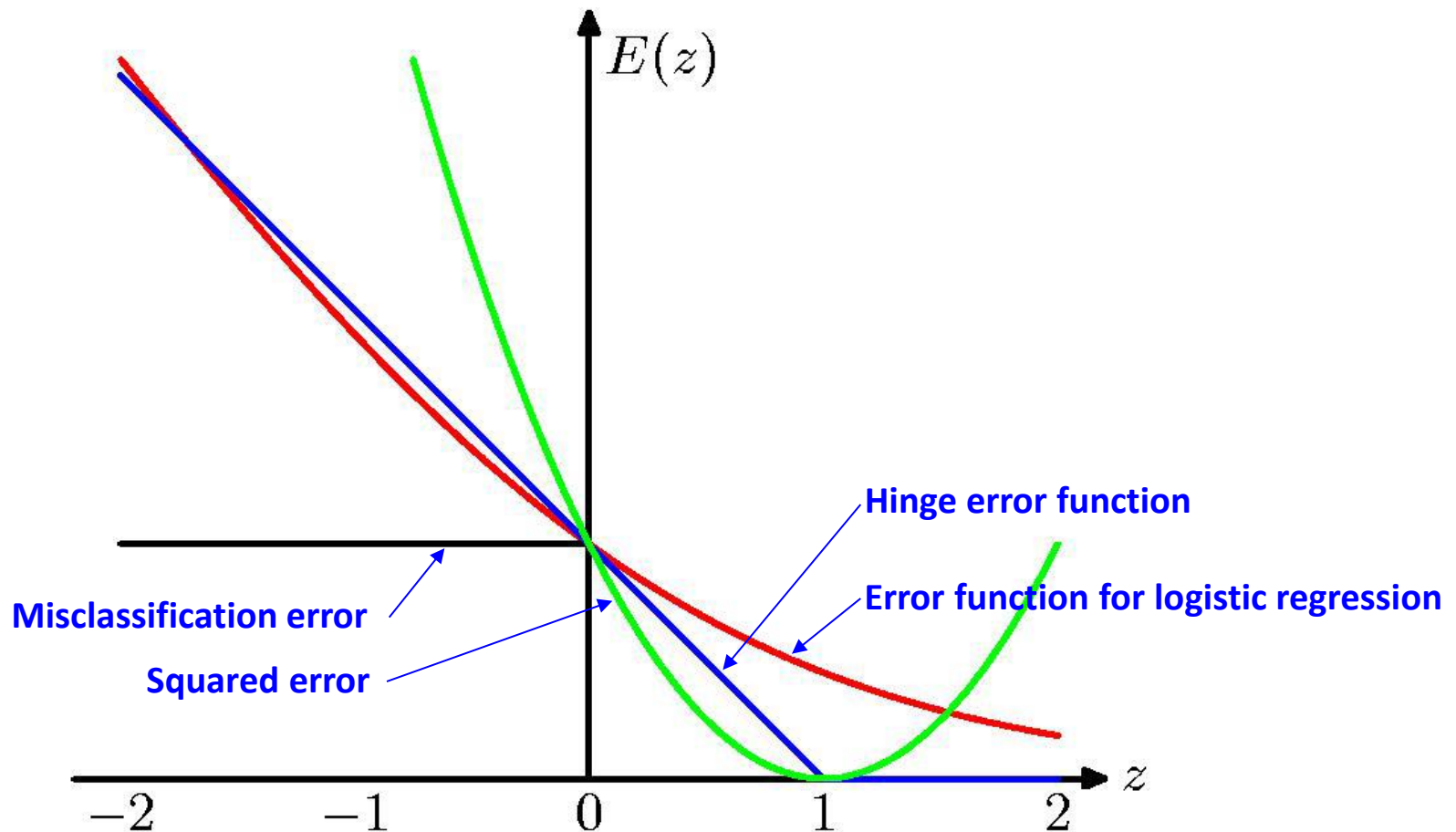
softplus:

$$\ln(1 + e^{-x})$$

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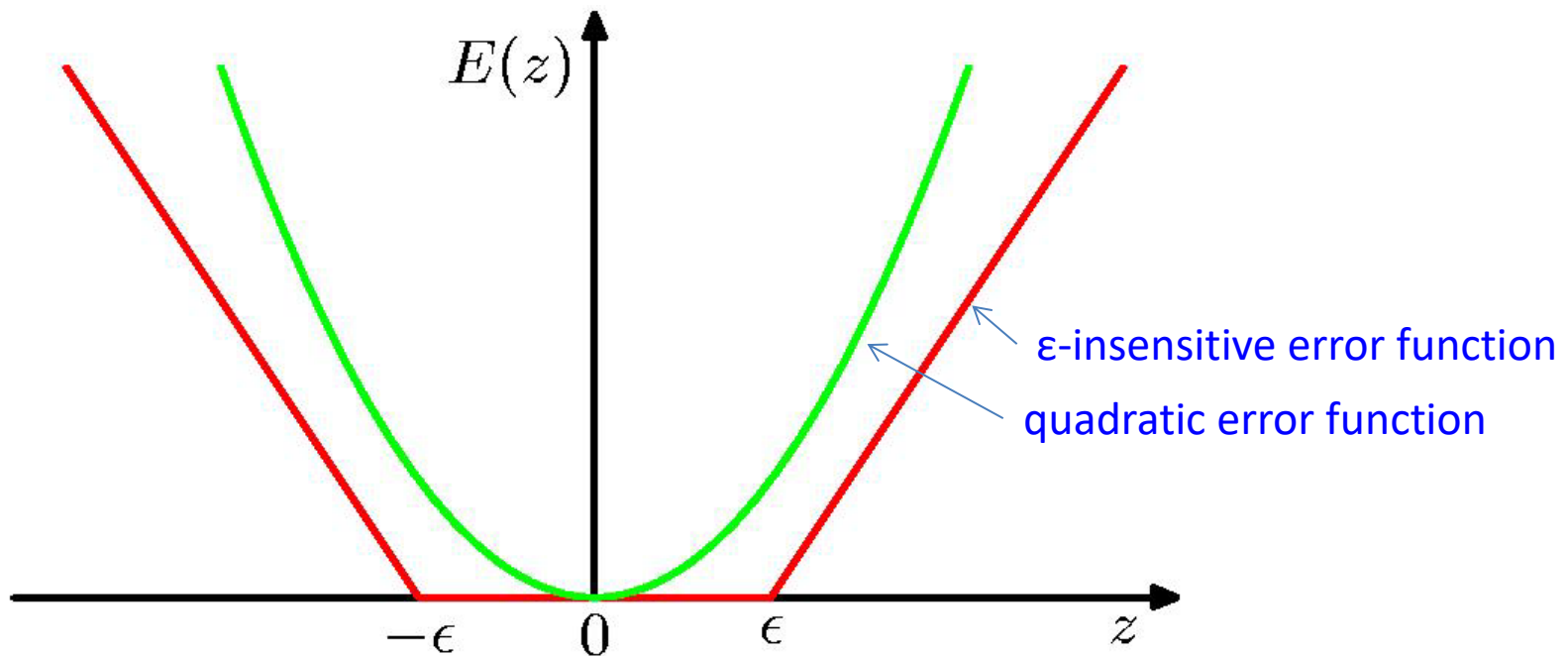
# Comparison of Error Functions

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# Comparison of Error Functions

---



# Reduction of Dimensionality (PCA)

---

Data                      Basis                      Coefficients

$\swarrow \quad \searrow \quad \swarrow$

$\mathbf{Y} = \mathbf{A}\mathbf{X}$

principal component analysis

$$\min_{A_i} A_i^T \text{COV}(Y_i) A_i$$

A: rotation

$$A_i^{*T} \text{COV}(Y_i) A_i^* = \lambda_i$$

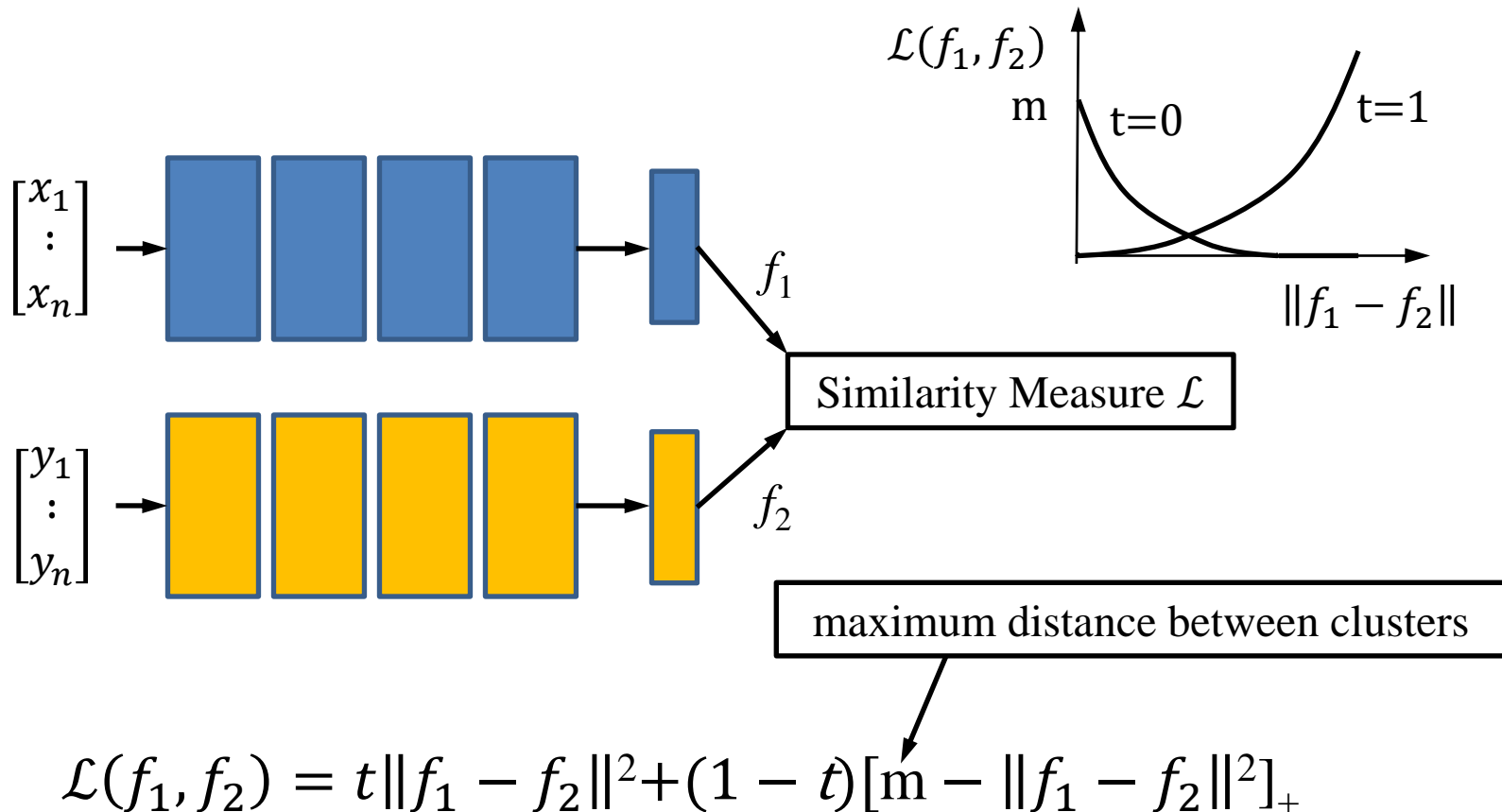
$A_i^*$ : optimal solution

$$s.t. \quad A_i^T A_i = 1 \quad E[Y_i] = \mathbf{0}$$

---

# Feature Extraction (Contrastive Loss)

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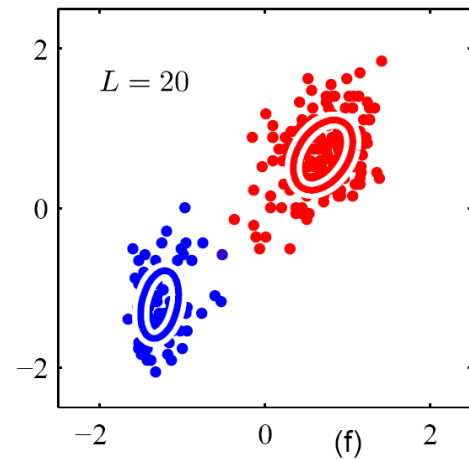
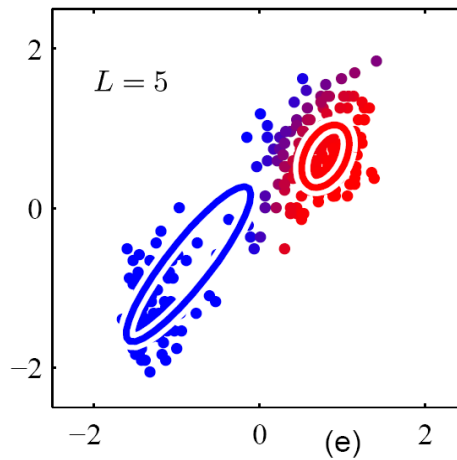
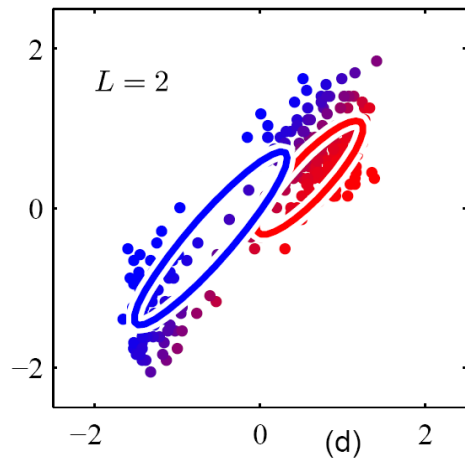
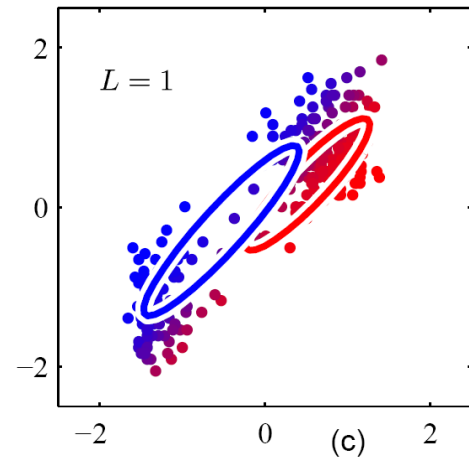
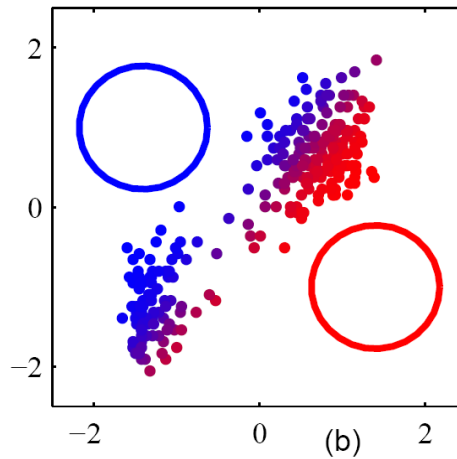
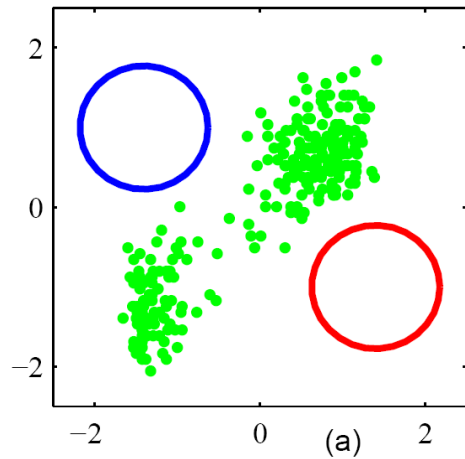


$t=1$ : two vectors belong to the same category;  $[ ]_+$ : non-negative

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# EM for Gaussian Mixtures

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# EM for Gaussian Mixtures

---

□ Given a Gaussian mixture model, the goal is to maximize the likelihood function with respect to the parameters

1. Initialize the means  $\mu_k$ , covariance  $\Sigma_k$  and mixing coefficients  $\pi_k$
2. E step

$$v(z_{nk}) = \frac{\pi_k N(\mathbf{x}_n | \mu_k, \Sigma_k)}{\sum_{j=1}^K \pi_j N(\mathbf{x}_n | \mu_j, \Sigma_j)}$$

3. M step

$$\mu_k^{new} = \frac{1}{N_k} \sum_{n=1}^N v(z_{nk}) \mathbf{x}_n$$

$$\Sigma_k^{new} = \frac{1}{N_k} \sum_{n=1}^N v(z_{nk}) (\mathbf{x}_n - \mu_k^{new})(\mathbf{x}_n - \mu_k^{new})^T$$

$$\pi_k^{new} = \frac{N_k}{N} \quad N_k = \sum_{n=1}^N v(z_{nk})$$

4. Evaluate the log likelihood

$$\ln p(\mathbf{X} | \mu, \Sigma, \Pi) = \sum_{n=1}^N \ln \left\{ \sum_{k=1}^K \pi_k N(\mathbf{x}_n | \mu_k, \Sigma_k) \right\}$$

---



# EM for Bernoulli Mixtures

---

$$\ln p(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\pi}) = \sum_{n=1}^N \ln \left\{ \sum_{k=1}^K \pi_k p(\mathbf{x}_n \mid \boldsymbol{\mu}_k) \right\}$$

$$p(\mathbf{x} \mid \mathbf{z}, \boldsymbol{\mu}) = \prod_{k=1}^K p(\mathbf{x} \mid \boldsymbol{\mu}_k)^{z_k} \quad (\mathbf{z} = (z_1, \dots, z_K)^T \text{ is a binary indicator variables})$$

$$p(\mathbf{z} \mid \boldsymbol{\pi}) = \prod_{k=1}^K \pi_k^{z_k}$$

(complete - data log likelihood function) :

$$\ln p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\mu}, \boldsymbol{\pi}) = \sum_{n=1}^N \sum_{k=1}^K z_{nk} \left\{ \ln \pi_k + \sum_{i=1}^D [x_{ni} \ln \mu_{ki} + (1 - x_{ni}) \ln (1 - \mu_{ki})] \right\}$$

$$E_z[\ln p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\mu}, \boldsymbol{\pi})] = \sum_{n=1}^N \sum_{k=1}^K \gamma(z_{nk}) \left\{ \ln \pi_k + \sum_{i=1}^D [x_{ni} \ln \mu_{ki} + (1 - x_{ni}) \ln (1 - \mu_{ki})] \right\}$$

$$(\text{E - step}) \quad \gamma(z_{nk}) = E[z_{nk}] = \frac{\pi_k p(\mathbf{x}_n \mid \boldsymbol{\mu}_k)}{\sum_{j=1}^K \pi_j p(\mathbf{x}_n \mid \boldsymbol{\mu}_j)}, \quad N_k = \sum_{n=1}^N \gamma(z_{nk}), \quad \bar{\mathbf{x}}_k = \frac{1}{N_k} \sum_{n=1}^N \gamma(z_{nk}) \mathbf{x}_n$$

$$(\text{M - step}) \quad \boldsymbol{\mu}_k = \bar{\mathbf{x}}_k, \quad \pi_k = \frac{N_k}{N}$$

\* In contrast to the mixture of Gaussians, there are no singularities in which the likelihood goes to infinity

---

# Hidden Markov Models

Conditional distribution for latent variable

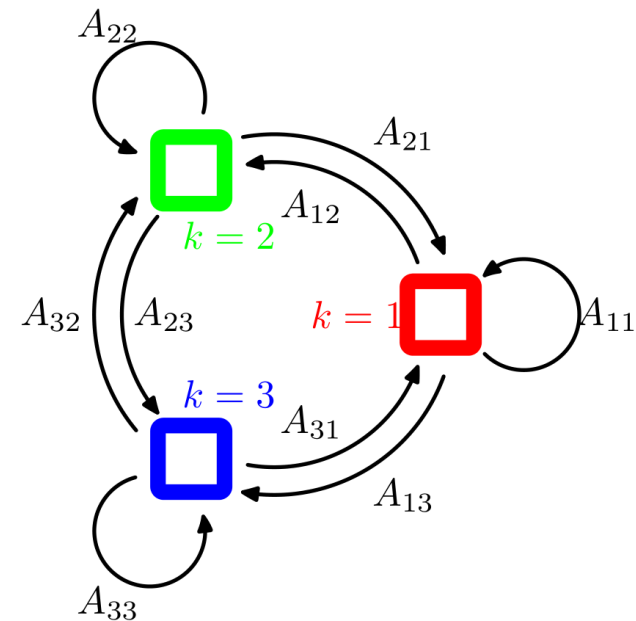
$$p(\mathbf{z}_n | \mathbf{z}_{n-1}, \mathbf{A}) = \prod_{k=1}^K \prod_{j=1}^K A_{jk}^{z_{n-1,j} z_{nk}}$$

$$p(\mathbf{z}_1 | \boldsymbol{\pi}) = \prod_{k=1}^K \pi_k^{z_{1k}}$$

$$\sum_k \pi_k = 1$$

A means transition probabilities

As in the case of a standard mixture model, the latent variables are the discrete multinomial variables  $\mathbf{z}_n$  using 1-of-K coding scheme



a model whose latent variables have three possible states corresponding to the three boxes. The black lines denote the elements of the transition matrix  $A_{jk}$

# EM for HMM

---

## EM algorithm

$$\gamma(\mathbf{z}_n) = p(\mathbf{z}_n | \mathbf{X}, \boldsymbol{\theta}^{\text{old}})$$

$$\xi(\mathbf{z}_{n-1}, \mathbf{z}_n) = p(\mathbf{z}_{n-1}, \mathbf{z}_n | \mathbf{X}, \boldsymbol{\theta}^{\text{old}})$$

$$\gamma(z_{nk}) = \mathbb{E}[z_{nk}] = \sum_{\mathbf{z}} \gamma(\mathbf{z}) z_{nk}$$

$$\xi(z_{n-1,j}, z_{nk}) = \mathbb{E}[z_{n-1,j} z_{nk}] = \sum_{\mathbf{z}} \gamma(\mathbf{z}) z_{n-1,j} z_{nk}$$

$$\pi_k = \frac{\gamma(z_{1k})}{\sum_{j=1}^K \gamma(z_{1j})}$$

$$A_{jk} = \frac{\sum_{n=2}^N \xi(z_{n-1,j}, z_{nk})}{\sum_{l=1}^K \sum_{n=2}^N \xi(z_{n-1,j}, z_{nl})}$$

$$\boldsymbol{\mu}_k = \frac{\sum_{n=1}^N \gamma(z_{nk}) \mathbf{x}_n}{\sum_{n=1}^N \gamma(z_{nk})}$$

$$\boldsymbol{\Sigma}_k = \frac{\sum_{n=1}^N \gamma(z_{nk}) (\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^T}{\sum_{n=1}^N \gamma(z_{nk})}$$

# Sum-Product v.s. Max-Product

---

## □ Sum-Product Algorithm (evaluation)

- ✓ Compute the joint distribution from the Product
- ✓ Infer marginal distributions from the Sum

$$p(x_1, x_2) = \sum_{x_3} p(x_1, x_3)p(x_2, x_3)$$

## □ Max-Product Algorithm (decoding)

- ✓ Compute the joint distribution from the Product
- ✓ Perform ML estimation from the Max

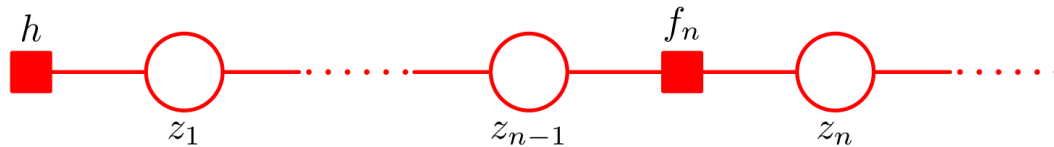
$$x_1^* = \max_{x_1} p(x_1, x_3)p(x_2, x_1)$$

---

# Sum-Product for HMMs

---

- Transforming the directed graph into a factor graph



$$h(\mathbf{z}_1) = p(\mathbf{z}_1)p(\mathbf{x}_1|\mathbf{z}_1)$$

$$f_n(\mathbf{z}_{n-1}, \mathbf{z}_n) = p(\mathbf{z}_n|\mathbf{z}_{n-1})p(\mathbf{x}_n|\mathbf{z}_n)$$

$$\mu_{\mathbf{z}_{n-1} \rightarrow f_n}(\mathbf{z}_{n-1}) = \mu_{f_{n-1} \rightarrow \mathbf{z}_{n-1}}(\mathbf{z}_{n-1})$$

$$\mu_{f_n \rightarrow \mathbf{z}_n}(\mathbf{z}_n) = \sum_{\mathbf{z}_{n-1}} f_n(\mathbf{z}_{n-1}, \mathbf{z}_n) \mu_{\mathbf{z}_{n-1} \rightarrow f_n}(\mathbf{z}_{n-1})$$

$$\mu_{f_n \rightarrow \mathbf{z}_n}(\mathbf{z}_n) = \sum_{\mathbf{z}_{n-1}} f_n(\mathbf{z}_{n-1}, \mathbf{z}_n) \mu_{f_{n-1} \rightarrow \mathbf{z}_{n-1}}(\mathbf{z}_{n-1})$$

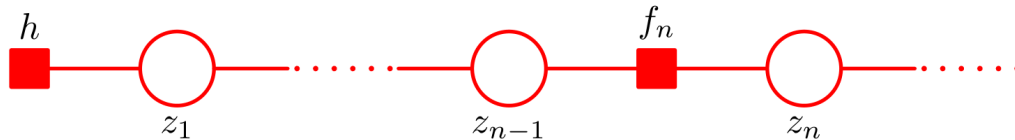
$$\alpha(\mathbf{z}_n) = \mu_{f_n \rightarrow \mathbf{z}_n}(\mathbf{z}_n)$$

---

# Sum-Product for HMMs

---

- Transforming the directed graph into a factor graph



$$\mu_{f_{n+1} \rightarrow f_n}(\mathbf{z}_n) = \sum_{\mathbf{z}_{n+1}} f_{n+1}(\mathbf{z}_n, \mathbf{z}_{n+1}) \mu_{f_{n+2} \rightarrow f_{n+1}}(\mathbf{z}_{n+1})$$

$$\beta(\mathbf{z}_n) = \mu_{f_{n+1} \rightarrow \mathbf{z}_n}(\mathbf{z}_n)$$

$$p(\mathbf{z}_n, \mathbf{X}) = \mu_{f_n \rightarrow \mathbf{z}_n}(\mathbf{z}_n) \mu_{f_{n+1} \rightarrow \mathbf{z}_n}(\mathbf{z}_n) = \alpha(\mathbf{z}_n) \beta(\mathbf{z}_n)$$

$$\gamma(\mathbf{z}_n) = \frac{p(\mathbf{z}_n, \mathbf{X})}{p(\mathbf{X})} = \frac{\alpha(\mathbf{z}_n) \beta(\mathbf{z}_n)}{p(\mathbf{X})}$$

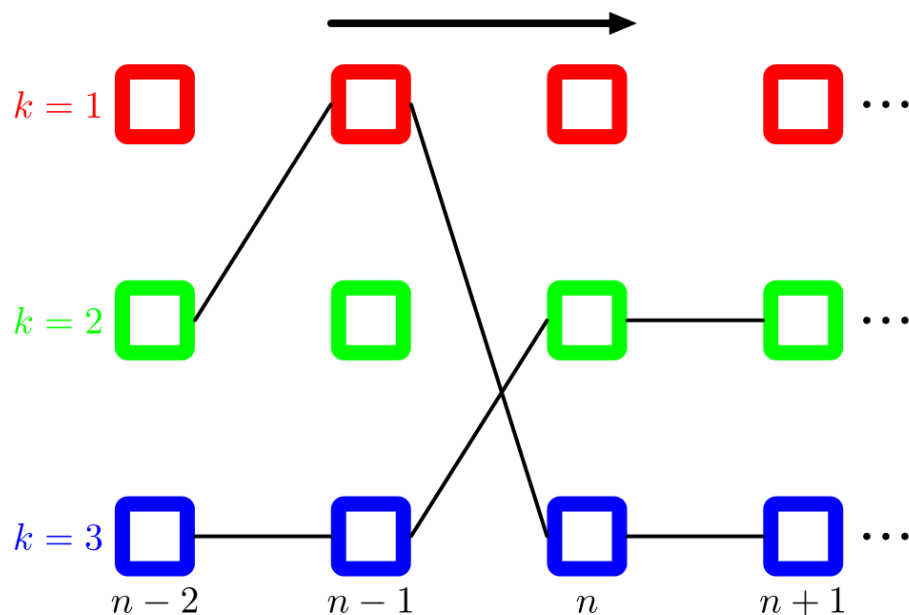
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# Latent Sequence Estimation

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## □ Decoding:

Given a HMM model  $\theta = \{\pi, \mathbf{A}, \phi\}$ , what is the most likely latent sequence  $\{\mathbf{z}_1, \dots, \mathbf{z}_N\}$  for an observation sequence  $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$  ?



# Viterbi Algorithm

---

$$\omega(\mathbf{z}_n) = \max_{\mathbf{z}_1, \dots, \mathbf{z}_{n-1}} \ln p(\mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{z}_1, \dots, \mathbf{z}_n)$$

$$\omega(\mathbf{z}_{n+1}) = \max_{\mathbf{z}_1, \dots, \mathbf{z}_n} \ln p(\mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}_{n+1}, \mathbf{z}_1, \dots, \mathbf{z}_n, \mathbf{z}_{n+1})$$

$$\omega(\mathbf{z}_{n+1}) = \ln p(\mathbf{x}_{n+1} | \mathbf{z}_{n+1}) + \max_{\mathbf{z}_n} \{ \ln p(\mathbf{z}_{n+1} | \mathbf{z}_n) + \omega(\mathbf{z}_n) \}$$

$$\omega(\mathbf{z}_1) = \ln p(\mathbf{z}_1) + \ln p(\mathbf{x}_1 | \mathbf{z}_1)$$

---



# Viterbi Algorithm

---

- Note that maximization over  $\mathbf{z}_n$  must be performed for each of  $K$  possible values of  $\mathbf{z}_{n+1}$
  - Denote this function by  $\psi(k_n)$ , where  $k \in \{1, \dots, K\}$
  - Once we find the most probable value of  $\mathbf{z}_N$ , we can trackback along the chain
- $$k_n^{\max} = \psi(k_{n+1}^{\max})$$
- Reduce the computational cost from  $O(K^N)$  to  $O(KN)$
-

# Example

---

- Given an HMM and an observation sequence, how to perform evaluation and decoding

Transition A	Emission B	Hidden States Z	Observations X
$\begin{bmatrix} 0.6 & 0.3 \\ 0.4 & 0.7 \end{bmatrix}$	$\begin{bmatrix} 0.8 & 0.1 \\ 0.2 & 0.9 \end{bmatrix}$	{bull, bear}	{up, down}

If Z is stationary, then  $\pi = [3/7, 4/7]$ . We also can assume  $\pi = [1/2, 1/2]$

An observation sequence: {up, up, down}

---

# Evaluation (Sum-Product)

---

$$\alpha(z_1) = p(z_1, x_1) = p(x_1|z_1)p(z_1)$$

$$\boxed{x_1=\text{up}, z_1=\text{bull or bear}} = \begin{bmatrix} 0.8 \\ 0.1 \end{bmatrix} \cdot \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} = \begin{bmatrix} 0.8 \times 0.5 \\ 0.1 \times 0.5 \end{bmatrix} = \begin{bmatrix} 0.4 \\ 0.05 \end{bmatrix}$$

$$\alpha(z_2) = p(z_2, x_1, x_2) = p(x_2|z_2) \sum_{z_1} p(z_2|z_1) \alpha(z_1)$$

$$\boxed{x_2=\text{up}, z_2=\text{bull or bear}} = \begin{bmatrix} 0.8 \\ 0.1 \end{bmatrix} \cdot \begin{bmatrix} 0.6 \times 0.4 + 0.3 \times 0.05 \\ 0.4 \times 0.4 + 0.7 \times 0.05 \end{bmatrix} = \begin{bmatrix} 0.204 \\ 0.0195 \end{bmatrix}$$

$$\alpha(z_3) = p(z_3, x_1, x_2, x_3) = p(x_3|z_3) \sum_{z_2} p(z_3|z_2) \alpha(z_2)$$

$$\boxed{x_3=\text{down}, z_2=\text{bull or bear}} = \begin{bmatrix} 0.2 \\ 0.9 \end{bmatrix} \cdot \begin{bmatrix} 0.6 \times 0.204 + 0.3 \times 0.0195 \\ 0.4 \times 0.204 + 0.7 \times 0.0195 \end{bmatrix} = \begin{bmatrix} 0.02565 \\ 0.085725 \end{bmatrix}$$

$$p(x_1, x_2, x_3) = \sum_{z_3} \alpha(z_3) = 0.111375$$

---

# Decoding (Max-Product)

---

$$\delta(z_1) = p(z_1, x_1) = p(x_1|z_1)p(z_1)$$

$$\boxed{x_1=\text{up}, z_1=\text{bull or bear}} = \begin{bmatrix} 0.8 \\ 0.1 \end{bmatrix} \cdot \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} = \begin{bmatrix} 0.8 \times 0.5 \\ 0.1 \times 0.5 \end{bmatrix} = \begin{bmatrix} 0.4 \\ 0.05 \end{bmatrix}$$

$$\delta(z_2) = p(z_2, x_1, x_2) = p(x_2|z_2) \max_{z_1} p(z_2|z_1)\delta(z_1)$$

$$\boxed{x_2=\text{up}, z_2=\text{bull or bear}} = \begin{bmatrix} 0.8 \\ 0.1 \end{bmatrix} \cdot \begin{bmatrix} 0.6 \times 0.4 \\ 0.4 \times 0.4 \end{bmatrix} = \begin{bmatrix} 0.192 \\ 0.016 \end{bmatrix} \leftarrow$$

$$\phi(z_2) = \arg \max_{z_1} p(z_2|z_1)\delta(z_1) = \begin{bmatrix} \text{bull} \rightarrow \text{bull} \\ \text{bull} \rightarrow \text{bear} \end{bmatrix} \leftarrow$$

$$\delta(z_3) = p(z_3, x_1, x_2, x_3) = p(x_3|z_3) \max_{z_2} p(z_3|z_2)\delta(z_2)$$

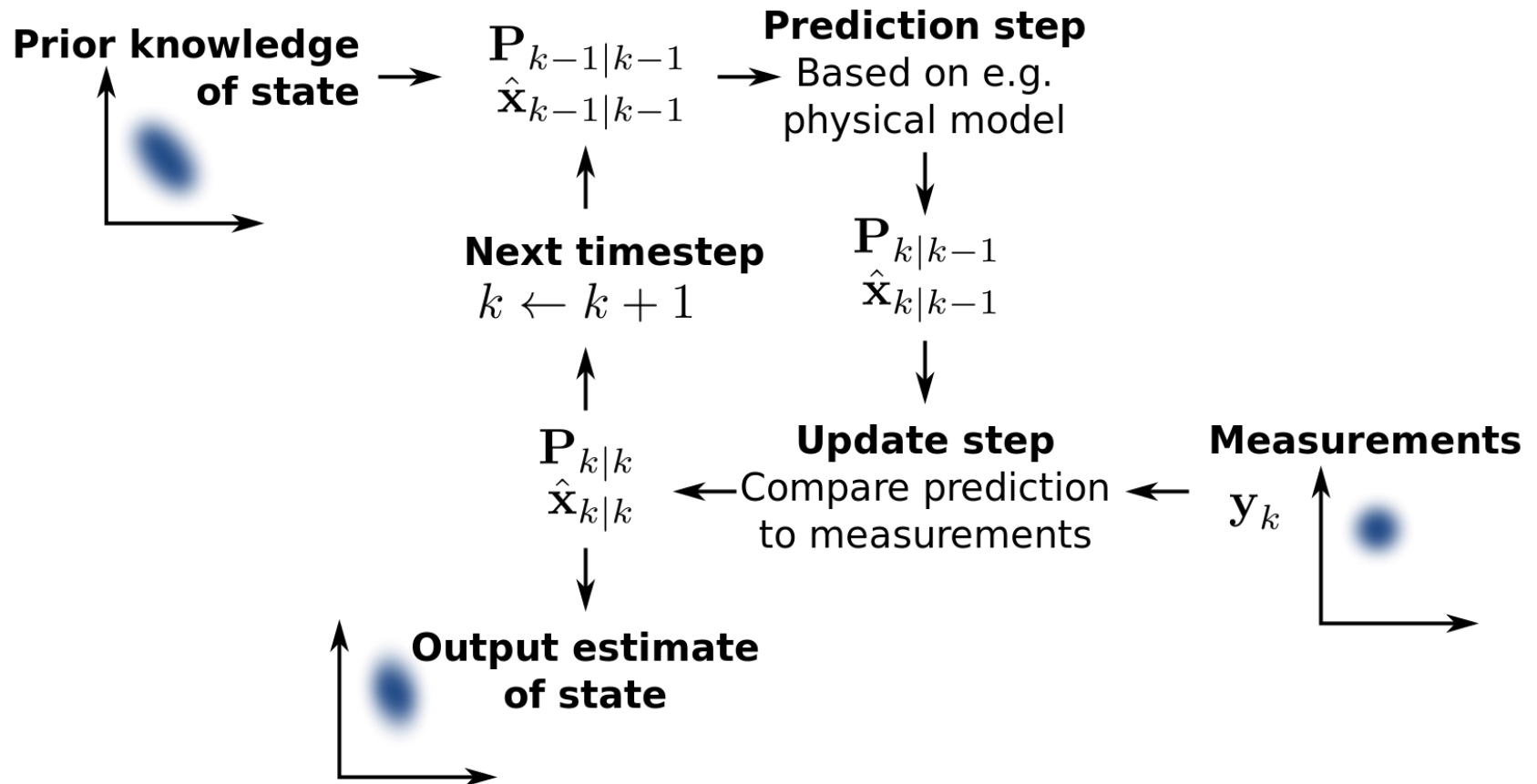
$$\boxed{x_3=\text{down}, z_2=\text{bull or bear}} = \begin{bmatrix} 0.2 \\ 0.9 \end{bmatrix} \cdot \begin{bmatrix} 0.6 \times 0.192 \\ 0.4 \times 0.192 \end{bmatrix} = \begin{bmatrix} 0.02304 \\ 0.06912 \end{bmatrix} \leftarrow$$

$$\phi(z_3) = \arg \max_{z_2} p(z_3|z_2)\delta(z_2) = \begin{bmatrix} \text{bull} \rightarrow \text{bull} \\ \text{bull} \rightarrow \text{bear} \end{bmatrix} \leftarrow$$

Optimal solution:  
bull  $\rightarrow$  bull  $\rightarrow$  bear

# Kalman Filtering

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# EM for LDS

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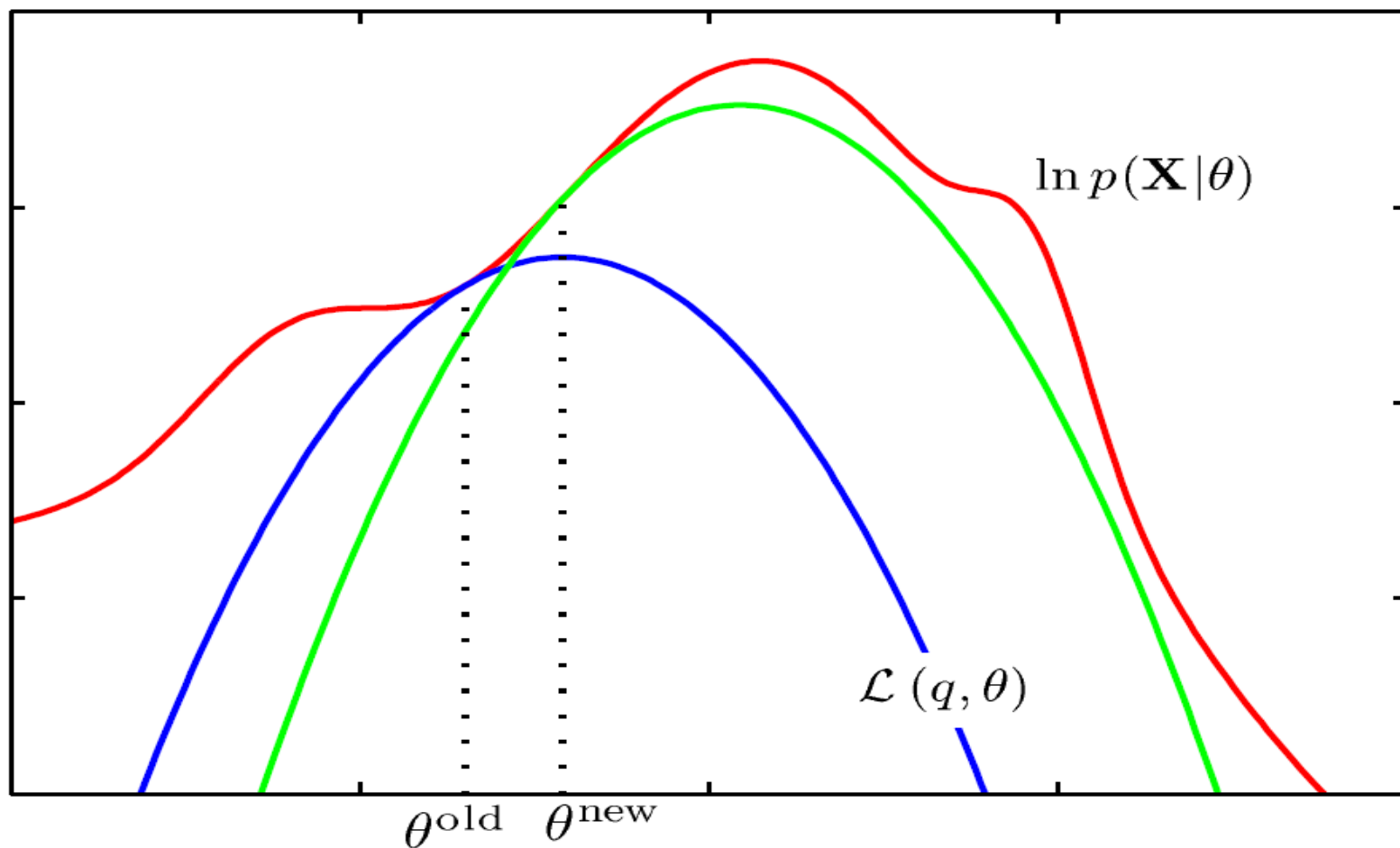
$$\begin{aligned}\ln p(\mathbf{X}, \mathbf{Z} | \boldsymbol{\theta}) &= \ln p(\mathbf{z}_1 | \boldsymbol{\mu}_0, \mathbf{V}_0) + \sum_{n=2}^N \ln p(\mathbf{z}_n | \mathbf{z}_{n-1}, \mathbf{A}, \boldsymbol{\Gamma}) \\ &\quad + \sum_{n=1}^N \ln p(\mathbf{x}_n | \mathbf{z}_n, \mathbf{C}, \boldsymbol{\Sigma})\end{aligned}$$

$$Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) = \mathbb{E}_{\mathbf{Z} | \boldsymbol{\theta}^{\text{old}}} [\ln p(\mathbf{X}, \mathbf{Z} | \boldsymbol{\theta})]$$

---

# EM Algorithm in General

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# The EM Algorithm in General (I)

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- ❑ Direct optimization of  $p(\mathbf{X}|\theta)$  is difficult while optimization of complete data likelihood  $p(\mathbf{X}, \mathbf{Z}|\theta)$  is significantly easier.
- ❑ Decomposition of the likelihood  $p(\mathbf{X}|\theta)$

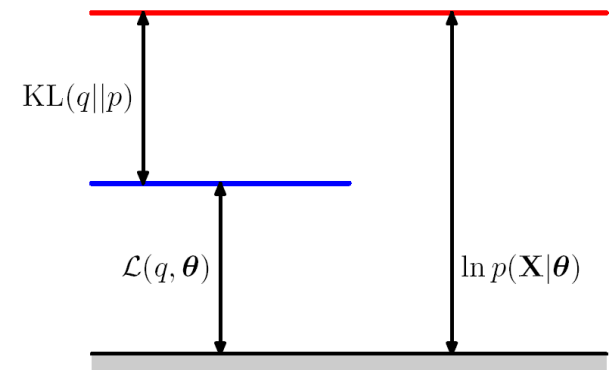
$$\ln p(\mathbf{X}, \mathbf{Z}|\theta) = \ln p(\mathbf{Z}|\mathbf{X}, \theta) + \ln p(\mathbf{X}|\theta)$$

$$\ln p(\mathbf{X}|\theta) = \mathcal{L}(q, \theta) + \text{KL}(q\|p)$$

$$\mathcal{L}(q, \theta) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} \right\}$$

$$\text{KL}(q\|p) = - \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{Z}|\mathbf{X}, \theta)}{q(\mathbf{Z})} \right\}$$

$$\text{KL}(q\|p) \geq 0 \quad \Rightarrow \quad \mathcal{L}(q, \theta) \leq \ln p(\mathbf{X}|\theta)$$





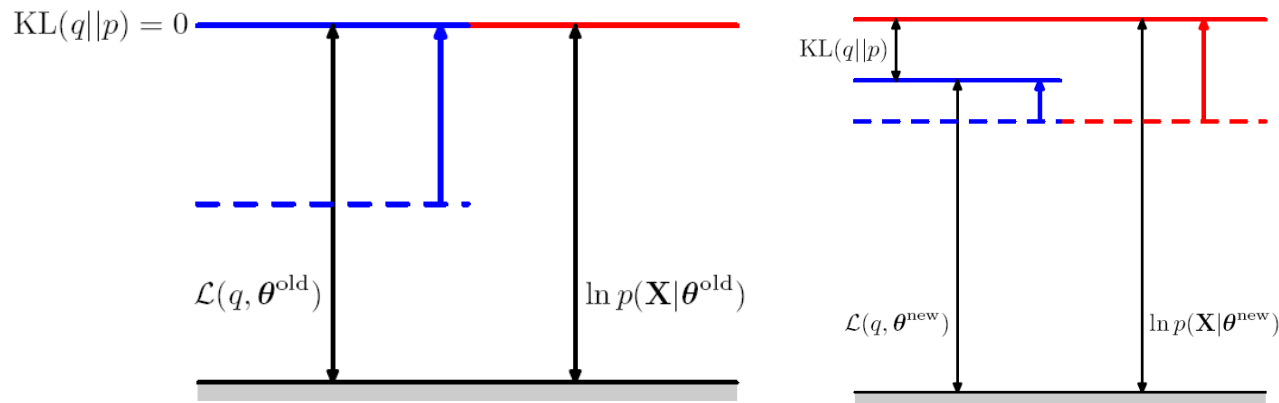
# The EM Algorithm in General (II)

- **(E step)** The lower bound  $\mathcal{L}(q, \theta_{\text{old}})$  is maximized while holding  $\theta_{\text{old}}$  fixed. Since  $\ln p(\mathbf{X}|\theta)$  does not depend on  $q(\mathbf{Z})$ ,  $\mathcal{L}(q, \theta_{\text{old}})$  will be the largest when  $\text{KL}(q||p)$  vanishes (i.e. when  $q(\mathbf{Z})$  is equal to the posterior distribution  $p(\mathbf{Z}|\mathbf{X}, \theta_{\text{old}})$ )
- **(M step)**  $q(\mathbf{Z})$  is fixed and the lower bound  $\mathcal{L}(q, \theta_{\text{old}})$  is maximized wrt.  $\theta$  to  $\theta_{\text{new}}$ . When the lower bound is increased,  $\theta$  is updated making  $\text{KL}(q||p)$  greater than 0. Thus the increase in the log likelihood function is greater than the increase in the lower bound.
- In the M step, the quantity being maximized is the expectation of the complete-data log-likelihood

$$\begin{aligned}
 \mathcal{L}(q, \theta) &= \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta^{\text{old}}) \ln p(\mathbf{X}, \mathbf{Z}|\theta) - \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta^{\text{old}}) \ln p(\mathbf{Z}|\mathbf{X}, \theta^{\text{old}}) \\
 &= \mathcal{Q}(\theta, \theta^{\text{old}}) + \text{const}
 \end{aligned}$$

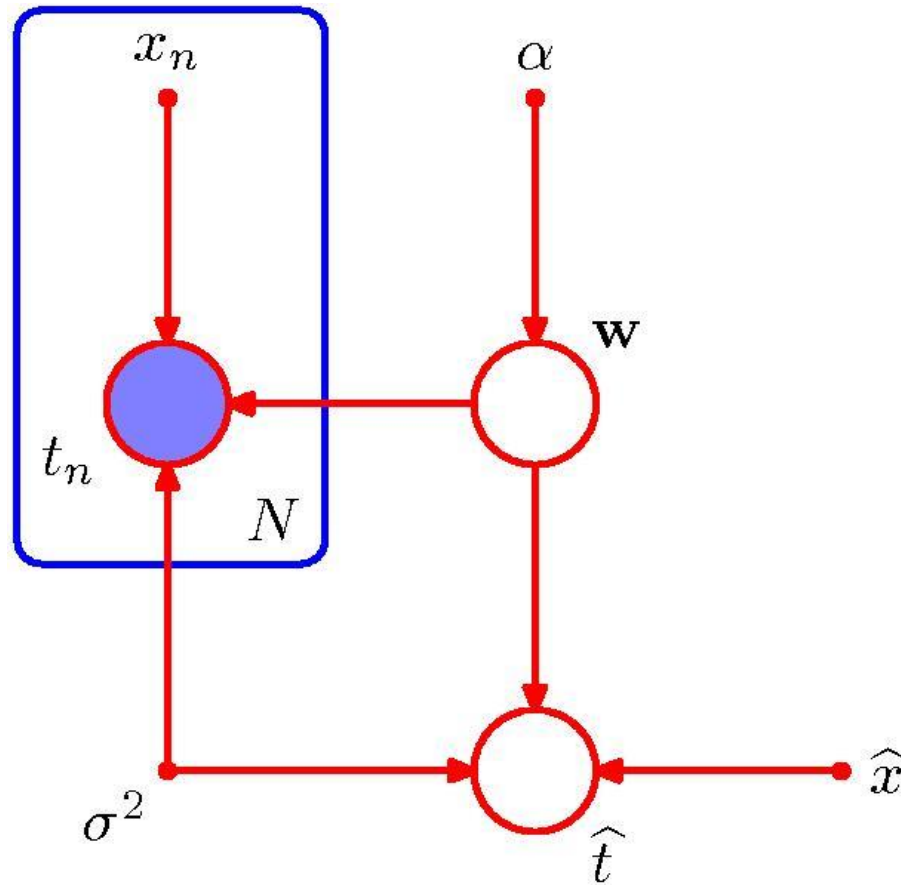
←

$q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \theta^{\text{old}})$



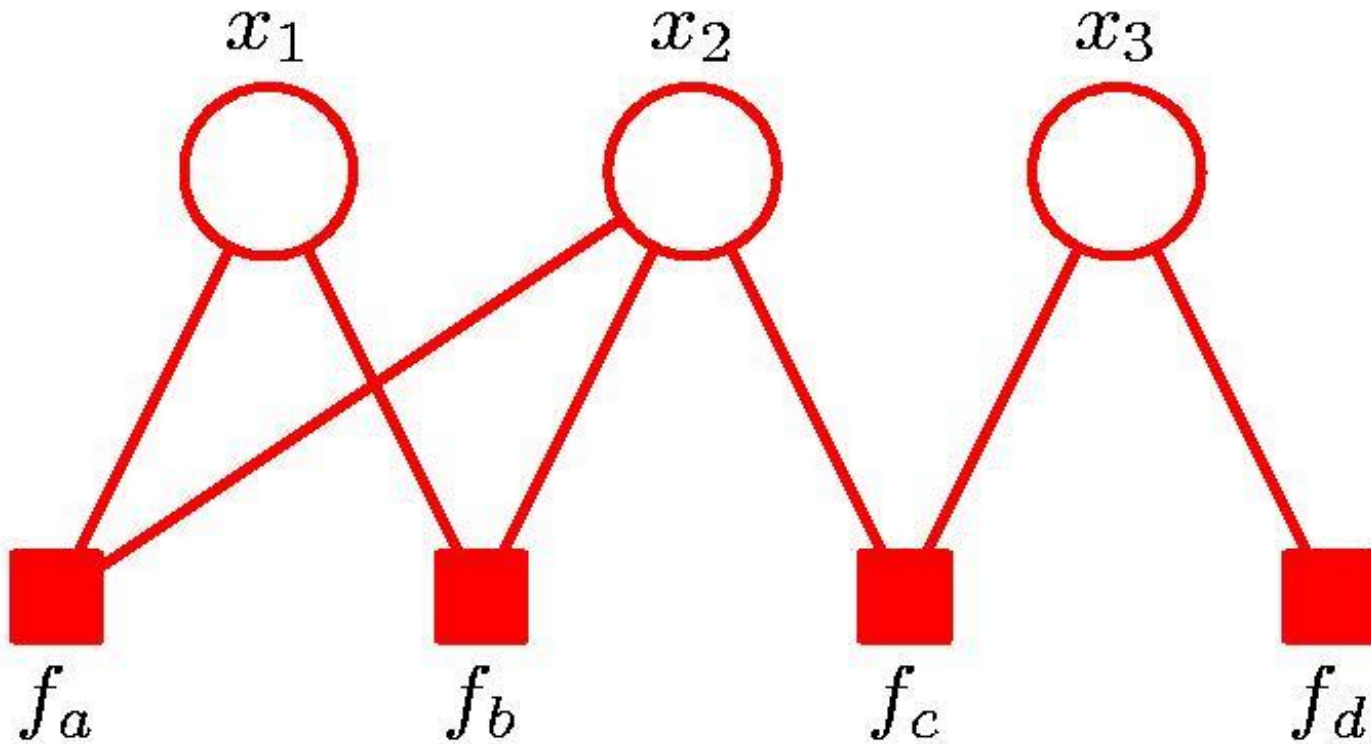
# Graphical Model – Bayesian Regression

---



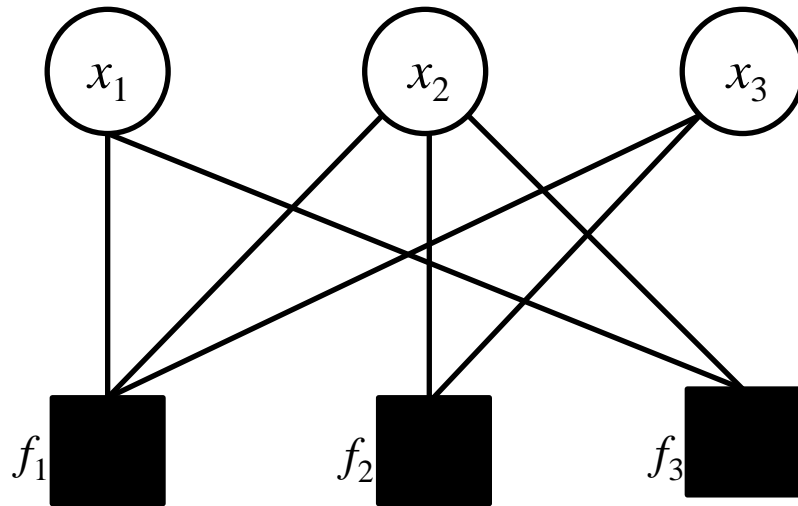
# Graphical Model – Factor Graph

---



# Factor Graph for Solving Equations

---



$$x_1 + 2x_2 + x_3 = 4 \quad x_2 + 2x_3 = 3 \quad x_1 + x_2 = 2$$

(1)  $x_1 = 1 \quad x_2 = 1 \quad x_3 = 0$

(2)  $f_1 \rightarrow x_1: x_1 = 4 - 2x_2 - x_3 = 2$   
 $f_1 \rightarrow x_2: x_2 = (4 - x_1 - x_3)/2 = 1.5$   
 $f_1 \rightarrow x_3: x_3 = 4 - 2x_2 - x_1 = 1$

$$f_2 \rightarrow x_2: x_2 = 3 - 2x_3 = 3$$

$$f_2 \rightarrow x_3: x_3 = 3 - 2x_2 = 1$$

$$f_3 \rightarrow x_1: x_1 = 2 - x_2 = 1$$

$$f_3 \rightarrow x_2: x_2 = 2 - x_1 = 1$$

(3)  $x_1 = (1+2+1)/3 = 4/3 \quad x_2 = (1+1.5+3+1)/4 = 6.5/4 \quad x_3 = (0+1+1)/3 = 2/3$

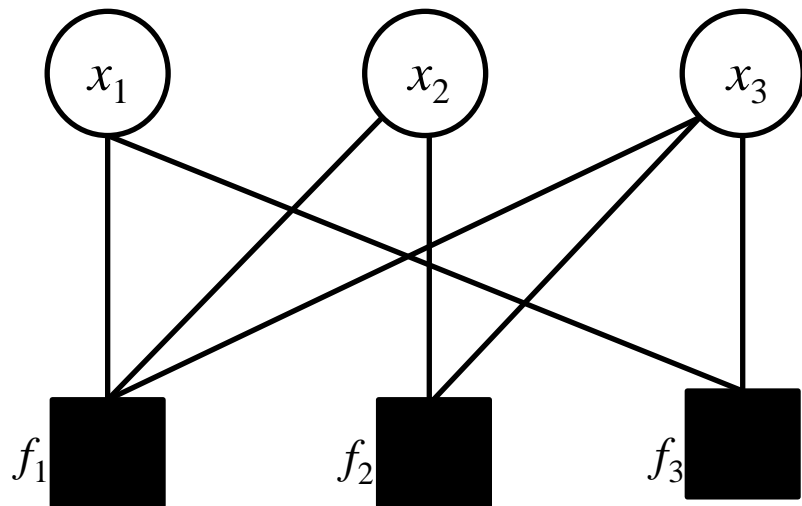
---

# Factor Graph for Computing Means

---

$$S_i = x_i N_i$$

$$(1) \quad S_1 = 11 \quad N_1 = 10 \quad S_2 = 10 \quad N_2 = 10 \quad S_3 = 18 \quad N_3 = 20$$



$$x_1 = x_2 = x_3$$

$$x_2 = x_3$$

$$x_1 = x_3$$

$$(2) \quad f_1 \rightarrow x_1: S_1 = 28 \quad N_1 = 30$$

$$f_1 \rightarrow x_2: S_2 = 29 \quad N_2 = 30$$

$$f_1 \rightarrow x_3: S_3 = 21 \quad N_3 = 20$$

$$f_2 \rightarrow x_2: S_2 = 18 \quad N_2 = 20$$

$$f_2 \rightarrow x_3: S_3 = 10 \quad N_3 = 10$$

$$f_3 \rightarrow x_1: S_1 = 18 \quad N_1 = 20$$

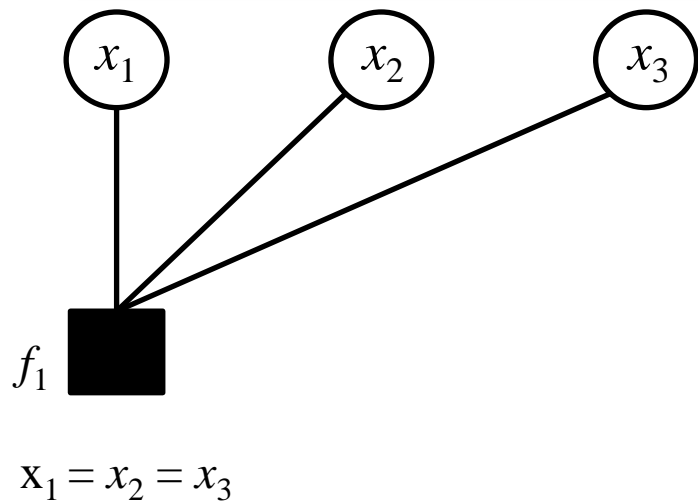
$$f_3 \rightarrow x_3: S_3 = 11 \quad N_3 = 10$$

$$(3) \quad S_1 = 57 \quad N_1 = 60 \quad S_2 = 57 \quad N_2 = 60 \quad S_3 = 60 \quad N_3 = 60$$


---

# Factor Graph for Belief Aggregation

---



$$(1) \quad x_1 \sim \mathcal{N}(m_1, \Sigma_1) \quad x_2 \sim \mathcal{N}(m_2, \Sigma_2)$$

$$x_3 \sim \mathcal{N}(m_3, \Sigma_3)$$

$$(2) \quad f_{1 \rightarrow x_1}:$$

$$\hat{\Sigma}_1^{-1} = \Sigma_2^{-1} + \Sigma_3^{-1} \quad \hat{\Sigma}_1^{-1} \hat{m}_1 = \Sigma_2^{-1} m_2 + \Sigma_3^{-1} m_3$$

$$f_{1 \rightarrow x_2}:$$

$$\hat{\Sigma}_2^{-1} = \Sigma_1^{-1} + \Sigma_3^{-1} \quad \hat{\Sigma}_2^{-1} \hat{m}_2 = \Sigma_1^{-1} m_1 + \Sigma_3^{-1} m_3$$

$$f_{1 \rightarrow x_3}:$$

$$\hat{\Sigma}_3^{-1} = \Sigma_1^{-1} + \Sigma_2^{-1} \quad \hat{\Sigma}_3^{-1} \hat{m}_3 = \Sigma_1^{-1} m_1 + \Sigma_2^{-1} m_2$$

$$(3)$$

$$\bar{\Sigma}_1^{-1} = \Sigma_1^{-1} + \hat{\Sigma}_1^{-1} \quad \bar{\Sigma}_1^{-1} \bar{m}_1 = \Sigma_1^{-1} m_1 + \hat{\Sigma}_1^{-1} \hat{m}_1$$

$$\bar{\Sigma}_2^{-1} = \Sigma_2^{-1} + \hat{\Sigma}_2^{-1} \quad \bar{\Sigma}_2^{-1} \bar{m}_2 = \Sigma_2^{-1} m_2 + \hat{\Sigma}_2^{-1} \hat{m}_2$$

$$\bar{\Sigma}_3^{-1} = \Sigma_3^{-1} + \hat{\Sigma}_3^{-1} \quad \bar{\Sigma}_3^{-1} \bar{m}_3 = \Sigma_3^{-1} m_3 + \hat{\Sigma}_3^{-1} \hat{m}_3$$


---

# Markov Decision Process

---

			+0
			-1
START			

# MDP Model

0	1	2	3
4	5	6	7
8	9	10	11

- a) Position 3: reward = 0 for any action
- b) Positions 5 and 7: wall, reward = -1
- c) reward = - 0.1 for each step in other states
- d) action = {up/0, down/1, left/2, right/3}

## transition probabilities:

$$\{x: \{u_1: (x', p(x'|x, u_1), r), u_2: (x', p(x'|x, u_2), r), \\ u_3: (x', p(x'|x, u_3), r), u_4: (x', p(x'|x, u_4), r) \} \}$$

```
{0: {0: (0, 1.0, -0.1), 1: (4, 1.0, -0.1), 3: (1, 1.0, -0.1), 2: (0, 1.0, -0.1)}, 1: {0: (1, 1.0, -0.1), 1: (1, 1.0, -1), 3: (2, 1.0, -0.1), 2: (0, 1.0, -0.1)}, 2: {0: (2, 1.0, -0.1), 1: (6, 1.0, -0.1), 3: (3, 1.0, -0.1), 2: (1, 1.0, -0.1)}, 3: {0: (3, 1.0, 0), 1: (3, 1.0, 0), 3: (3, 1.0, 0), 2: (3, 1.0, 0)}, 4: {0: (0, 1.0, -0.1), 1: (8, 1.0, -0.1), 3: (4, 1.0, -1), 2: (4, 1.0, -0.1)}, 5: {0: (1, 1.0, -0.1), 1: (9, 1.0, -0.1), 3: (6, 1.0, -0.1), 2: (4, 1.0, -0.1)}, 6: {0: (2, 1.0, -0.1), 1: (10, 1.0, -0.1), 3: (6, 1.0, -1), 2: (6, 1.0, -1)}, 7: {0: (3, 1.0, -0.1), 1: (11, 1.0, -0.1), 3: (7, 1.0, -1), 2: (6, 1.0, -0.1)}, 8: {0: (4, 1.0, -0.1), 1: (8, 1.0, -0.1), 3: (9, 1.0, -0.1), 2: (8, 1.0, -0.1)}, 9: {0: (9, 1.0, -1), 1: (9, 1.0, -0.1), 3: (10, 1.0, -0.1), 2: (8, 1.0, -0.1)}, 10: {0: (6, 1.0, -0.1), 1: (10, 1.0, -0.1), 3: (11, 1.0, -0.1), 2: (9, 1.0, -0.1)}, 11: {0: (11, 1.0, -1), 1: (11, 1.0, -0.1), 3: (11, 1.0, -0.1), 2: (10, 1.0, -0.1)}}
```



# Value Iteration (I)

---

Value Function  $V^0$

0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0

0	1	2	3
4	5	6	7
8	9	10	11

$$V^0(0) = 0.0$$

$$V^1(0) = -0.1$$

$$r(0, \text{up}) + V^0(0) * p(0|0, \text{up}) = -0.1 + (-0.0) * 1 = -0.1$$

$$r(0, \text{do}) + V^0(4) * p(4|0, \text{do}) = -0.1 + (-0.0) * 1 = -0.1$$

$$r(0, \text{rig}) + V^0(1) * p(1|0, \text{rig}) = -0.1 + (-0.0) * 1 = -0.1$$

$$r(0, \text{lef}) + V^0(0) * p(0|0, \text{lef}) = -0.1 + (-0.0) * 1 = -0.1$$

$$V^0(1) = 0.0$$

$$V^1(1) = -0.1$$

$$r(1, \text{up}) + V^0(1) * p(1|1, \text{up}) = -0.1 + (-0.0) * 1 = -0.1$$

$$r(1, \text{do}) + V^0(1) * p(1|1, \text{do}) = -1.0 + (-0.0) * 1 = -1.0$$

$$r(1, \text{rig}) + V^0(2) * p(2|1, \text{rig}) = -0.1 + (-0.0) * 1 = -0.1$$

$$r(1, \text{lef}) + V^0(0) * p(0|1, \text{lef}) = -0.1 + (-0.0) * 1 = -0.1$$

---

# Value Iteration (II)

---

Value Function  $V^1$

- 0.1	- 0.1	- 0.1	0.0
- 0.1	0.0	- 0.1	0.0
- 0.1	- 0.1	- 0.1	- 0.1

$$V^1(0) = - 0.1$$

$$V^2(0) = - 0.2$$

$$r(0, \text{up}) + V^1(0) * p(0|0, \text{up}) = - 0.1 + (- 0.1) * 1 = - 0.2$$

$$r(0, \text{do}) + V^1(4) * p(4|0, \text{do}) = - 0.1 + (- 0.1) * 1 = - 0.2$$

$$r(0, \text{rig}) + V^1(1) * p(1|0, \text{rig}) = - 0.1 + (- 0.1) * 1 = - 0.2$$

$$r(0, \text{lef}) + V^1(0) * p(0|0, \text{lef}) = - 0.1 + (- 0.1) * 1 = - 0.2$$

0	1	2	3
4	5	6	7
8	9	10	11

$$V^1(1) = - 0.1$$

$$V^2(1) = - 0.2$$

$$r(1, \text{up}) + V^1(1) * p(1|1, \text{up}) = - 0.1 + (- 0.1) * 1 = - 0.2$$

$$r(1, \text{do}) + V^1(1) * p(1|1, \text{do}) = - 1.0 + (- 0.1) * 1 = - 1.1$$

$$r(1, \text{rig}) + V^1(2) * p(2|1, \text{rig}) = - 0.1 + (- 0.1) * 1 = - 0.2$$

$$r(1, \text{lef}) + V^1(0) * p(0|1, \text{lef}) = - 0.1 + (- 0.1) * 1 = - 0.2$$

---

# Value Iteration (III)

---

Value Function  $V^2$

- 0.2	- 0.2	- 0.1	0.0
- 0.2	0.0	- 0.2	0.0
- 0.2	- 0.2	- 0.2	- 0.2

$$V^2(0) = - 0.2$$

$$V^3(0) = - 0.3$$

$$r(0, \text{up}) + V^2(0) * p(0|0, \text{up}) = - 0.1 + (- 0.2) * 1 = - 0.3$$

$$r(0, \text{do}) + V^2(4) * p(4|0, \text{do}) = - 0.1 + (- 0.2) * 1 = - 0.3$$

$$r(0, \text{rig}) + V^2(1) * p(1|0, \text{rig}) = - 0.1 + (- 0.2) * 1 = - 0.3$$

$$r(0, \text{lef}) + V^2(0) * p(0|0, \text{lef}) = - 0.1 + (- 0.2) * 1 = - 0.3$$

0	1	2	3
4	5	6	7
8	9	10	11

$$V^2(1) = - 0.2$$

$$V^3(1) = - 0.2$$

$$r(1, \text{up}) + V^2(1) * p(1|1, \text{up}) = - 0.1 + (- 0.2) * 1 = - 0.3$$

$$r(1, \text{do}) + V^2(1) * p(1|1, \text{do}) = - 1.0 + (- 0.2) * 1 = - 1.2$$

$$r(1, \text{rig}) + V^2(2) * p(2|1, \text{rig}) = - 0.1 + (- 0.1) * 1 = - 0.2$$

$$r(1, \text{lef}) + V^2(0) * p(0|1, \text{lef}) = - 0.1 + (- 0.2) * 1 = - 0.3$$

---

# Value Iteration (IV)

---

Value Function  $V^3$

- 0.3	- 0.2	- 0.1	0.0
- 0.3	0.0	- 0.2	0.0
- 0.3	- 0.3	- 0.3	- 0.3

$$V^3(0) = - 0.2$$

$$V^4(0) = - 0.3$$

$$r(0, \text{up}) + V^3(0) * p(0|0, \text{up}) = - 0.1 + (- 0.3) * 1 = - 0.4$$

$$r(0, \text{do}) + V^3(4) * p(4|0, \text{do}) = - 0.1 + (- 0.3) * 1 = - 0.4$$

$$r(0, \text{rig}) + V^3(1) * p(1|0, \text{rig}) = - 0.1 + (- 0.2) * 1 = - 0.3$$

$$r(0, \text{lef}) + V^3(0) * p(0|0, \text{lef}) = - 0.1 + (- 0.3) * 1 = - 0.4$$

0	1	2	3
4	5	6	7
8	9	10	11

$$V^3(1) = - 0.2$$

$$V^4(1) = - 0.2$$

$$r(1, \text{up}) + V^3(1) * p(1|1, \text{up}) = - 0.1 + (- 0.2) * 1 = - 0.3$$

$$r(1, \text{do}) + V^3(1) * p(1|1, \text{do}) = - 1.0 + (- 0.2) * 1 = - 1.2$$

$$r(1, \text{rig}) + V^3(2) * p(2|1, \text{rig}) = - 0.1 + (- 0.1) * 1 = - 0.2$$

$$r(1, \text{lef}) + V^3(0) * p(0|1, \text{lef}) = - 0.1 + (- 0.3) * 1 = - 0.4$$

---

# Value Iteration (V)

---

Value Function  $V^4$

- 0.3	- 0.2	- 0.1	0.0
- 0.4	0.0	- 0.2	0.0
- 0.4	- 0.4	- 0.3	- 0.4

$$V^4(0) = - 0.2$$

$$V^5(0) = - 0.3$$

$$r(0, \text{up}) + V^1(0) * p(0|0, \text{up}) = - 0.1 + (- 0.3) * 1 = - 0.4$$

$$r(0, \text{do}) + V^1(4) * p(4|0, \text{do}) = - 0.1 + (- 0.4) * 1 = - 0.5$$

$$r(0, \text{rig}) + V^1(1) * p(1|0, \text{rig}) = - 0.1 + (- 0.2) * 1 = - 0.3$$

$$r(0, \text{lef}) + V^1(0) * p(0|0, \text{lef}) = - 0.1 + (- 0.3) * 1 = - 0.4$$

0	1	2	3
4	5	6	7
8	9	10	11

$$V^4(1) = - 0.2$$

$$V^5(1) = - 0.2$$

$$r(1, \text{up}) + V^1(1) * p(1|1, \text{up}) = - 0.1 + (- 0.2) * 1 = - 0.3$$

$$r(1, \text{do}) + V^1(1) * p(1|1, \text{do}) = - 1.0 + (- 0.2) * 1 = - 1.2$$

$$r(1, \text{rig}) + V^1(2) * p(2|1, \text{rig}) = - 0.1 + (- 0.1) * 1 = - 0.2$$

$$r(1, \text{lef}) + V^1(0) * p(0|1, \text{lef}) = - 0.1 + (- 0.3) * 1 = - 0.4$$

---

# Stationary Value Function

---

Stationary Value Function

- 0.3	- 0.2	- 0.1	0.0
- 0.4	0.0	- 0.2	0.0
- 0.5	- 0.4	- 0.3	- 0.4

$$V(0) = - 0.3$$

$$r(0, \text{up}) + V(0) * p(0|0, \text{up}) = - 0.1 + (- 0.3) * 1 = - 0.4$$

$$r(0, \text{do}) + V(4) * p(4|0, \text{do}) = - 0.1 + (- 0.4) * 1 = - 0.5$$

$$r(0, \text{rig}) + V(1) * p(1|0, \text{rig}) = - 0.1 + (- 0.2) * 1 = - 0.3$$

$$r(0, \text{lef}) + V(0) * p(0|0, \text{lef}) = - 0.1 + (- 0.3) * 1 = - 0.4$$

0	1	2	3
4	5	6	7
8	9	10	11

$$V(1) = - 0.2$$

$$r(1, \text{up}) + V(1) * p(1|1, \text{up}) = - 0.1 + (- 0.2) * 1 = - 0.3$$

$$r(1, \text{do}) + V(1) * p(1|1, \text{do}) = - 1.0 + (- 0.2) * 1 = - 1.0$$

$$r(1, \text{rig}) + V(2) * p(2|1, \text{rig}) = - 0.1 + (- 0.1) * 1 = - 0.2$$

$$r(1, \text{lef}) + V(0) * p(0|1, \text{lef}) = - 0.1 + (- 0.3) * 1 = - 0.4$$

---

# Optimal Policy for Value Iteration

---

Stationary Value Function

-0.3	-0.2	-0.1	0.0
-0.4	-0.0	-0.2	-0.0
-0.5	-0.4	-0.3	-0.4

$$V(0) = -0.3$$

Optimal Action: right →

$$r(0, \text{up}) + V(0) * p(0|0, \text{up}) = -0.1 + (-0.3) * 1 = -0.4$$

$$r(0, \text{do}) + V(4) * p(4|0, \text{do}) = -0.1 + (-0.4) * 1 = -0.5$$

$$r(0, \text{rig}) + V(1) * p(1|0, \text{rig}) = -0.1 + (-0.2) * 1 = -0.3$$

$$r(0, \text{lef}) + V(0) * p(1|0, \text{lef}) = -0.1 + (-0.3) * 1 = -0.4$$

Optimal Policy

→	→	→	●
↑	□	↑	□
↑ →	→	↑	←

$$V(1) = -0.2$$

Optimal Action: right →

$$r(1, \text{up}) + V(1) * p(1|1, \text{up}) = -0.1 + (-0.2) * 1 = -0.3$$

$$r(1, \text{do}) + V(1) * p(1|1, \text{do}) = -1.0 + (-0.0) * 1 = -1.0$$

$$r(1, \text{rig}) + V(2) * p(2|1, \text{rig}) = -0.1 + (-0.1) * 1 = -0.2$$

$$r(1, \text{lef}) + V(0) * p(0|1, \text{lef}) = -0.1 + (-0.3) * 1 = -0.4$$


---

# Policy Iteration

---

- ❑ Often the optimal policy has been reached long before the value function has converged.
- ❑ Policy iteration (1) calculates a new policy based on the current value function and (2) then calculates a new value function based on this policy.

(1) Policy improvement  $\pi^* = \operatorname{argmax}_{\pi} R_T^{\pi}(x_t)$

(2) Policy evaluation  $R_T^{\pi}(x_t) = E \left[ \sum_{\tau=1}^T \gamma^{\tau} r_{t+\tau} \mid u_{t+\tau} = \pi(z_{1:t+\tau-1} u_{1:t+\tau-1}) \right]$

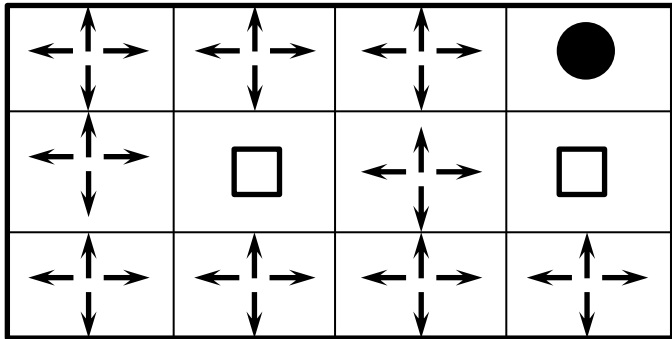
- ❑ Often converges faster to the optimal policy.
-



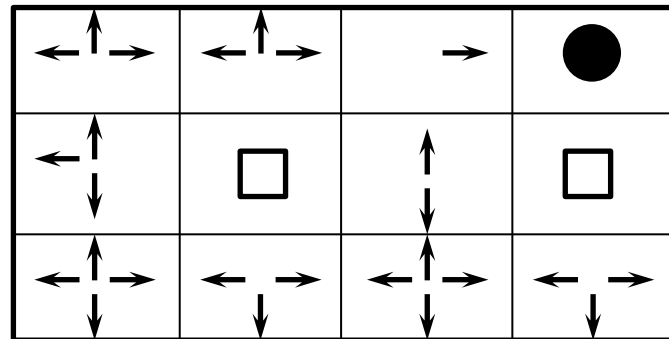
# Policy Iteration (I)

---

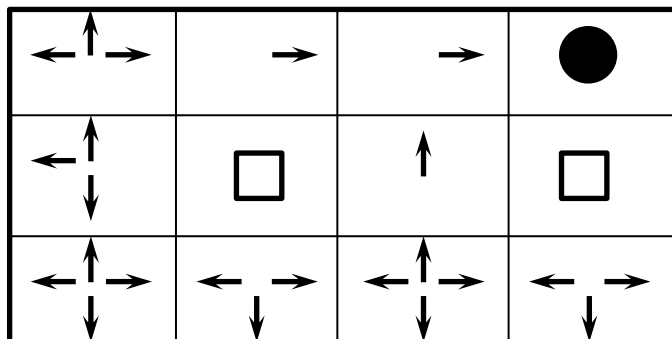
Policy  $\pi^0$



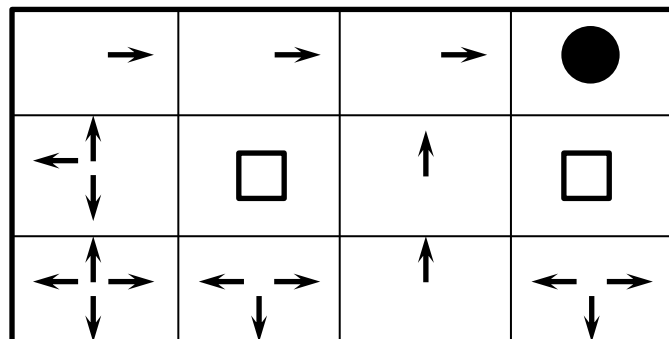
Policy  $\pi^1$



Policy  $\pi^2$



Policy  $\pi^3$



# Policy Iteration (II)

---

Policy  $\pi^4$

→	→	→	●
↑	□	↑	□
↕	→	↑	←

Policy  $\pi^5$

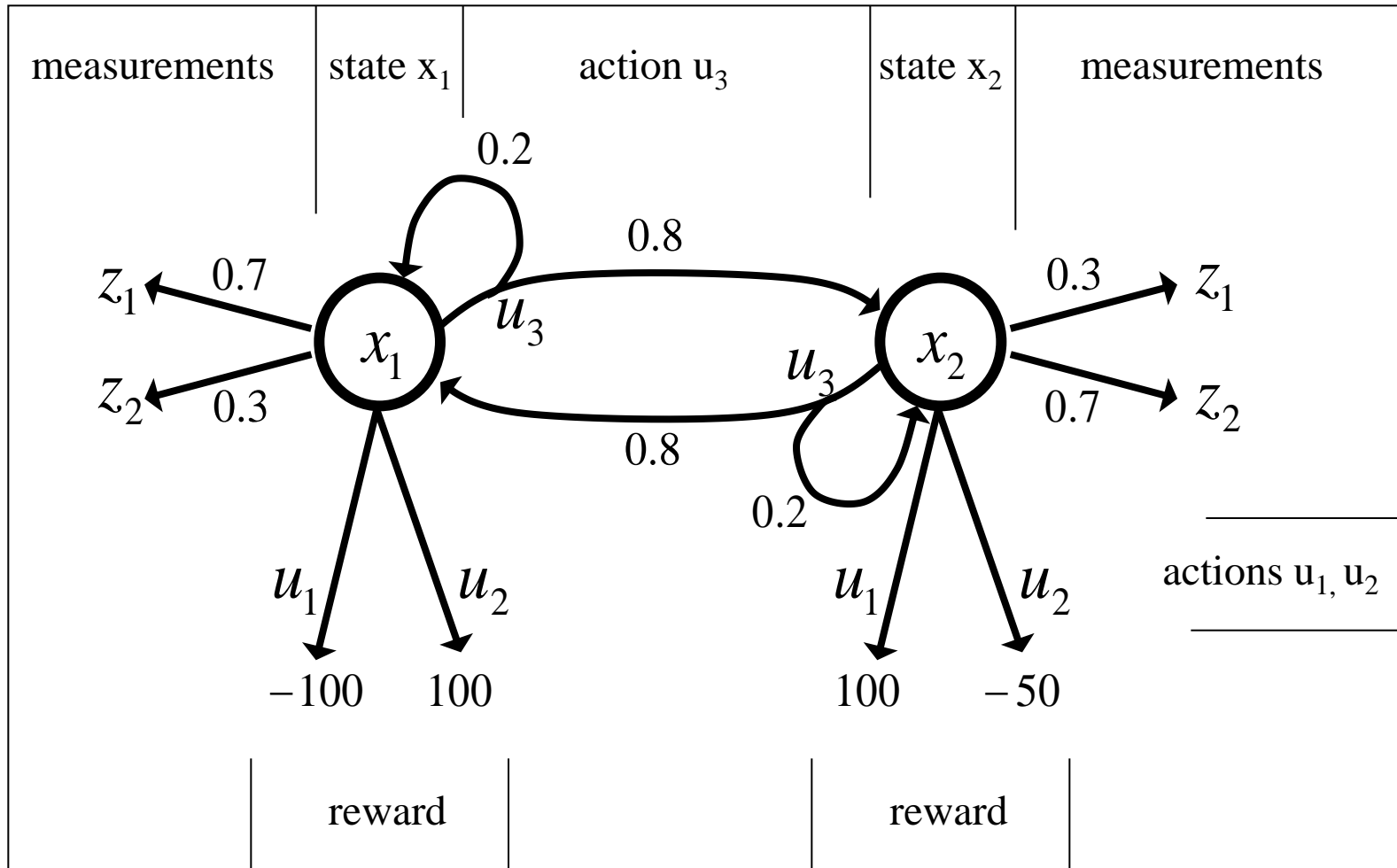
→	→	→	●
↑	□	↑	□
↑→	→	↑	←

Value Function

-0.3	-0.2	-0.1	0.0
-0.4	-0.0	-0.2	-0.0
-0.5	-0.4	-0.3	-0.4

---

# Partially Observable MDP



# More Course Links

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## **Stanford Machine Learning:**

<https://see.stanford.edu/Course/CS229/47>

**MIT Machine Learning:** <https://ocw.mit.edu/courses/electrical-engineering-and-computer-science/6-867-machine-learning-fall-2006/index.htm>

**Stanford CNN for Vision:** <http://cs231n.stanford.edu>

**Stanford Deep Learning:** <http://cs230.stanford.edu/syllabus.html>

**MIT Deep Learning:** <http://introtodeeplearning.com/>

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