Machine Learning
CS 4900/5900

Lecture 01

Razvan C. Bunescu

School of Electrical Engineering and Computer Science

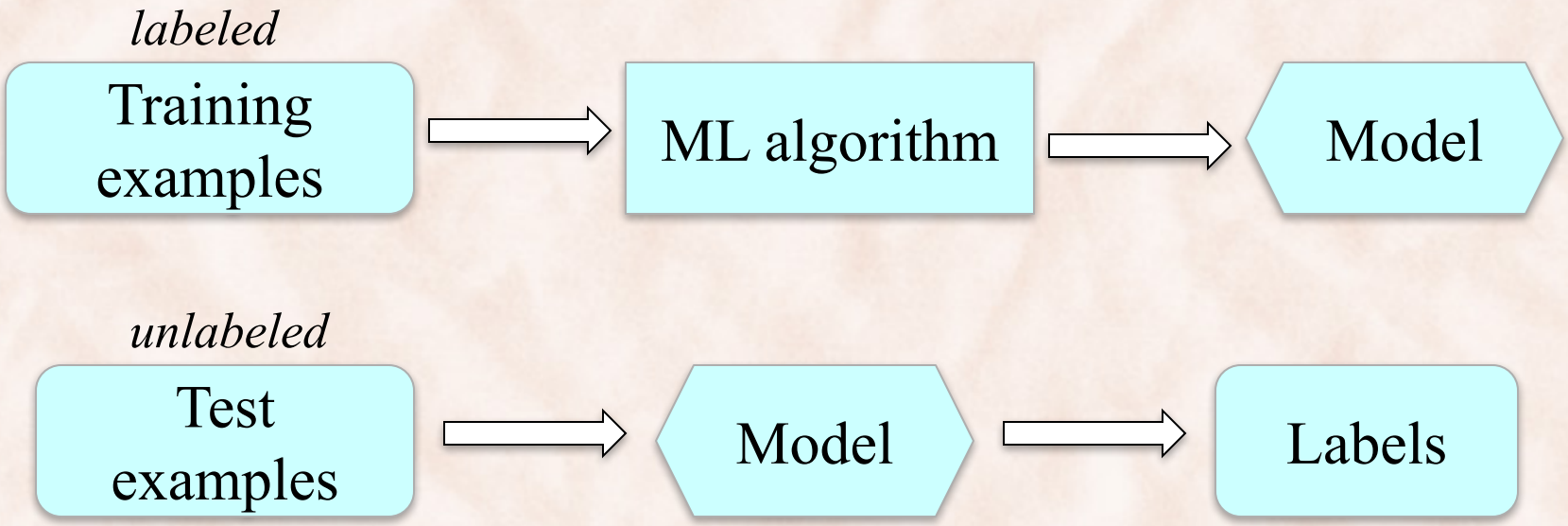
bunescu@ohio.edu

What is (Human) Learning?

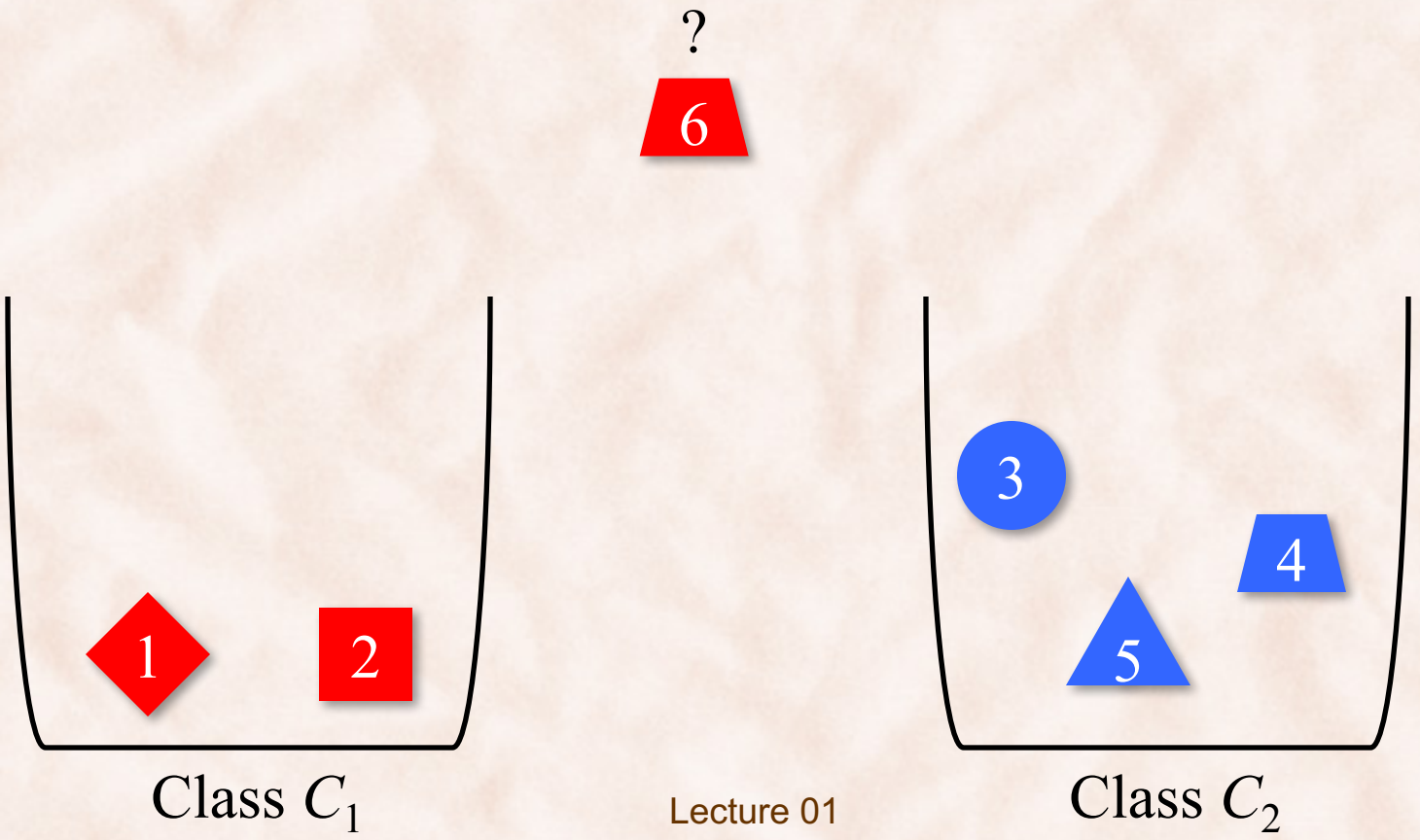
- Merriam-Webster:
  - ***learn*** = to acquire knowledge, understanding, or skill … by study, instruction, or ***experience***.
- Why do we learn?
  - to ***improve performance*** on a given ***task***.
- What (tasks) do we learn:
  1. categorize email, recognize faces, diagnose diseases, translate, …
  2. clustering (fish, insects, birds, mice, humans), summarization, sound source separation, …
  3. walk, play backgammon, ride bikes, drive cars, fly helicopters, …

What is Machine Learning?

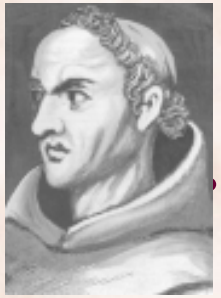
- **Machine Learning** = constructing computer programs that *automatically improve with experience*:
  - Supervised Learning i.e. learning from labeled examples.



What is Learning?



Occam's Razor



William of Occam (1288 – 1348)

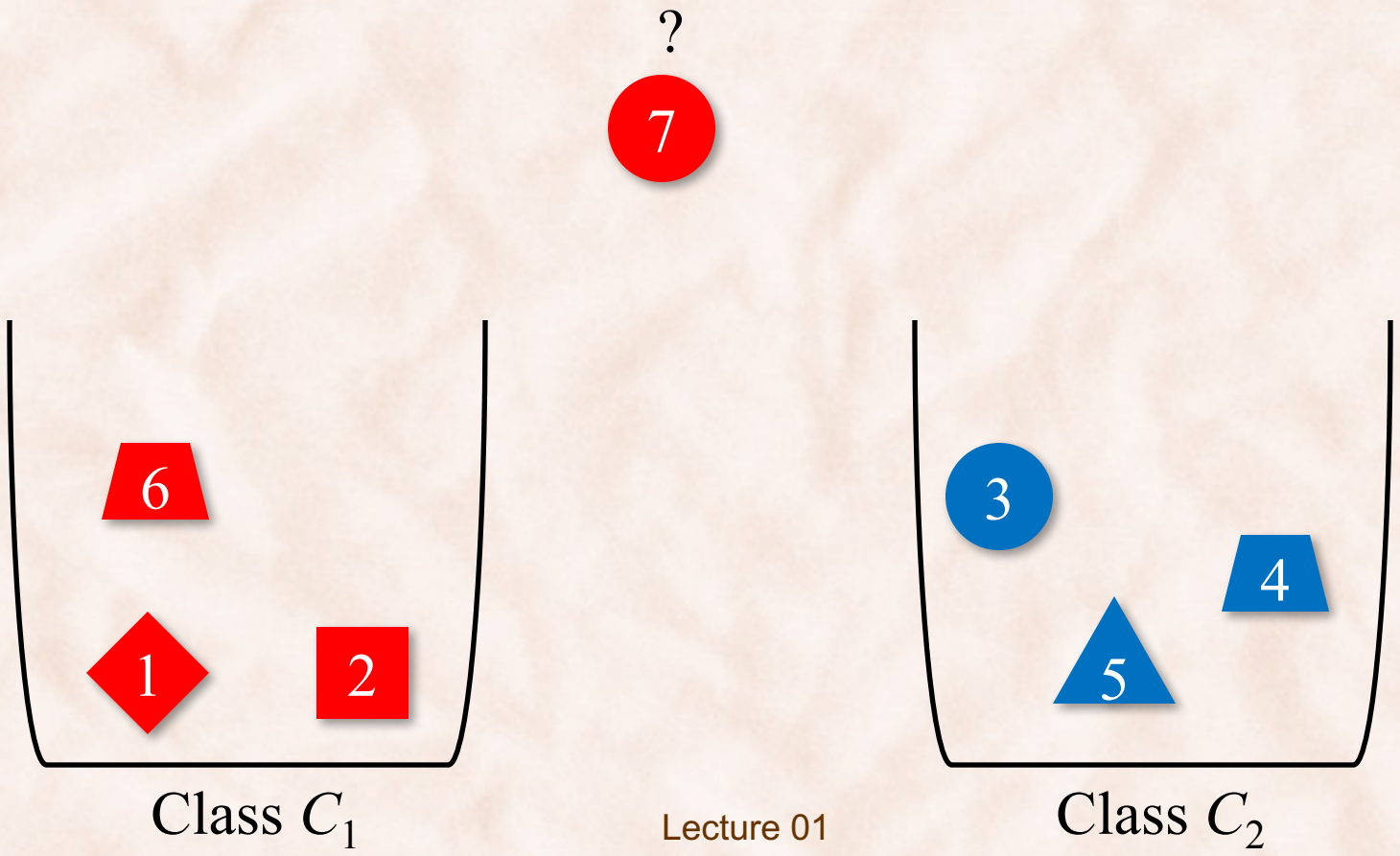
English Franciscan friar, theologian and philosopher.

- "*Entia non sunt multiplicanda praeter necessitatem*"
  - Entities must not be multiplied beyond necessity.

i.e. Do not make things needlessly complicated.

i.e. Prefer the simplest hypothesis that fits the data.

What is Learning?



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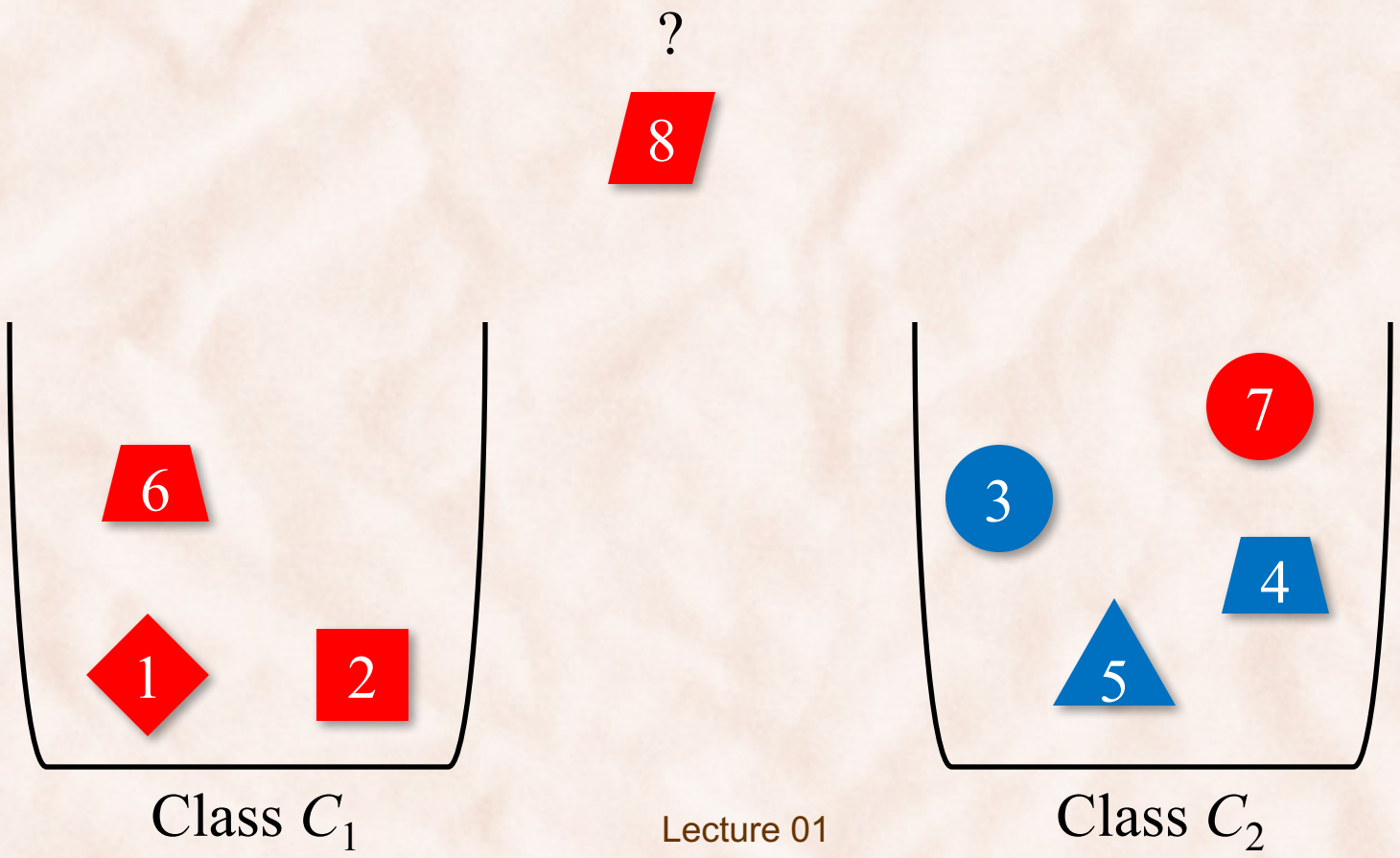

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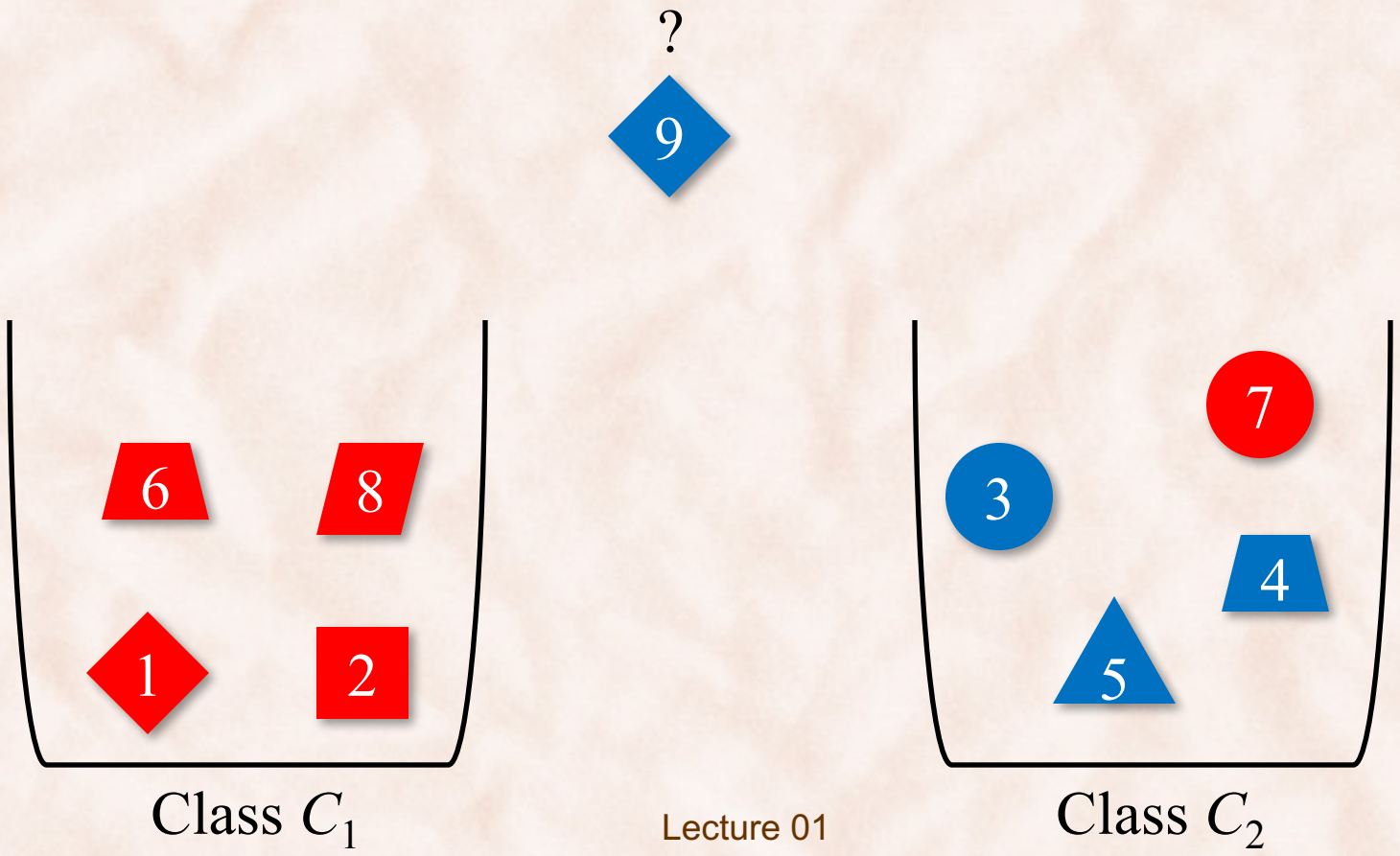

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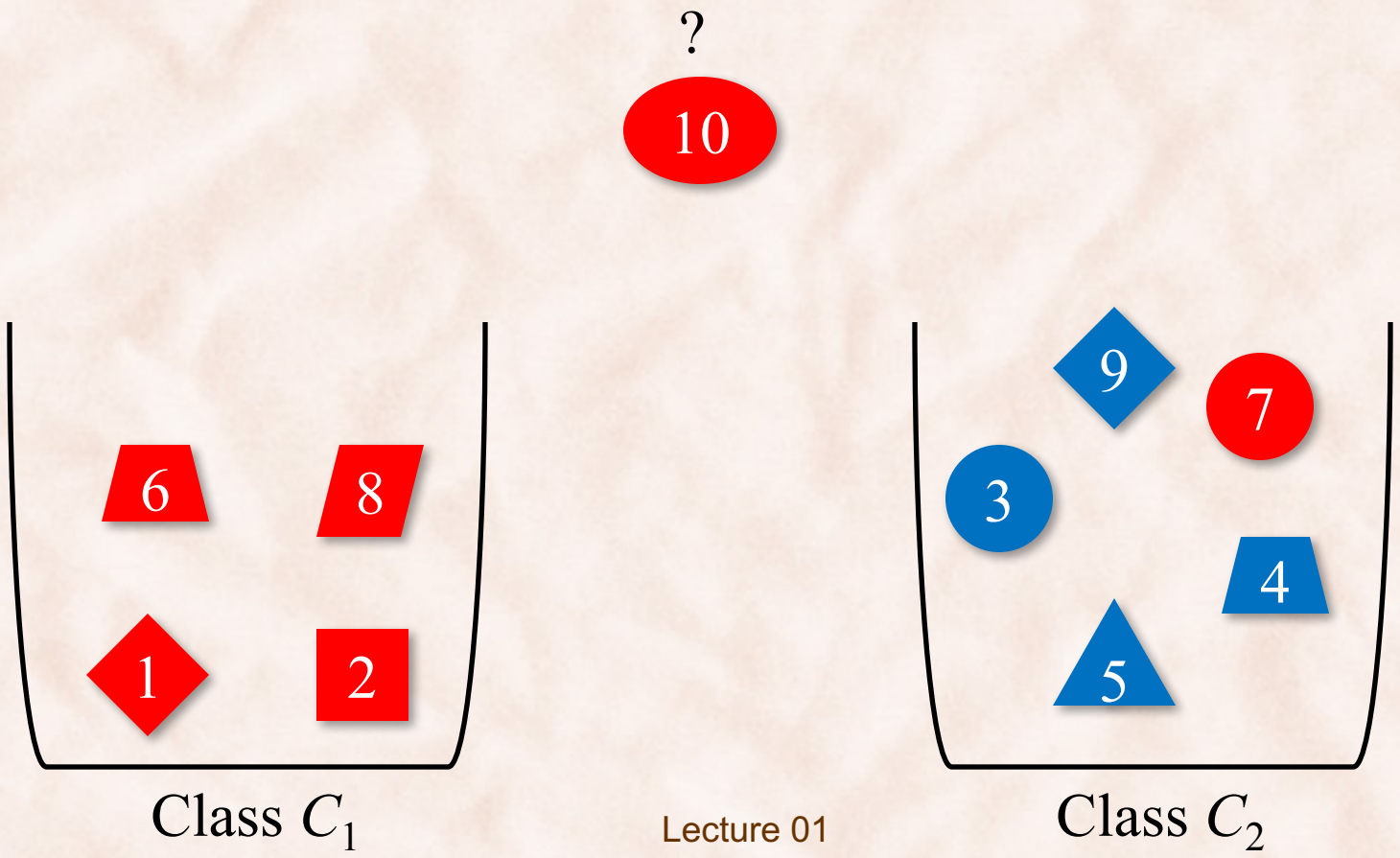
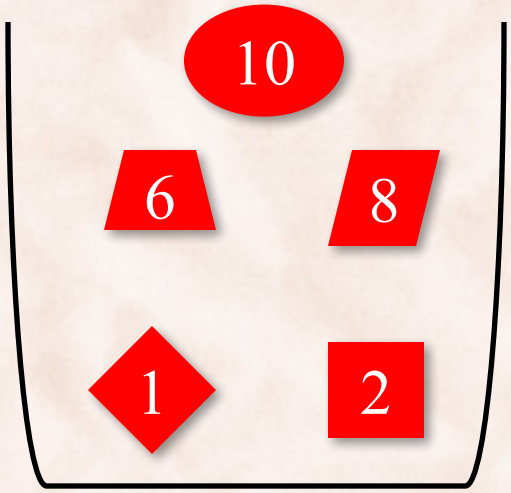
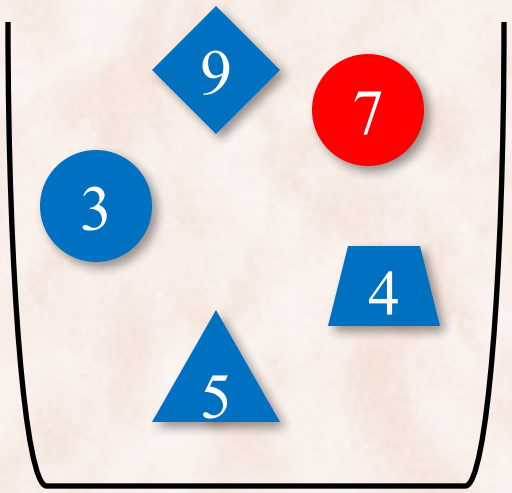


What is Learning?



Class C_1



Class C_2

ML Concepts & Notation

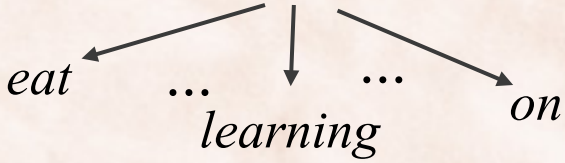
- A (labeled) example (**x**, t) consists of:
  - Instance / observation / raw feature vector **x**.
  - Label t.

- Examples:
  1. Digit recognition:

instance **x** = ?

label t = ?

  2. Language modelling:
     - "machine ..... is a hot topic in AI"



instance **x** = ?

label t = ?

ML Concepts & Notation

- Often, a raw observation $\mathbf{x}$ is pre-processed and further transformed into a feature vector $\varphi(\mathbf{x}) = [\varphi_1(\mathbf{x}), \varphi_1(\mathbf{x}), \ldots, \varphi_K(\mathbf{x})]^T$.
  - Where do the features φ_k come from?
    - Feature engineering, e.g. in polynomial curve fitting:
      - manual, can be time consuming (e.g. SIFT).
    - (Unsupervised) feature learning, e.g. in modern computer vision
      - automatic, used in deep learning models.

ML Concepts & Notation

- A training dataset is a set of (training) examples $(\mathbf{x}_1,t_1)$, $(\mathbf{x}_2,t_2)$, … $(\mathbf{x}_N,t_N)$:
  - The data matrix X contains all instance vectors $\mathbf{x}_1$, $\mathbf{x}_2$, …, $\mathbf{x}_N$ row-wise.
  - The label vector $\mathbf{t} = [t_1, t_2, \ldots, t_N]^T$.

- A test dataset is a set of (test) examples $(\mathbf{x}_{N+1},t_{N+1})$, …, $(\mathbf{x}_{N+M},t_{N+M})$:
  - **Must be different from the training examples**!

ML Concepts & Notation

- There is a function f that maps an instance $\mathbf{x}$ to its label $t = f(\mathbf{x})$.
  - f is unknown / not given.
  - But we observe samples from f: $(\mathbf{x}_1,t_1)$, $(\mathbf{x}_2,t_2)$, … $(\mathbf{x}_N,t_N)$.

- Learning means finding a model h that maps an instance $\mathbf{x}$ to a label $h(\mathbf{x}) \approx f(\mathbf{x})$, i.e. close to the true label of $\mathbf{x}$.
  - Machine learning = finding a model h that approximates well the unknown function f.
  - Machine learning = function approximation!

ML Concepts & Notation

- Machine learning is inductive:
  - Inductive hypothesis: if a model performs well on training examples, it is expected to also perform well on unseen (test) examples.

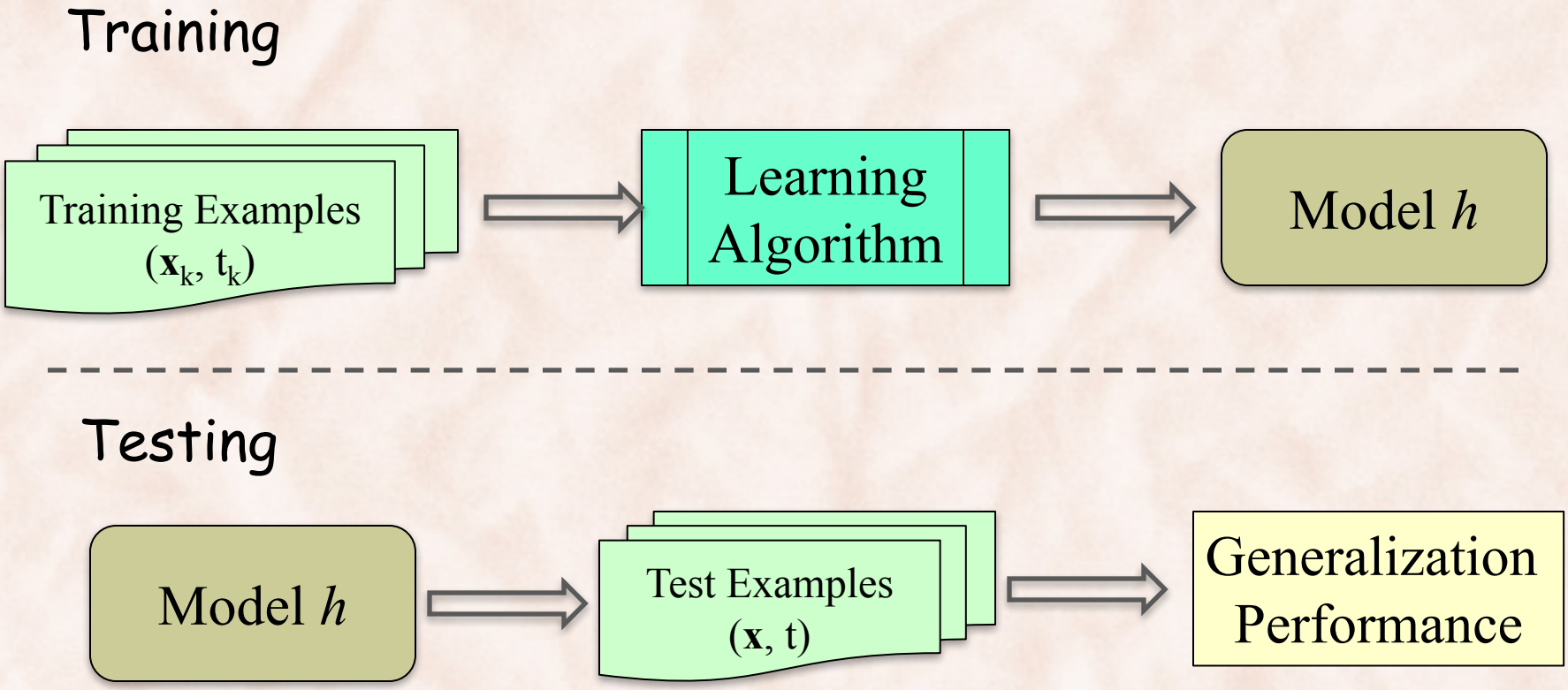
- The model y is often specified through a set of parameters $\mathbf{w}$:
  - $\mathbf{x}$ is mapped by the model to $h(\mathbf{x}, \mathbf{w})$.

- The objective function $J(\mathbf{w})$ captures how poorly the model does on the training dataset:
  - Want to find $\hat{\mathbf{w}} = \underset{\mathbf{w}}{\operatorname{argmin}} J(\mathbf{w})$
    - Machine learning = optimization!

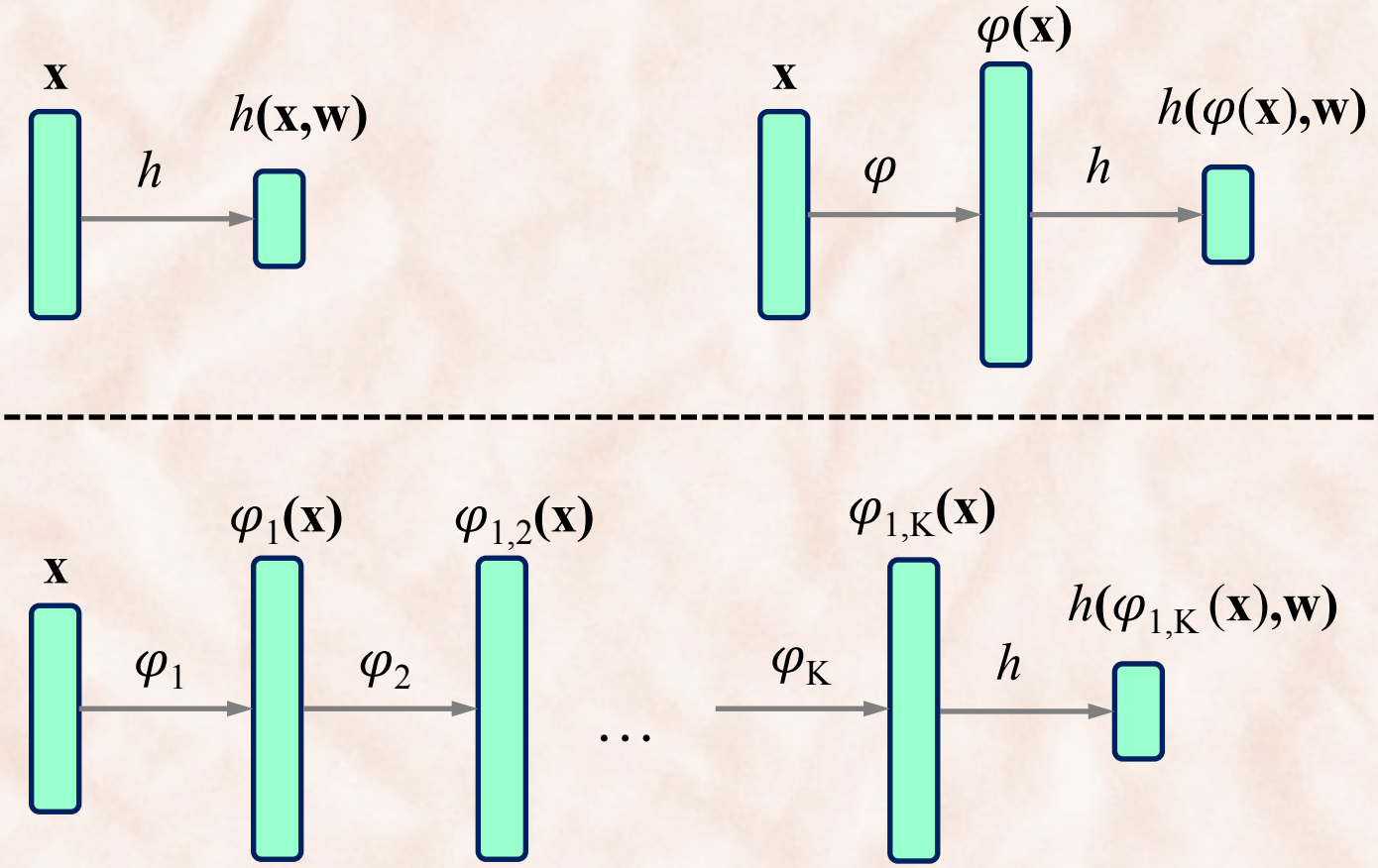
Fitting vs. Generalization

- Fitting performance = how well the model performs on training examples.
- Generalization performance = how well the model performs on unseen (test) examples.
- We are interested in **Generalization**:
  - Prefer finding patterns to memorizing examples!
    - Overfitting:
    - Regularization:

Supervised Learning



Machine Learning vs. Deep Learning



What is Machine Learning?

- **Machine Learning** = constructing computer programs that *automatically improve with experience*:
  - Supervised Learning i.e. learning from labeled examples:
    - Classification
    - Regression
  - Unsupervised Learning i.e. learning from unlabeled examples:
    - Clustering.
    - Dimensionality reduction (visualization).
    - Density estimation.
  - Reinforcement Learning i.e. learning with delayed feedback.

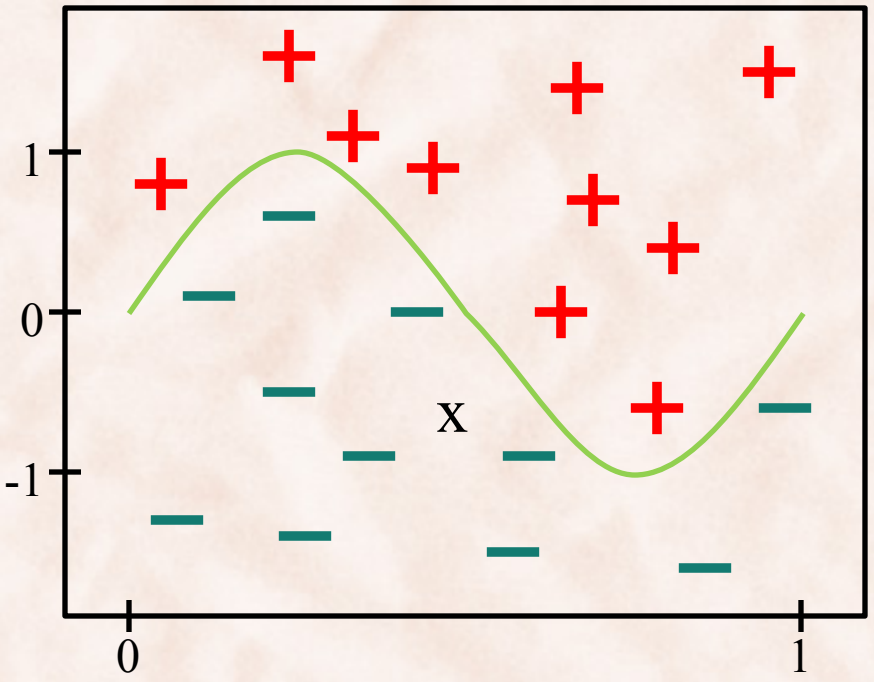
Supervised Learning

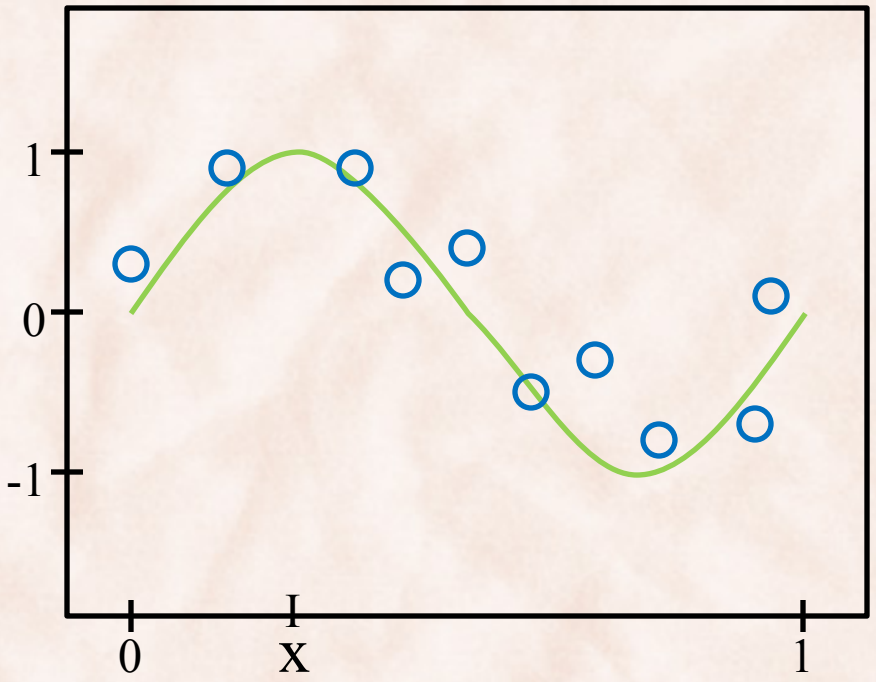
- Task = learn a function f : X $\rightarrow$ T that maps input instances $\mathbf{x} \in$ X to output targets $t \in$ T:
  - **Classification**:
    - The output $t \in$ T is one of a finite set of discrete categories.
  - **Regression**:
    - The output $t \in$ T is continuous, or has a continuous component.

- Supervision = set of training examples:

$$(\mathbf{x}_1, t_1),\ (\mathbf{x}_2, t_2),\ \ldots\ (\mathbf{x}_n, t_n)$$

Classification vs. Regression





Classification: Junk Email Filtering

[Sahami, Dumais & Heckerman, AAAI'98]

From: Tammy Jordan
jordant@oak.cats.ohiou.edu
Subject: Spring 2015 Course

CS690: Machine Learning

Instructor: Razvan Bunescu
Email: bunescu@ohio.edu
Time and Location: Tue, Thu 9:00 AM , ARC 101
Website: http://ace.cs.ohio.edu/~razvan/courses/ml6830

Course description:
Machine Learning is concerned with the design and analysis of algorithms that enable computers to automatically find patterns in the data. This introductory course will give an overview …

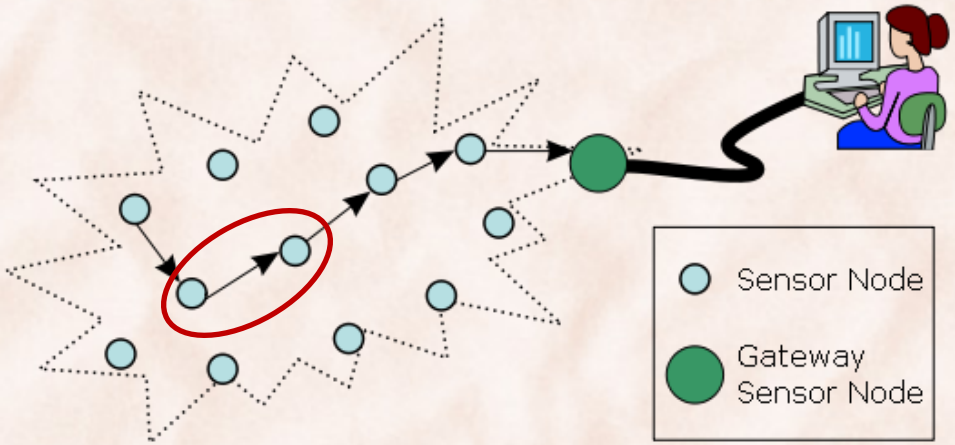
From: UK National Lottery
edreyes@uknational.co.uk
Subject: Award Winning Notice

UK NATIONAL LOTTERY. GOVERNMENT ACCREDITED LICENSED LOTTERY. REGISTERED UNDER THE UNITED KINGDOM DATA PROTECTION ACT;

We happily announce to you the draws of (UK NATIONAL LOTTERY PROMOTION) International programs held in London , England Your email address attached to ticket number :3456 with serial number :7576/06 drew the lucky number 4-2-274, which subsequently won you the lottery in the first category …

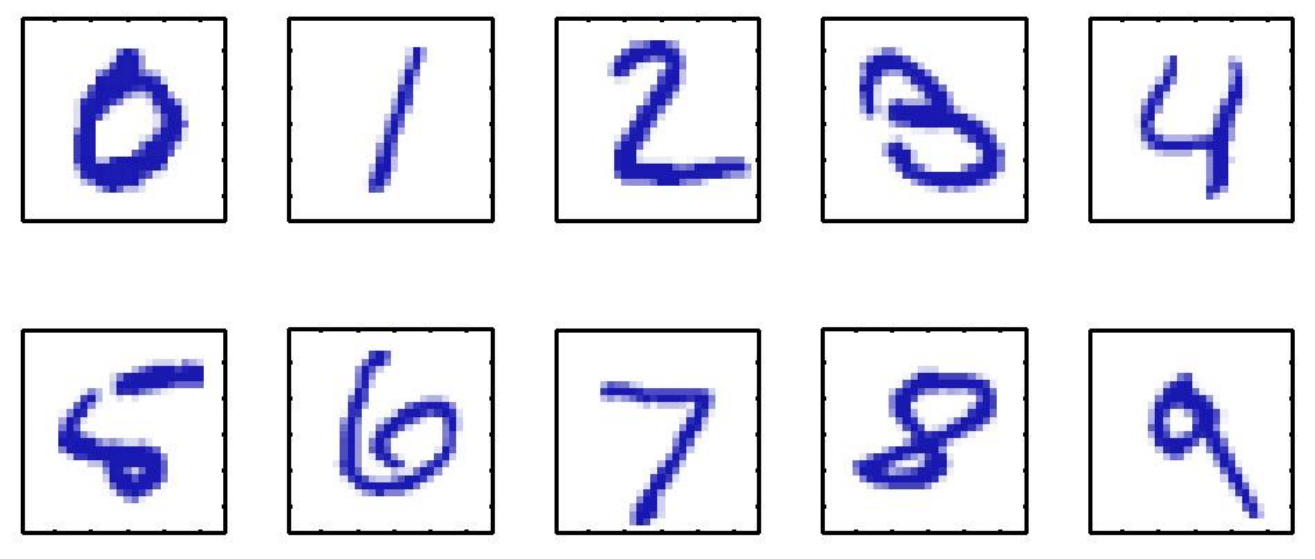
- Email filtering:
  - Provide emails labeled as *{Spam, Ham}*.
  - Train *Naïve Bayes* model to discriminate between the two.

Classification: Routing in Wireless Sensor Networks [Wang, Martonosi & Peh, SECON'06]



- Link quality prediction:
  - Provide a set of training links:
    - received signal strength, send/forward buffer sizes
    - node depth from base station, forward/backward probability
    - LQI = Link Quality Indication, binarized as {Good, Bad}
  - Train *Decision Trees* model to predict LQ using runtime features.

Classification: Handwritten Zip Code Recognition [Le Cun et al., Neural Computation '89]



- Handwritten digit recognition:
  - Provide images of handwritten digits, labeled as {0, 1, …, 9}.
  - Train *Neural Network* model to recognize digits from input images.

Classification: Medical Diagnosis

[Krishnapuram et al., GENSIPS'02]

- Cancer diagnosis from gene expression signatures:
  - Create database of gene expression profiles (X) from tissues of known cancer status (Y):
    - Human accute leukemia dataset:
      - http://www.broadinstitute.org/cgi-bin/cancer/datasets.cgi
    - Colon cancer microarray data:
      - http://microarray.princeton.edu/oncology
  - Train *Logistic Regression* / *SVM* / *RVM* model to classify the gene expression of a tissue of unknown cancer status.

ML for Software Verification / ATP

- Software verification requires theorem proving.
- Proving a mathematical theorem requires finding and using relevant previous theorems and definitions:
  - The space of existing theorems and definitions is huge.
  - Use machine learning to narrow the search space to relevant theorems and definitions:
    - "Premise Selection for Mathematics by Corpus Analysis and *Kernel Methods*", Alama et al., JAR 2012.
    - "DeepMath – *Deep Sequence* Models for Premise Selection", Alemi et al., NIPS 2016.

Software Verification / ATP for ML

- An ML model is a program i.e. ML algorithms induce programs.
- ML models such as (Deep) Neural Networks may lack robustness:
  - Adversarial methods can fool the networks, e.g. classifying a school bus as an ostrich.
  - Software verification / ATP methods can be used to prove an ML model has (or not) desirable properties:
    - "Reluplex: An Efficient SMT Solver for *Verifying Deep Neural Networks*", Katz et al., CAV 2017
      - Used to prove adversarial robustness for collision avoidance system for unmanned aircraft.

Classification: Other Examples

- Handwritten letter recognition
- Face recognition
- Credit card applications/transactions
- Recommender systems: books, music, …
- Fraud detection in e-commerce
- Worm detection in network packets
- Tone recognition
- Chord Recognition
- Named Entity Recognition

Regression: Examples

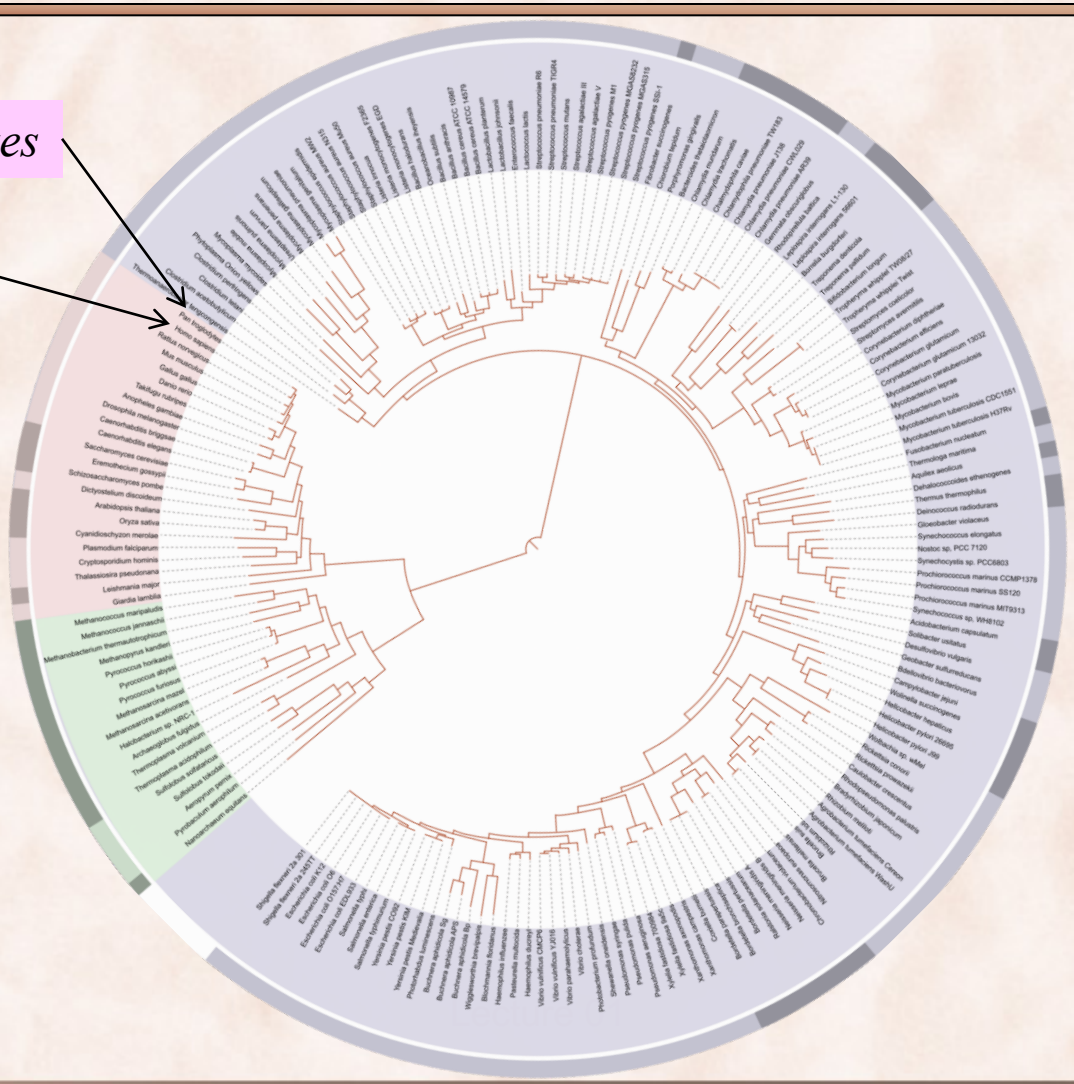
1. Stock market prediction:
   - Use the current stock market conditions ($x \in X$) to predict tomorrow's value of a particular stock ($t \in T$).
2. Oil price, GDP, income prediction.
3. Chemical processes:
   - Predict the yield in a chemical process based on the concentrations of reactants, temperature and pressure.

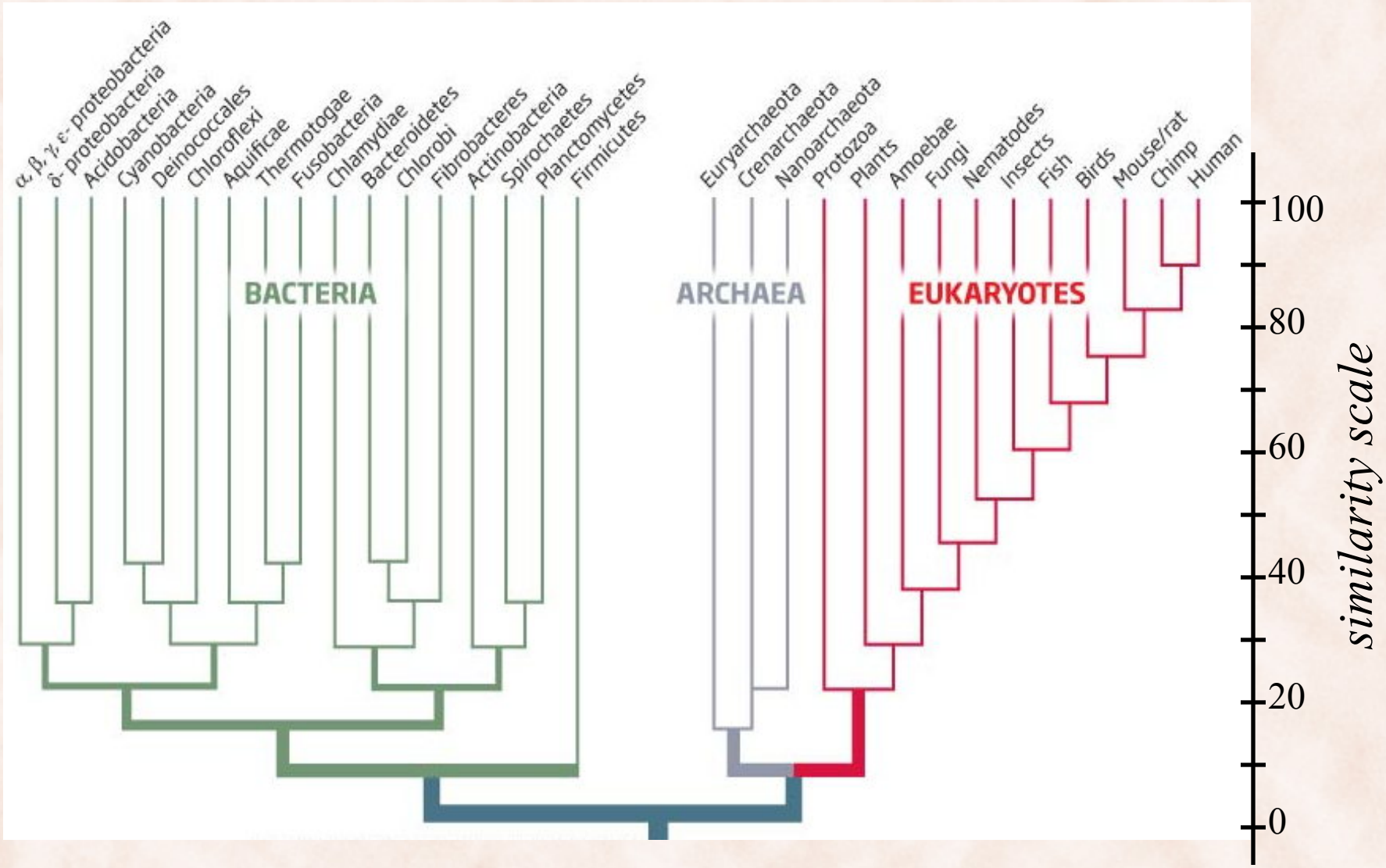
- Algorithms:
  - *Linear Regression*, *Neural Networks*, *Support Vector Machines*, …

Unsupervised Learning: Hierarchical Clustering

Pan Troglodytes

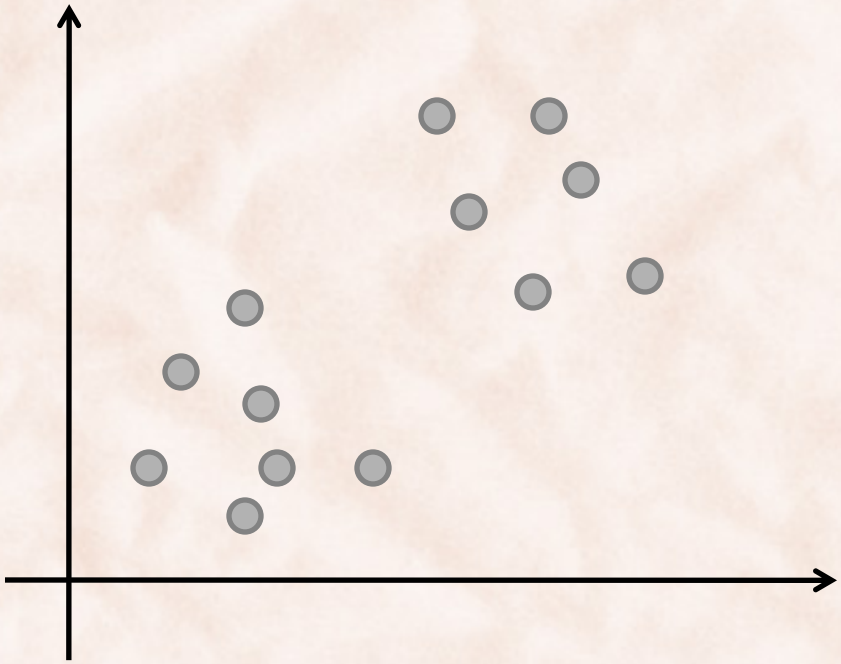
Homo Sapiens




α, β, γ, ε- proteobacteria
δ- proteobacteria
Acidobacteria
Cyanobacteria
Deinococcales
Chloroflexi
Aquificae
Thermotogae
Fusobacteria
Chlamydiae
Bacteroidetes
Chlorobi
Fibrobacteres
Actinobacteria
Spirochaetes
Planctomycetes
Firmicutes
BACTERIA
Euryarchaeota
Crenarchaeota
Nanoarchaeota
ARCHAEA
Protozoa
Plants
Amoebae
Fungi
Nematodes
Insects
Fish
Birds
Mouse/rat
Chimp
Human
EUKARYOTES
100
80
60
40
20
0
similarity scale

Unsupervised Learning: Clustering

- Partition unlabeled examples into disjoint clusters such that:
  - Examples in the same cluster are very similar.
  - Examples in different clusters are very different.



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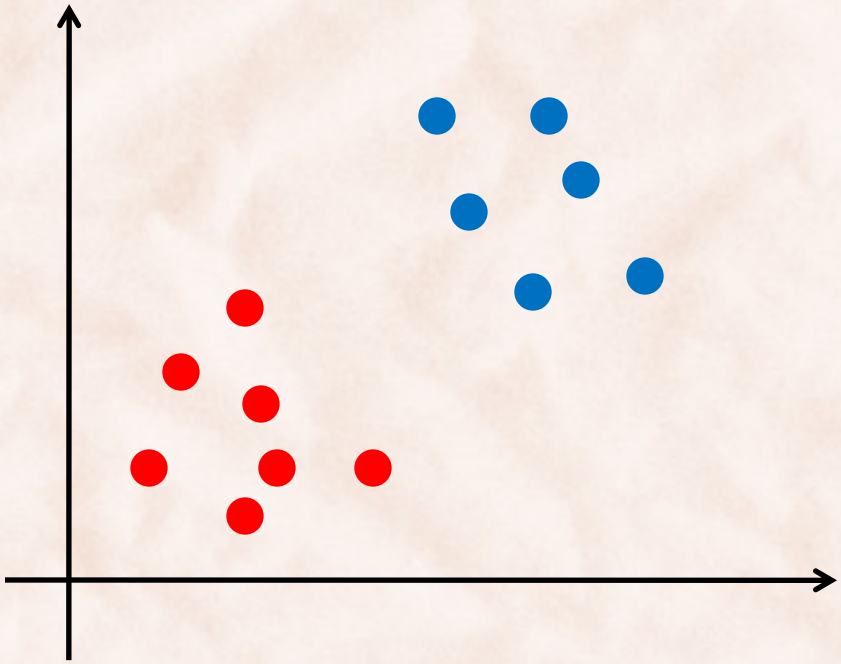
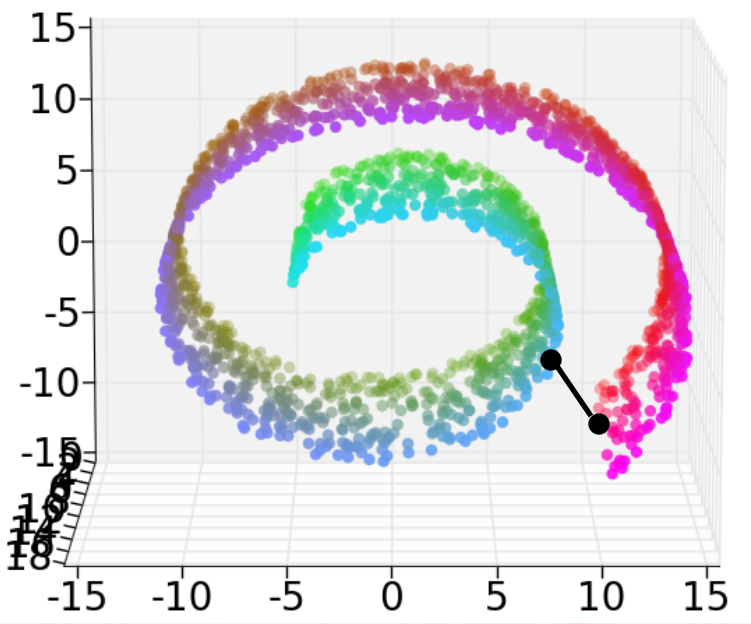
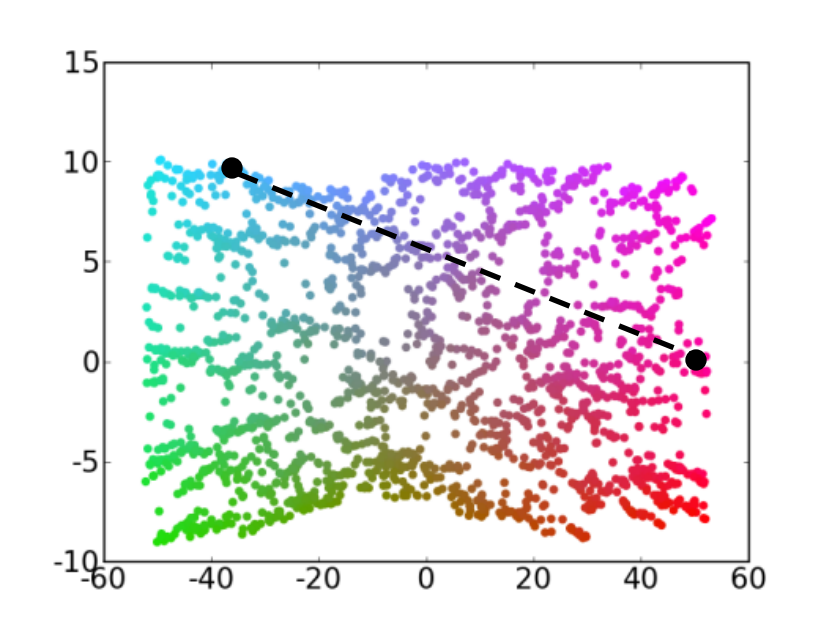


- Need to provide:
  - number of clusters ($k = 2$)
  - similarity measure (Euclidean)

Unsupervised Learning: Dimensionality Reduction

- Manifold Learning:
  - Data lies on a low-dimensional manifold embedded in a high-dimensional space.
  - Useful for *feature extraction* and *visualization*.





Reinforcement Learning

- Interaction between agent and environment modeled as a sequence of *actions* & *states*:
  - Learn *policy* for mapping states to actions in order to maximize a *reward*.
  - Reward given at the end state => *delayed reward*.
  - States may be only *partially observable*.
  - Trade-off between *exploration* and *exploitation*.
- Examples:
  - Backgammon [Tesauro, CACM'95].
  - Aerobatic helicopter flight [Abbeel, NIPS'07].
  - 49 Atari games, using deep RL [Mnih et al., Nature'15].

Reinforcement Learning: TD-Gammon

[Tesauro, CACM'95]

- Learn to play Backgammon:
  - Immediate reward:
    - +100 if win
    - –100 if lose
    - 0 for all other states
  - *Temporal Difference Learning* with a *Multilayer Perceptron*.
  - Trained by playing 1.5 million games against itself.
  - Played competitively against top-ranked players in international tournaments.

Relevant Disciplines

- Mathematics:
  - Probability & Statistics
  - Information Theory
  - Linear Algebra
  - Optimization
- Algorithms:
  - Computational Complexity
- Artificial Intelligence
  - Search
- Psychology
- Neurobiology

Readings

- PRML 1.2, 2.1 – 2.1.1, 2.2 – 2.2.1, 2.3 (2.3.4, 2.3.9).
- PRML Appendix B and C.

Machine Learning
CS 4900/5900

Lecture 02

Razvan C. Bunescu

School of Electrical Engineering and Computer Science

bunescu@ohio.edu

Supervised Learning

- **Task** = learn an (unknown) function $t : X \rightarrow T$ that maps input instances $\mathbf{x} \in X$ to output targets $t(\mathbf{x}) \in T$:
  - **Classification**:
    - The output $t(\mathbf{x}) \in T$ is one of a finite set of discrete categories.
  - **Regression**:
    - The output $t(\mathbf{x}) \in T$ is continuous, or has a continuous component.

- Target function $t(\mathbf{x})$ is known (only) through (noisy) set of training examples:

$$(\mathbf{x}_1,t_1), (\mathbf{x}_2,t_2), \ldots (\mathbf{x}_n,t_n)$$

Supervised Learning

- **Task** = learn an (unknown) function $t : X \rightarrow T$ that maps input instances $\mathbf{x} \in X$ to output targets $t(\mathbf{x}) \in T$:
  - function t is known (only) through (noisy) set of training examples:
    - Training/Test data: $(\mathbf{x}_1,t_1)$, $(\mathbf{x}_2,t_2)$, … $(\mathbf{x}_n,t_n)$

- **Task** = build a function $h(\mathbf{x})$ such that:
  - h matches t well on the *training data*:

    => h is able to fit data that it has seen.
  - h also matches target t well on *test data*:

    => h is able to generalize to unseen data.

Parametric Approaches to Supervised Learning

- **Task** = build a function $h(\mathbf{x})$ such that:
  - h matches t well on the training data:
    => h is able to fit data that it has seen.
  - h also matches t well on test data:
    => h is able to generalize to unseen data.

- **Task** = choose h from a "nice" *class of functions* that depend on a vector of parameters $\mathbf{w}$:
  - $h(\mathbf{x}) \equiv h_{\mathbf{w}}(\mathbf{x}) \equiv h(\mathbf{w},\mathbf{x})$
  - **what classes of functions are "nice"?**

Linear Regression

1. Univariate Linear Regression
   - House price prediction

2. Linear Regression with Polynomial Features
   - Polynomial curve fitting
   - Regularization
   - Ridge regression

3. Multivariate Linear Regression
   - House price prediction
   - Normal equations

House Price Prediction

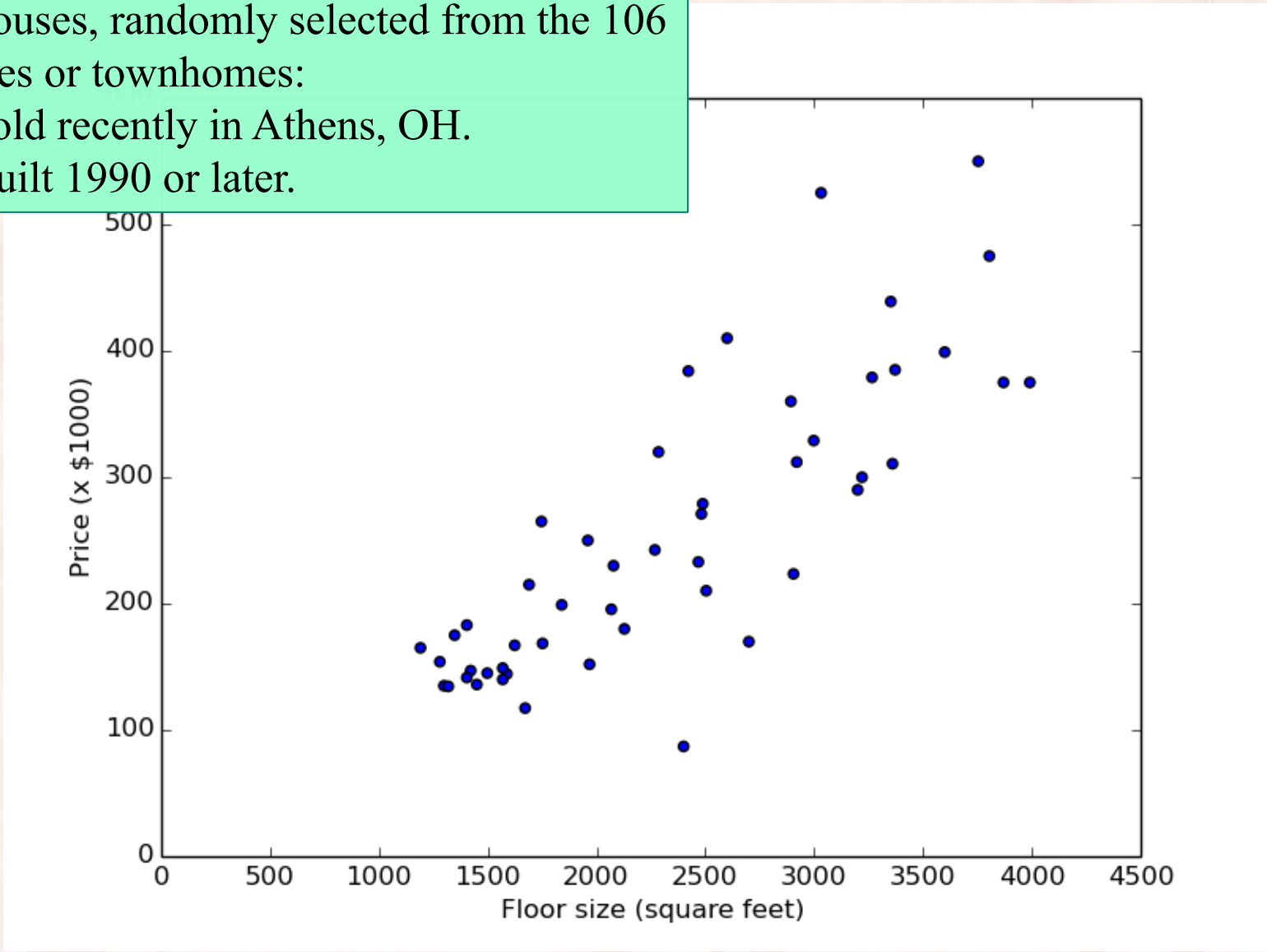
- Given the floor size in square feet, predict the selling price:
  - x is the size, t is the price
  - Need to learn a function h such that $h(x) \approx t(x)$.

- Is this classification or regression?
  - **Regression**, because price is real valued.
    - and there are many possible prices.
  - Univariate regression, because one input value.
  - Would a problem with only two labels $t_1 = 0.5$ and $t_2 = 1.0$ still be regression?

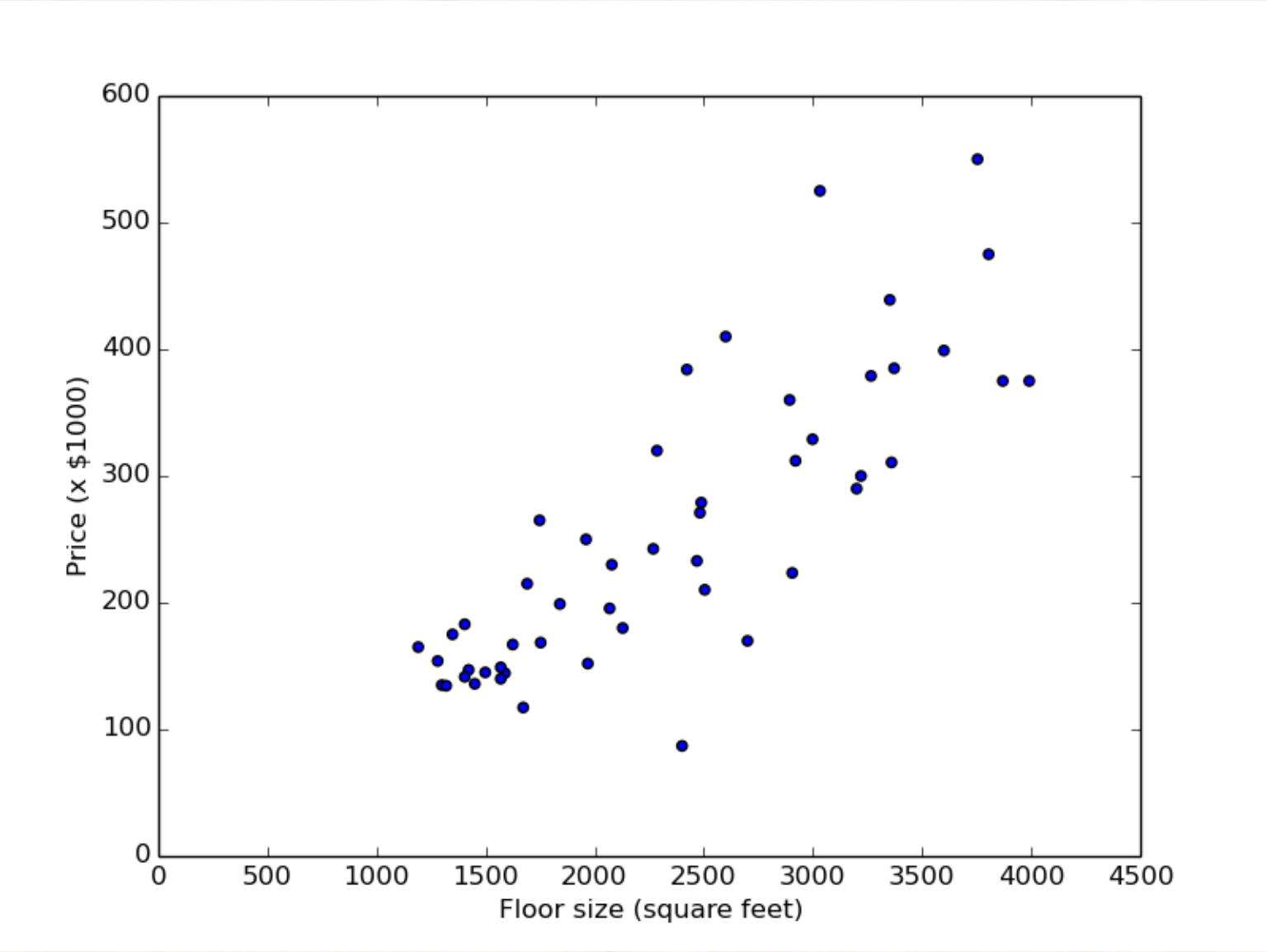
House Prices in Athens

50 houses, randomly selected from the 106 houses or townhomes:

- sold recently in Athens, OH.
- built 1990 or later.



House Prices in Athens

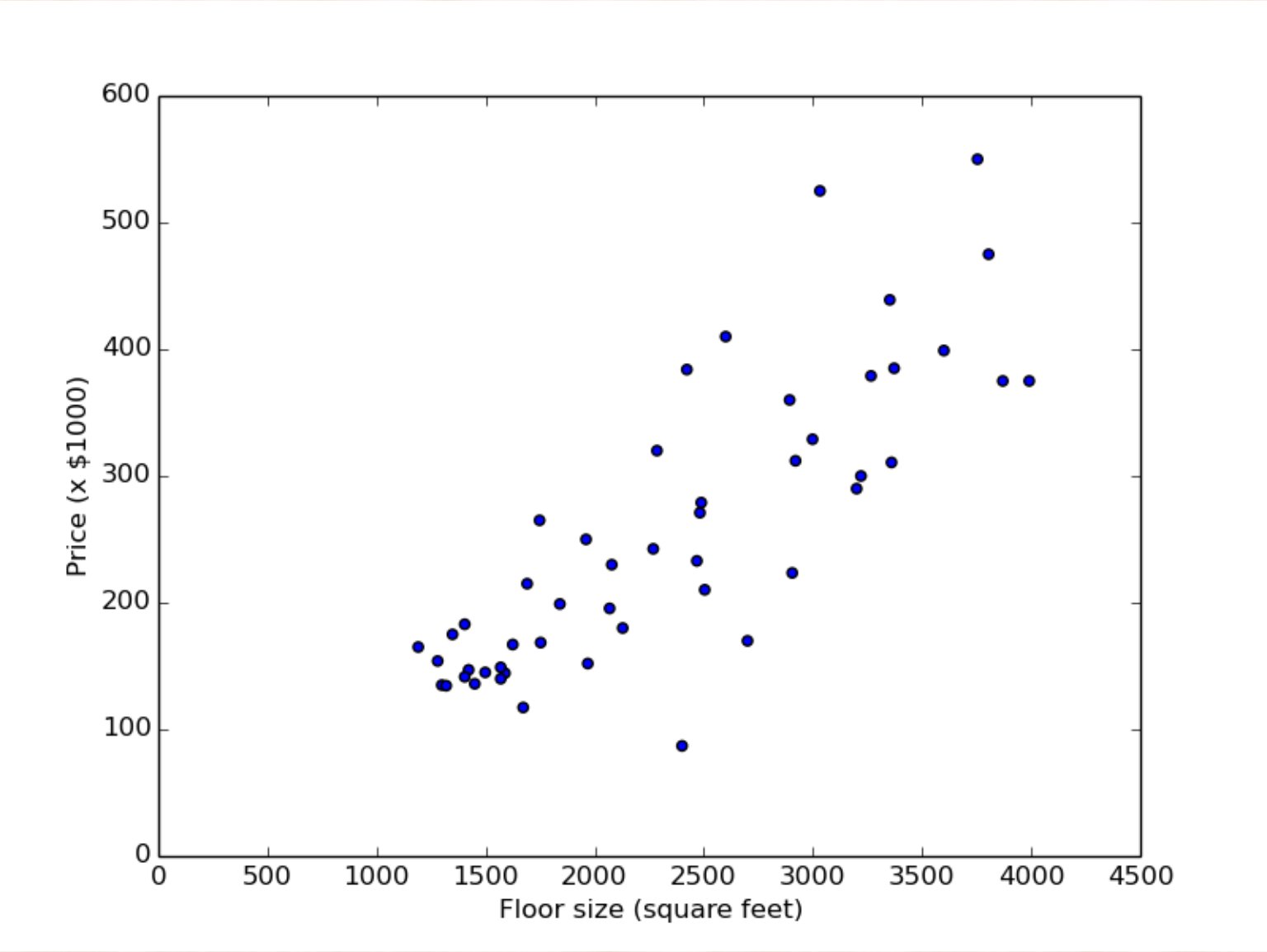


Parametric Approaches to Supervised Learning

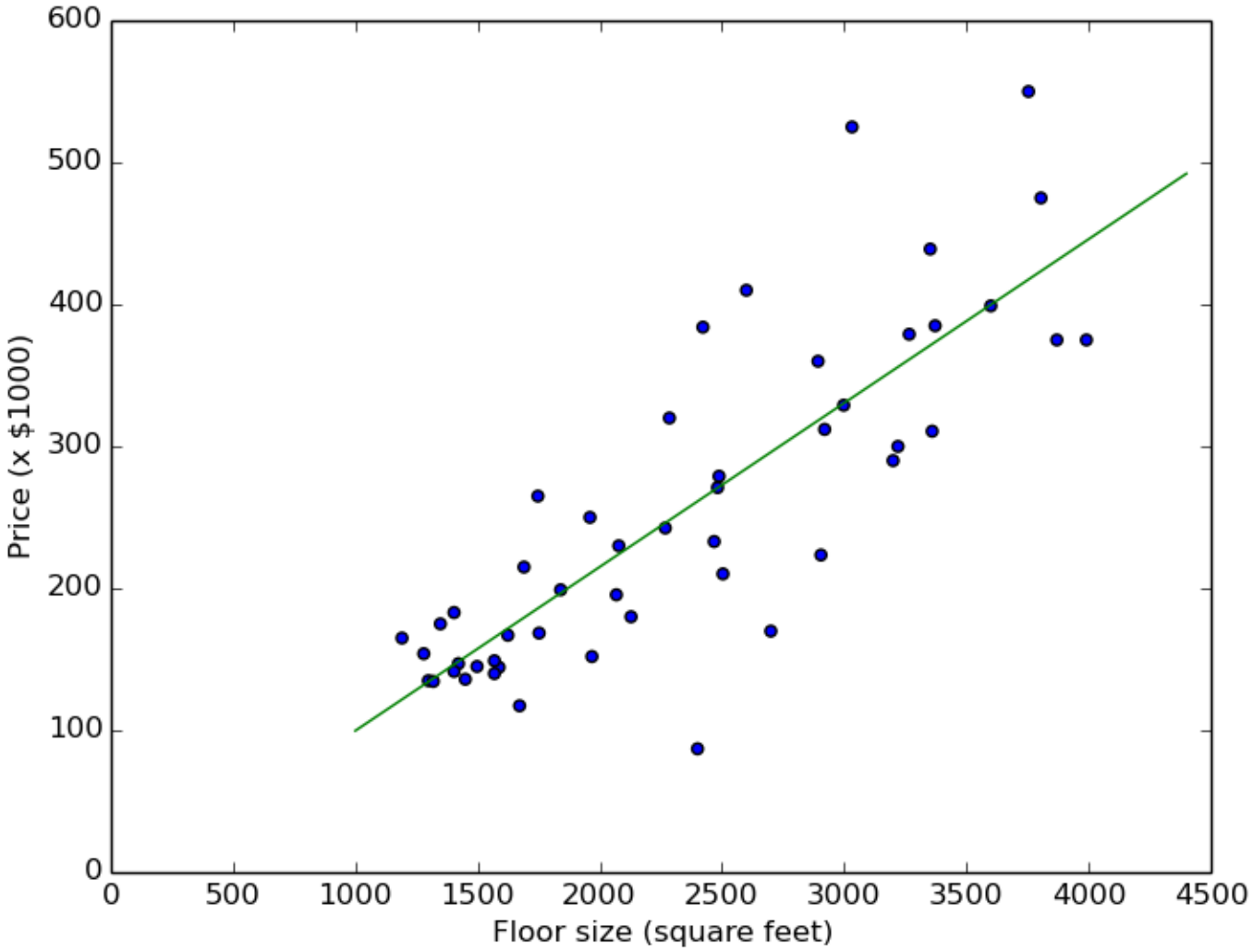
- **Task** = build a function $h(\mathbf{x})$ such that:
  - h matches t well on the training data:
    => h is able to fit data that it has seen.
  - h also matches t well on test data:
    => h is able to generalize to unseen data.

- **Task** = choose h from a "nice" *class of functions* that depend on a vector of parameters $\mathbf{w}$:
  - $h(\mathbf{x}) \equiv h_{\mathbf{w}}(\mathbf{x}) \equiv h(\mathbf{w},\mathbf{x})$
  - **what classes of functions are "nice"?**

House Prices in Athens



House Prices in Athens



Univariate Linear Regression

- Use a linear function approximation:
  - $h_{\mathbf{w}}(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} = [w_0, w_1]^{\mathrm{T}}[1, x] = w_1 x + w_0$.
    - w_0 is the intercept (or the bias term).
    - w_1 controls the slope.
  - Learning = optimization:
    - Find **w** that obtains the best fit on the training data, i.e. find **w** that minimizes the **sum of square errors**:

$$J(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N}\left(h_{\mathbf{w}}(\mathbf{x}_{\mathrm{n}}) - t_n\right)^2$$

$$\hat{\mathbf{w}} = \underset{\mathbf{w}}{\operatorname{argmin}}\, J(\mathbf{w})$$

Univariate Linear Regression

- Learning = finding the "right" parameters $\mathbf{w}^T = [w_0, w_1]$
  - Find $\mathbf{w}$ that minimizes an *error function* $E(\mathbf{w}) = J(\mathbf{w})$ which measures the misfit between $h(\mathbf{x}_n, \mathbf{w})$ and t_n.
  - Expect that $h(\mathbf{x}, \mathbf{w})$ performing well on training examples $\mathbf{x}_n \Rightarrow$ $h(\mathbf{x}, \mathbf{w})$ will perform well on arbitrary test examples $\mathbf{x} \in$ X.

Inductive Learning Hyphotesis

- Sum-of-Squares error function:

$$J(\mathbf{w}) = \frac{1}{2N} \sum_{n=1}^{N} (h_{\mathbf{w}}(\mathbf{x}_n) - t_n)^2$$

Minimizing Sum-of-Squares Error

- Sum-of-Squares error function:

why squared?

$$J(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N}(h_{\mathbf{w}}(\mathbf{x}_n) - t_n)^2$$

- How do we find $\mathbf{w}^*$ that minimizes $E(\mathbf{w})$?

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} J(\mathbf{w})$$

- Least Square solution is found by solving a system of 2 linear equations:

$$w_0 N + w_1 \sum_{n=1}^{N} x_n = \sum_{n=1}^{N} t_n$$

$$w_0 \sum_{n=1}^{N} x_n + w_1 \sum_{n=1}^{N} x_n^2 = \sum_{n=1}^{N} t_n x_n$$

Machine Learning
CS 4900/5900

Lecture 03

Razvan C. Bunescu

School of Electrical Engineering and Computer Science

bunescu@ohio.edu

Machine Learning is Optimization

- Parametric ML involves minimizing an **objective function** $J(\mathbf{w})$:
  - Also called **cost function**, **loss function**, or **error function**.
  - Want to find $\hat{\mathbf{w}} = \underset{\mathbf{w}}{\operatorname{argmin}} J(\mathbf{w})$

- Numerical optimization procedure:
  1. Start with some guess for $\mathbf{w}^0$, set $\tau = 0$.
  2. Update $\mathbf{w}^\tau$ to $\mathbf{w}^{\tau+1}$ such that $J(\mathbf{w}^{\tau+1}) \leq J(\mathbf{w}^\tau)$.
  3. Increment $\tau = \tau + 1$.
  4. Repeat from 2 until J cannot be improved anymore.

Gradient-based Optimization

- How to update $\mathbf{w}^{\tau}$ to $\mathbf{w}^{\tau+1}$ such that $J(\mathbf{w}^{\tau+1}) \leq J(\mathbf{w}^{\tau})$?

- Move $\mathbf{w}$ in the direction of **steepest descent**:

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} + \eta \mathbf{g}$$

  - $\mathbf{g}$ is the direction of steepest descent, i.e. direction along which J decreases the most.
  - η is the learning rate and controls the magnitude of the change.

Gradient-based Optimization

- Move $\mathbf{w}$ in the direction of **steepest descent**:

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} + \eta\mathbf{g}$$

- What is the direction of steepest descent of $J(\mathbf{w})$ at $\mathbf{w}^{\tau}$?
  - The gradient $\nabla J(\mathbf{w})$ is in the direction of steepest ascent.
  - Set $\mathbf{g} = -\nabla J(\mathbf{w})$ => the **gradient descent** update:

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta\nabla J(\mathbf{w}^{\tau})$$

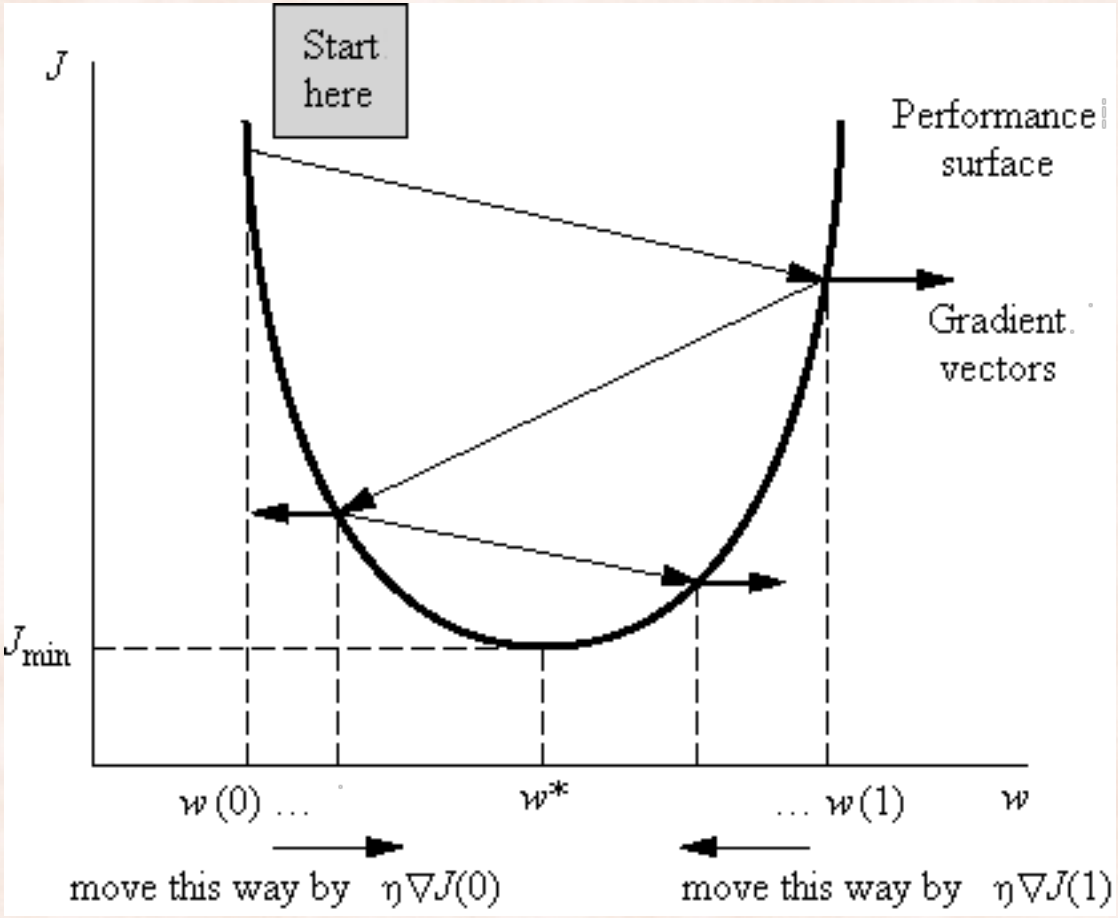
Gradient Descent Algorithm

- Want to minimize a function $J : R^n \rightarrow R$.
  - J is differentiable and convex.
  - compute gradient of J i.e. *direction of steepest increase*:

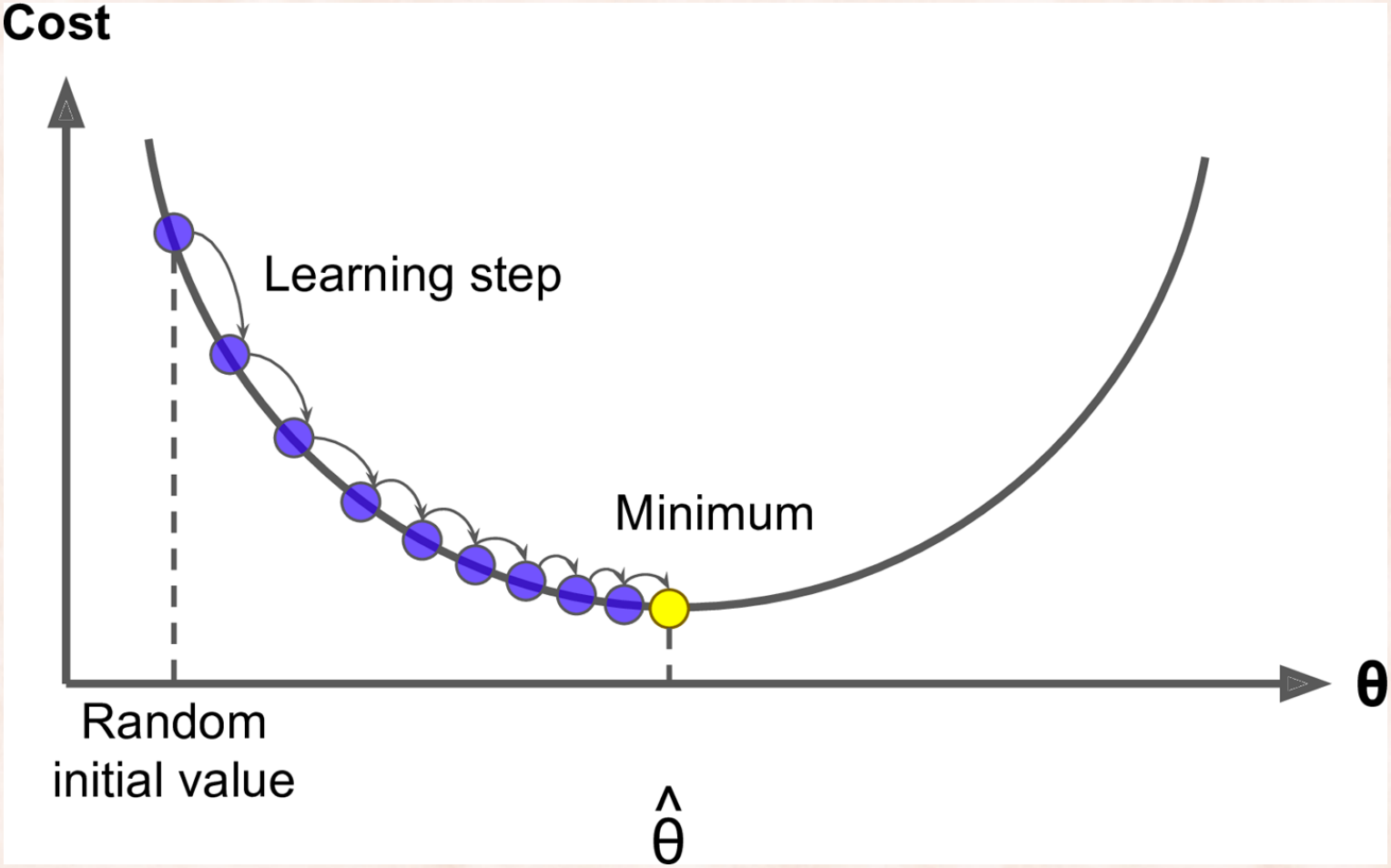
$$\nabla J(\mathbf{w}) = \left[\frac{\partial J}{\partial w_1}, \frac{\partial J}{\partial w_2}, \ldots, \frac{\partial J}{\partial w_n}\right]$$

1. Set learning rate $\eta = 0.001$ (or other small value).
2. Start with some guess for $\mathbf{w}^0$, set $\tau = 0$.
3. Repeat for epochs E or until J does not improve:
4. $\quad \tau = \tau + 1.$
5. $\quad \mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \nabla J(\mathbf{w}^{\tau})$

Gradient Descent: Large Updates



Gradient Descent: Small Updates



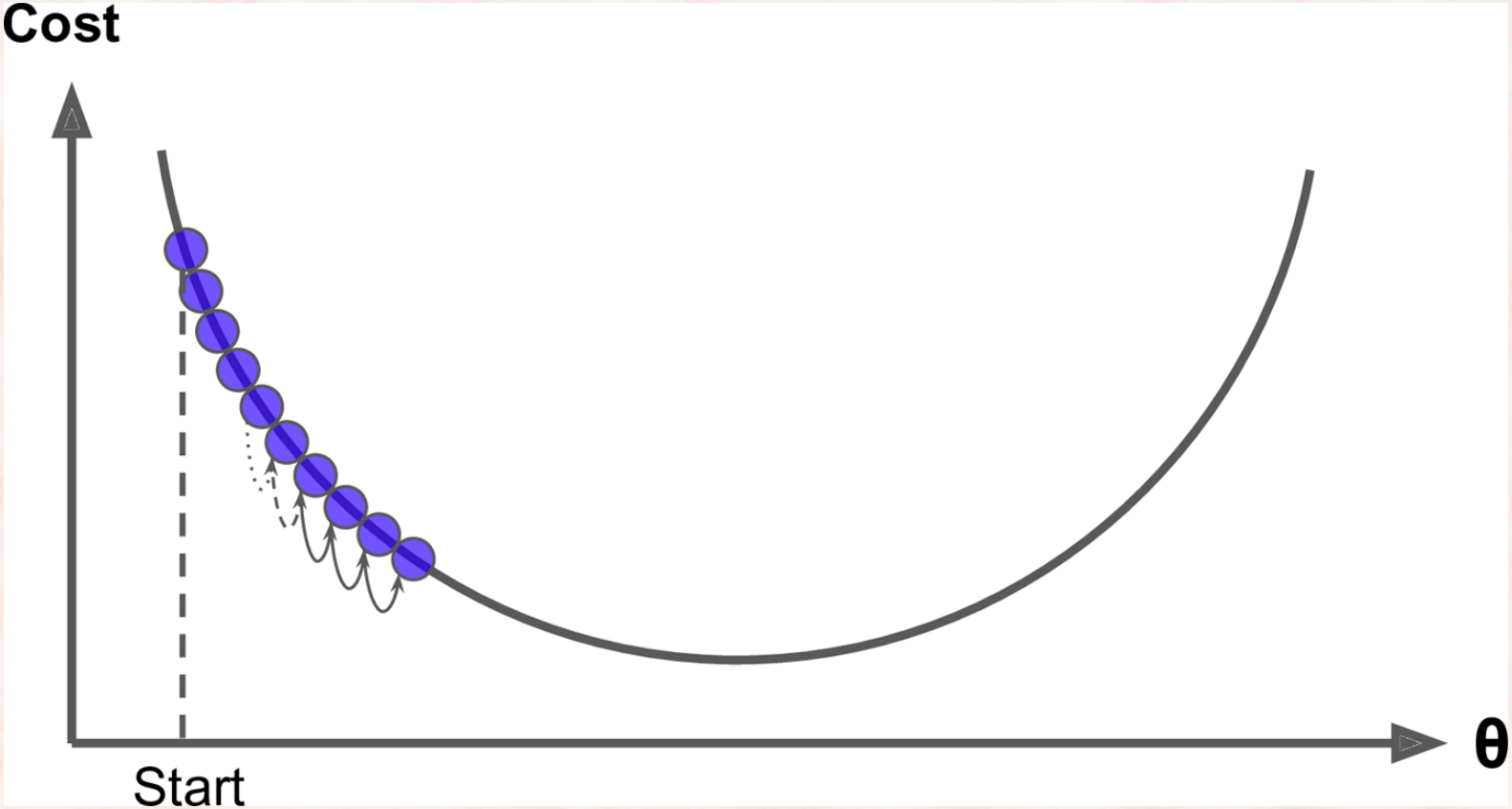
https://www.safaribooksonline.com/library/view/hands-on-machine-learning

The Learning Rate

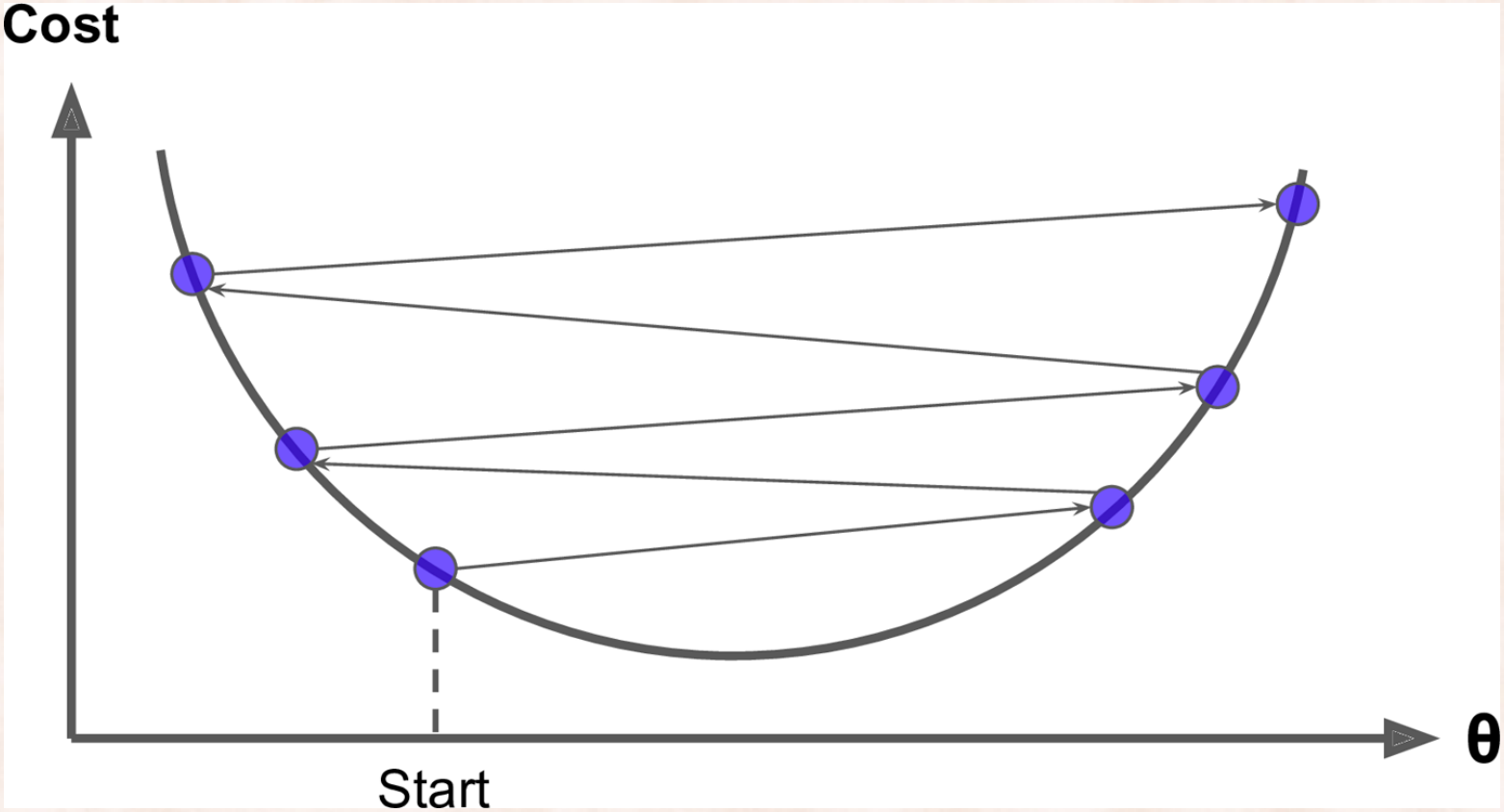
1. Set **learning rate** $\eta = 0.001$ (or other small value).
2. Start with some guess for $\mathbf{w}^0$, set $\tau = 0$.
3. Repeat for epochs E or until J does not improve:
4. $\tau = \tau + 1$.
5. $\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \nabla J(\mathbf{w}^{\tau})$

- How big should the **learning rate** be?
  - If learning rate too small => slow convergence.
  - If learning rate too big => oscillating behavior => may not even converge.

Learning Rate too Small



Learning Rate too Large

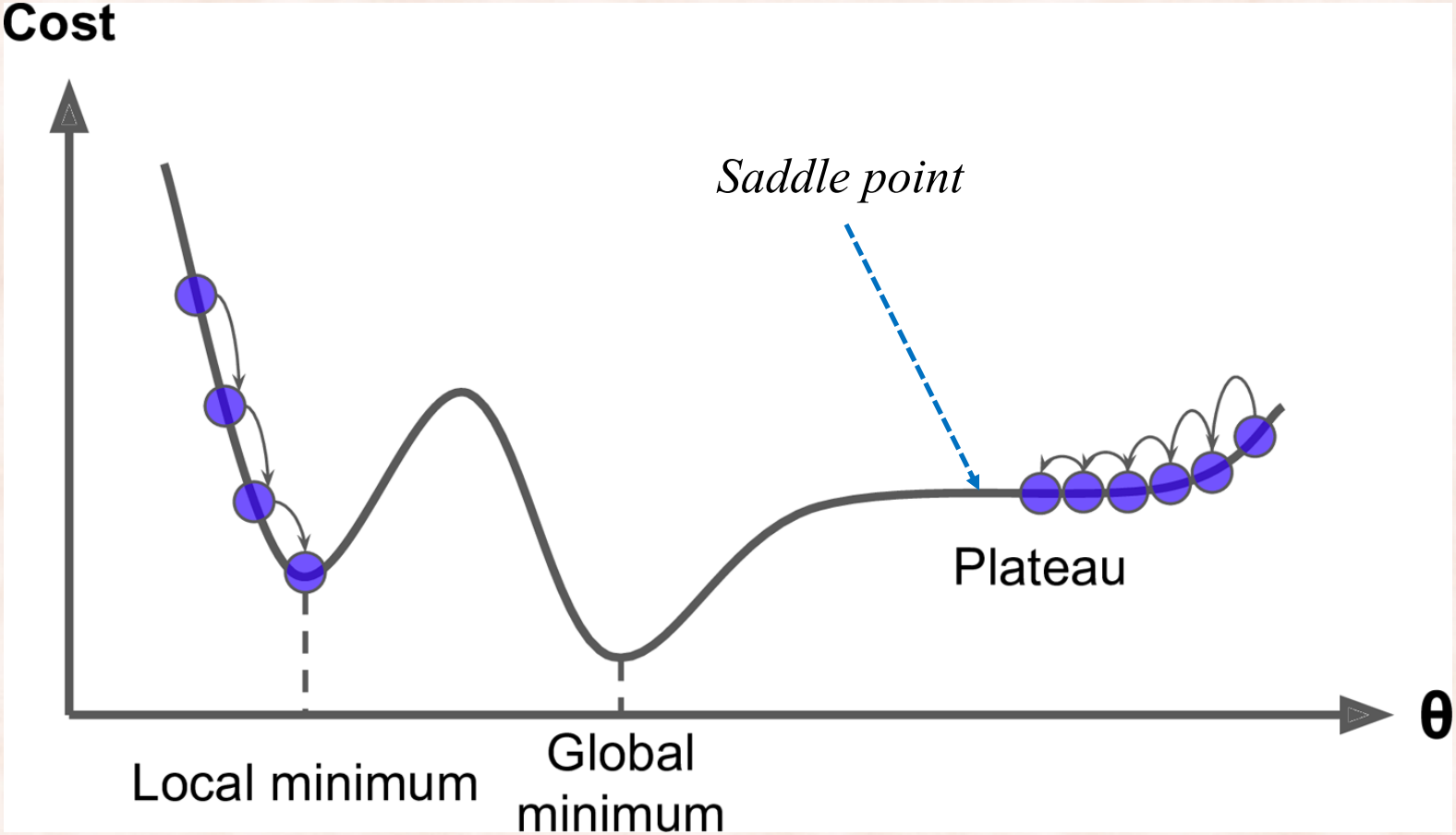


The Learning Rate

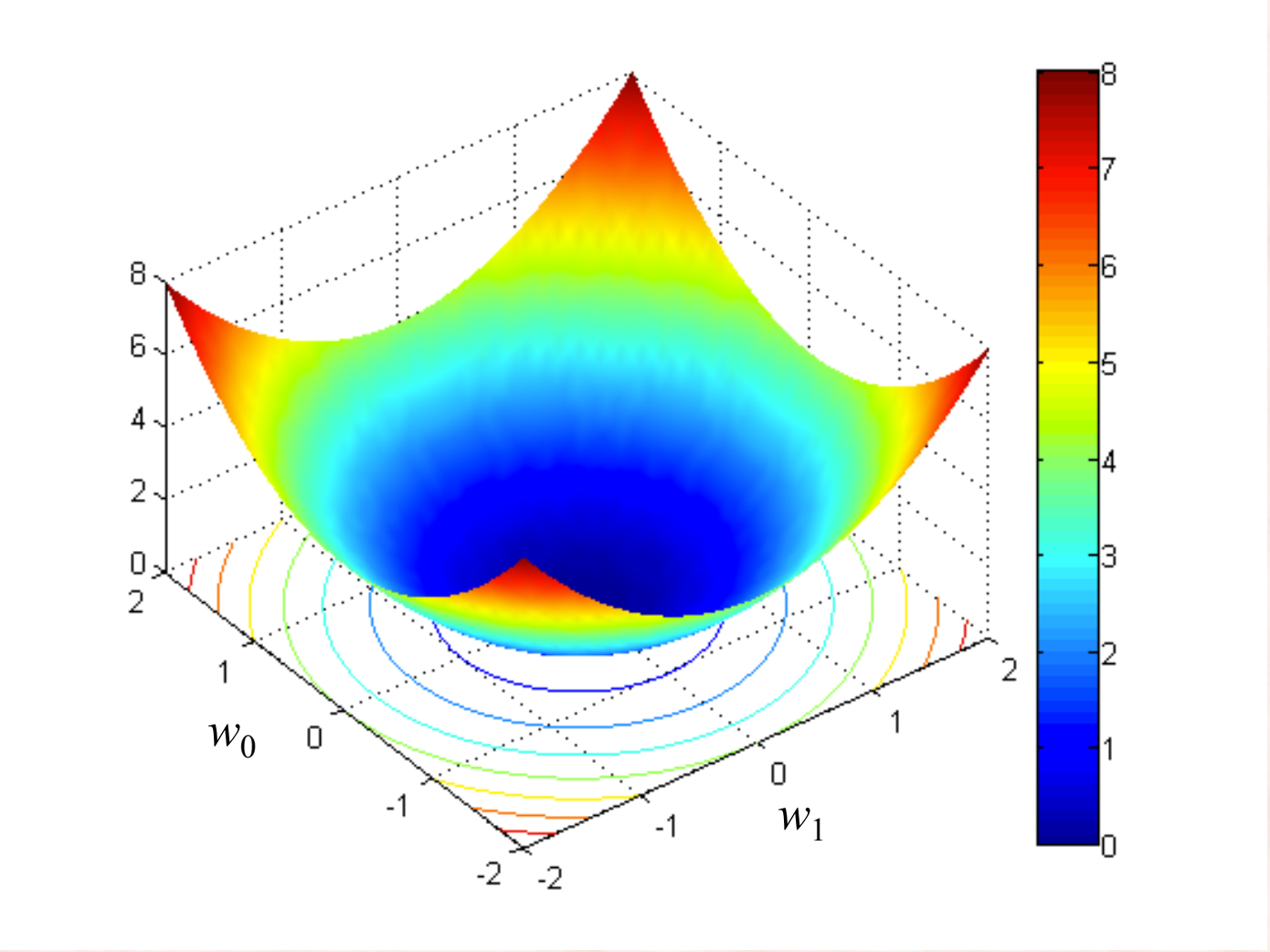
- How big should the **learning rate** be?
  - If learning rate too big => oscillating behavior.
  - If learning rate too small => hinders convergence.

- Use **line search** (backtracking line search, conjugate gradient, …).
- Use **second order methods** (Newton's method, L-BFGS, ...).
  - Requires computing or estimating the Hessian.
- Use a simple learning rate **annealing schedule**:
  - Start with a relatively large value for the learning rate.
  - Decrease the learning rate as a function of the number of epochs or as a function of the improvement in the objective.
- Use **adaptive learning rates**:
  - Adagrad, Adadelta, RMSProp, Adam.

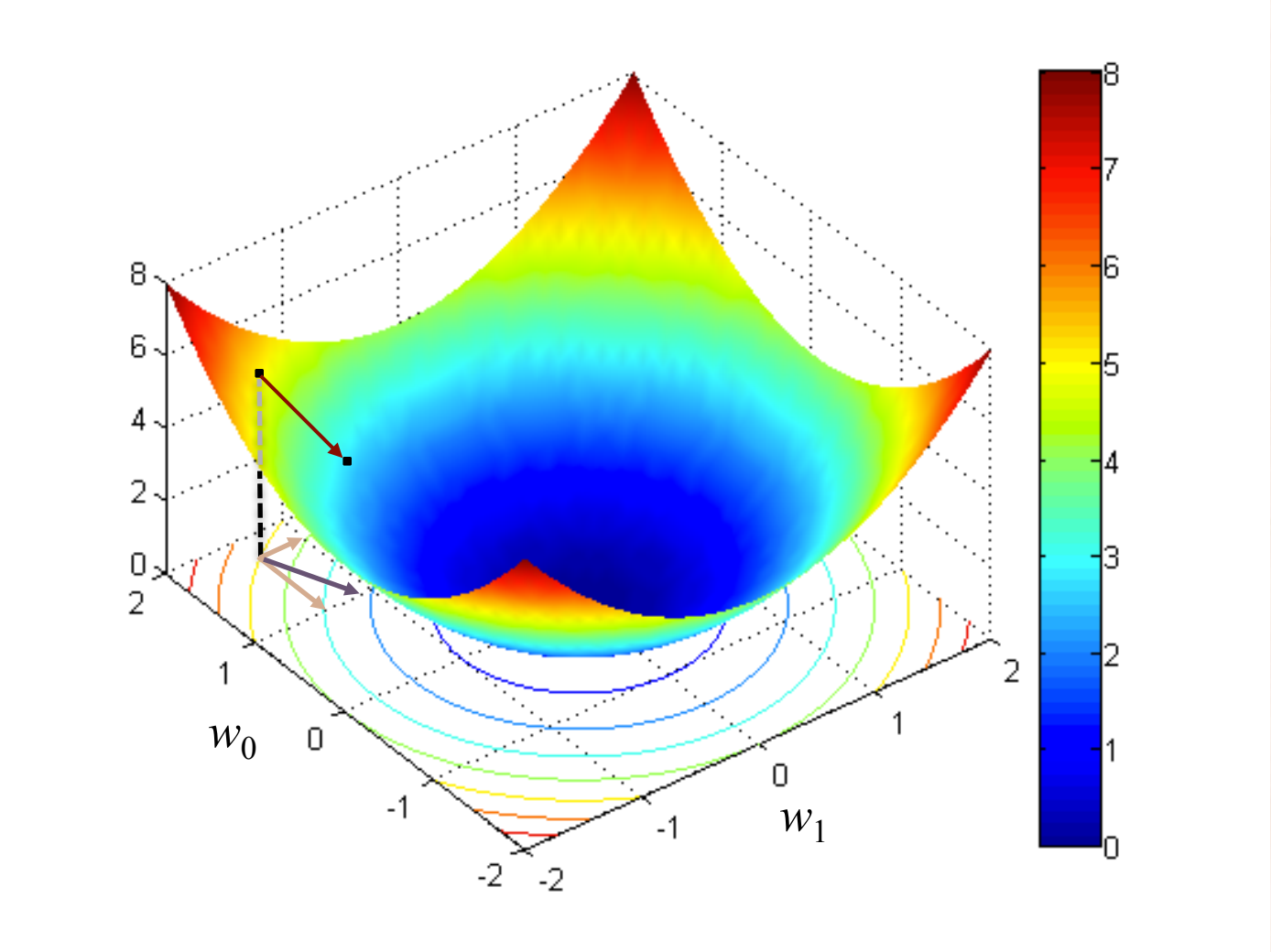
Gradient Descent: Nonconvex Objective



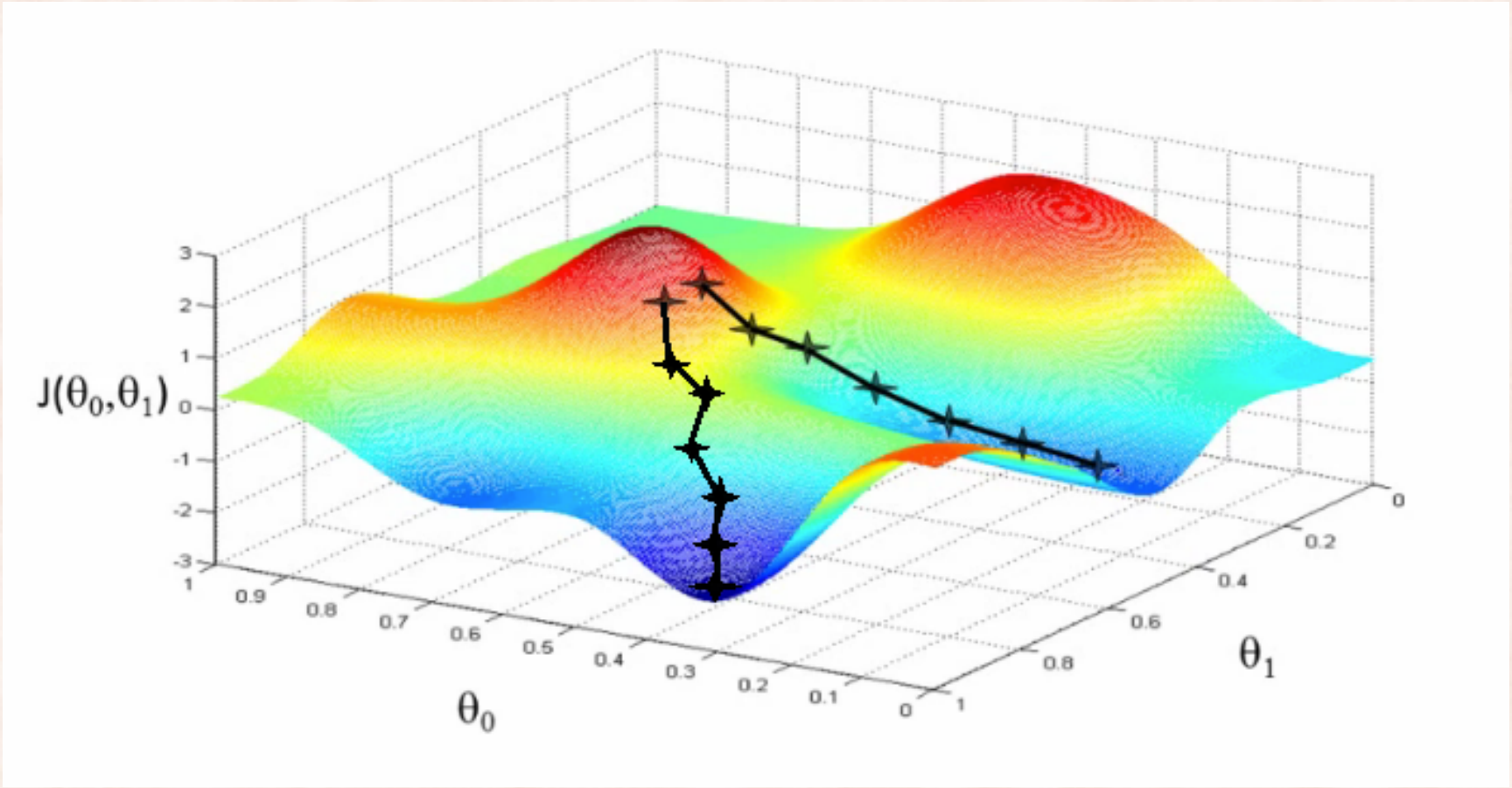
Convex Multivariate Objective



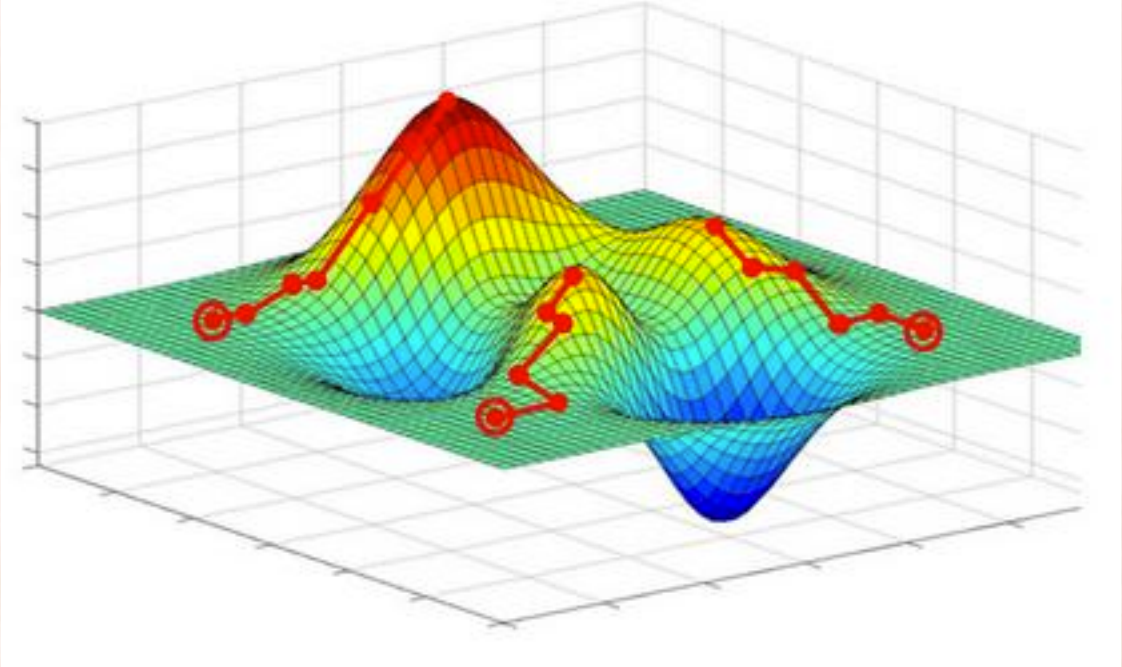
Gradient Step and Contour Lines



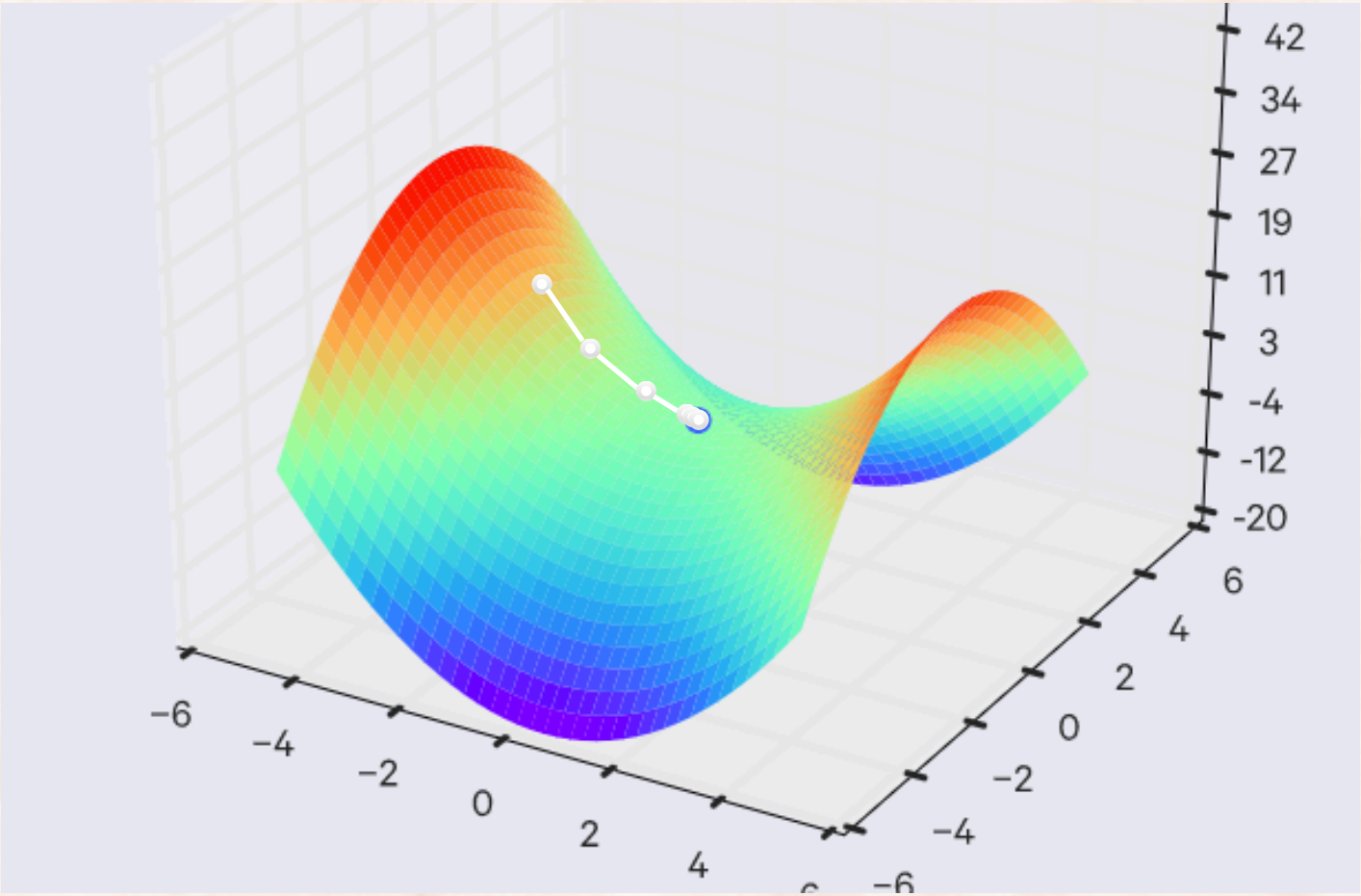
Gradient Descent: Nonconvex Objectives



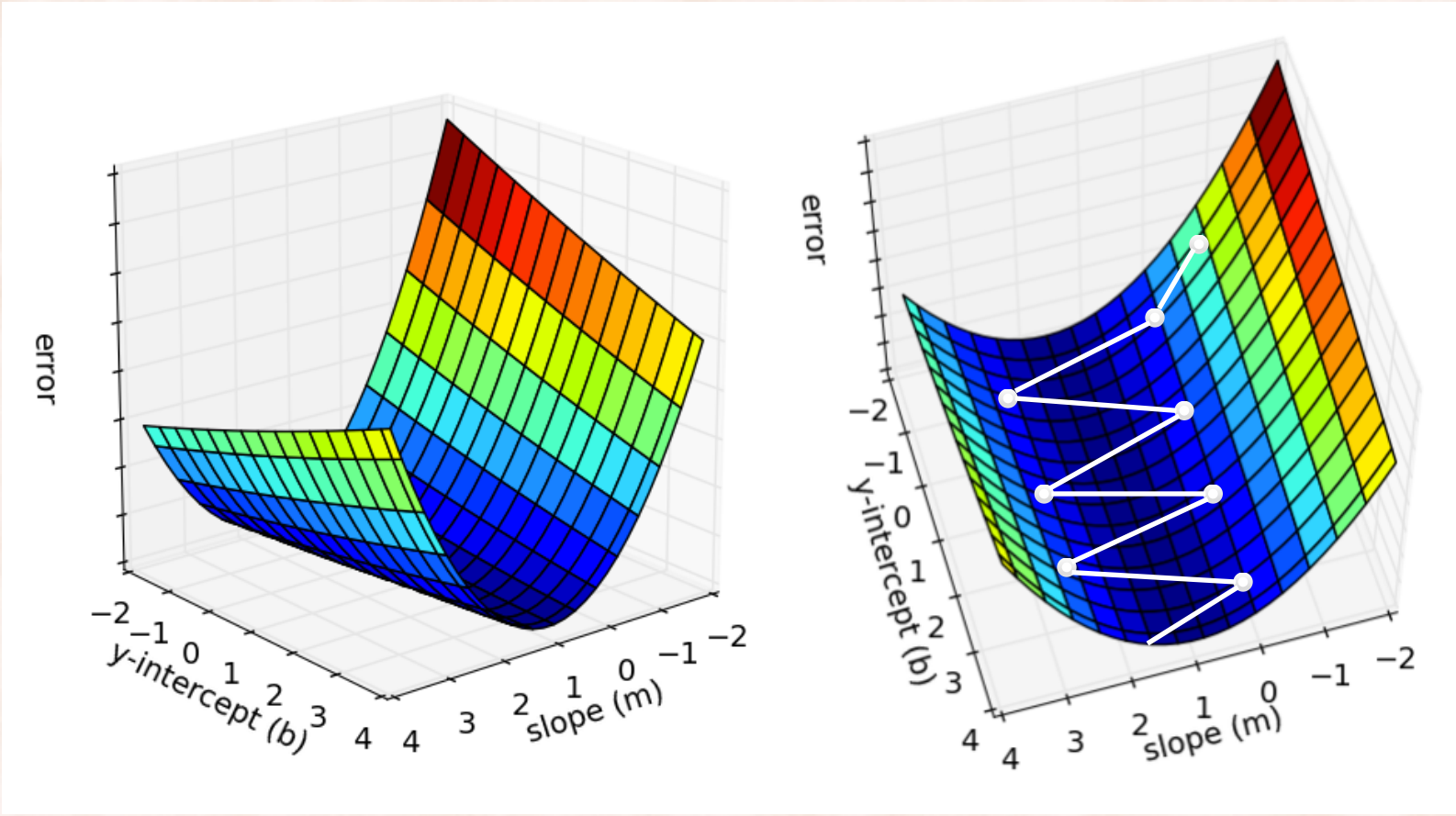
Gradient Descent & Plateaus



Gradient Descent & Saddle Points



Gradient Descent & Ravines



Gradient Descent & Ravines

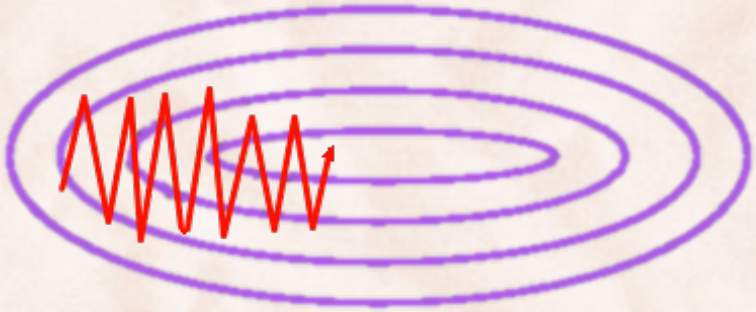
- **Ravines** are areas where the surface curves much more steeply in one dimension than another.
  - Common around local optima.
  - GD oscillates across the slopes of the ravines, making slow progress towards the local optimum along the bottom.
- Use **momentum** to help accelerate GD in the relevant directions and dampen oscillations:
  - Add a fraction of the past **update vector** to the current update vector.
    - The momentum term increases for dimensions whose previous gradients point in the same direction.
    - It reduces updates for dimensions whose gradients change sign.
    - Also reduces the risk of getting stuck in local minima.

Gradient Descent & Momentum

Vanilla Gradient Descent:

$$\mathbf{v}^{\tau+1} = \eta \nabla J(\mathbf{w}^{\tau})$$

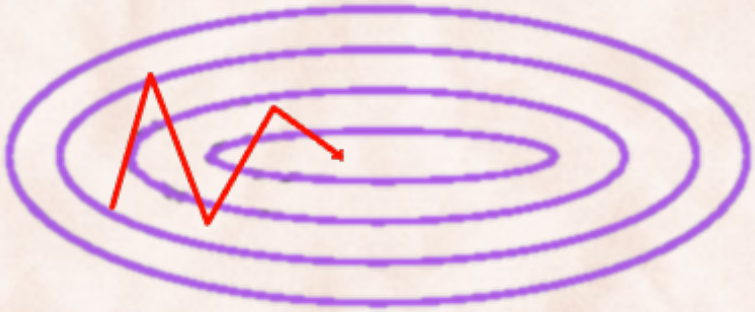
$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \mathbf{v}^{\tau+1}$$



Gradient Descent w/ Momentum:

$$\mathbf{v}^{\tau+1} = \gamma \mathbf{v}^{\tau} + \eta \nabla J(\mathbf{w}^{\tau})$$

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \mathbf{v}^{\tau+1}$$



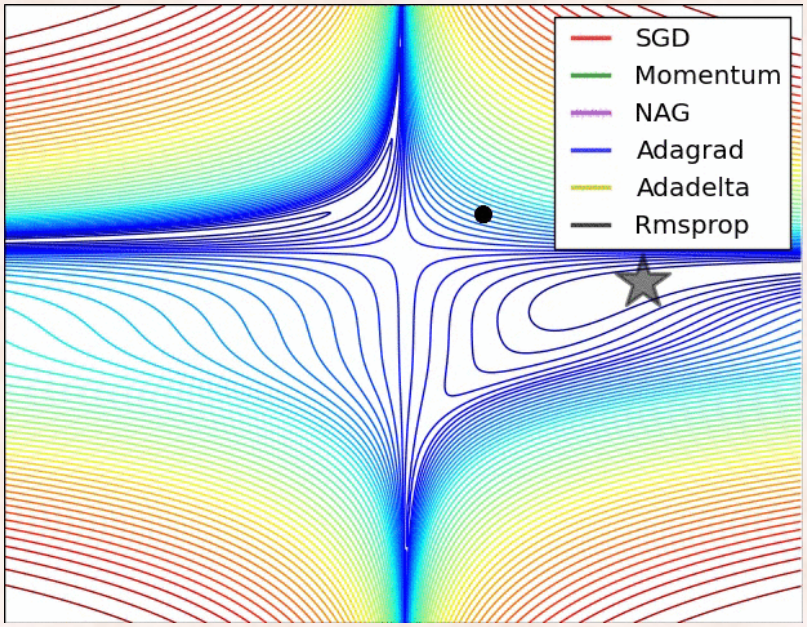
Gradient Descent Optimization Algorithms

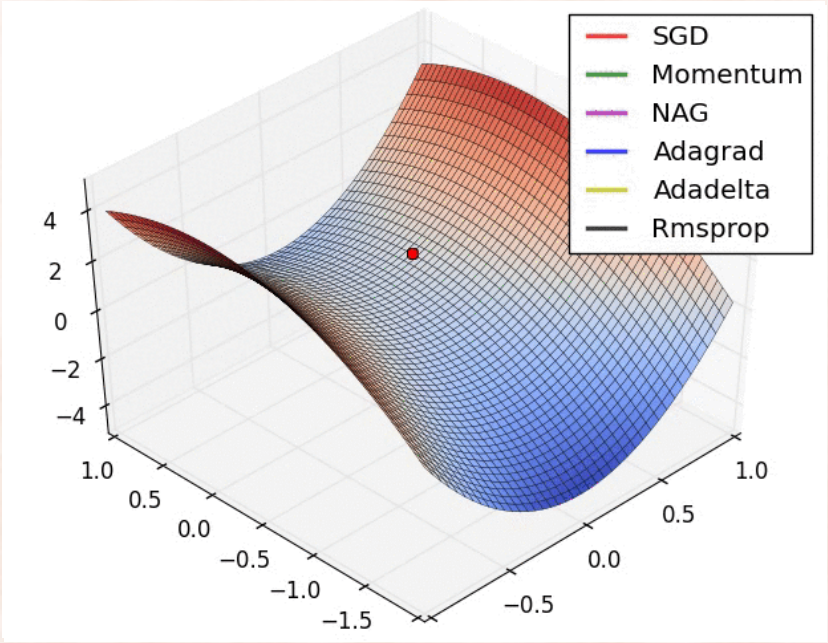
- **Momentum**.
- **Nesterov Accelerated Gradient** (NAG).
- Adaptive learning rates methods:
  - **Adagrad**.
  - **Adadelta**.
  - **RMSProp**.
  - **Adaptive Moment Estimation** (Adam)

Sebastian Ruder, CoRR 2016 . An overview of gradient descent optimization algorithms

Visualization

- Adagrad, RMSprop, Adadelta, and Adam are very similar algorithms that do well in similar circumstances.
  - Insofar, **Adam** might be the best overall choice.





https://imgur.com/a/Hqolp

Variants of Gradient Descent

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \nabla J(\mathbf{w}^{\tau})$$

- Depeding on how much data is used to compute the gradient at each step:
  - **Batch gradient descent**:
    - Use all the training examples.
  - **Stochastic gradient descent** (SGD).
    - Use one training example, update after each.
  - **Minibatch gradient descent**.
    - Use a constant number of training examples (minibatch).

Batch Gradient Descent

- Sum-of-squares error:

$$J(\mathbf{w}) = \frac{1}{2N} \sum_{n=1}^{N} \left(h_{\mathbf{w}}(\mathbf{x}^{(n)}) - t_n \right)^2$$

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \nabla J(\mathbf{w}^{\tau})$$

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \sum_{n=1}^{N} \left(h_{\mathbf{w}}(\mathbf{x}^{(n)}) - t_n \right) \mathbf{x}^{(n)}$$

Stochastic Gradient Descent

- Sum-of-squares error:

$$J(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N}\left(h_{\mathbf{w}}(\mathbf{x}^{(n)}) - t_n\right)^2 = \frac{1}{2N}\sum_{n=1}^{N} J\left(\mathbf{w}^{\tau}, \mathbf{x}^{(n)}\right)$$

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta\, \nabla J\left(\mathbf{w}^{\tau}, \mathbf{x}^{(n)}\right)$$

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta\left(h_{\mathbf{w}}(\mathbf{x}^{(n)}) - t_n\right)\mathbf{x}^{(n)}$$

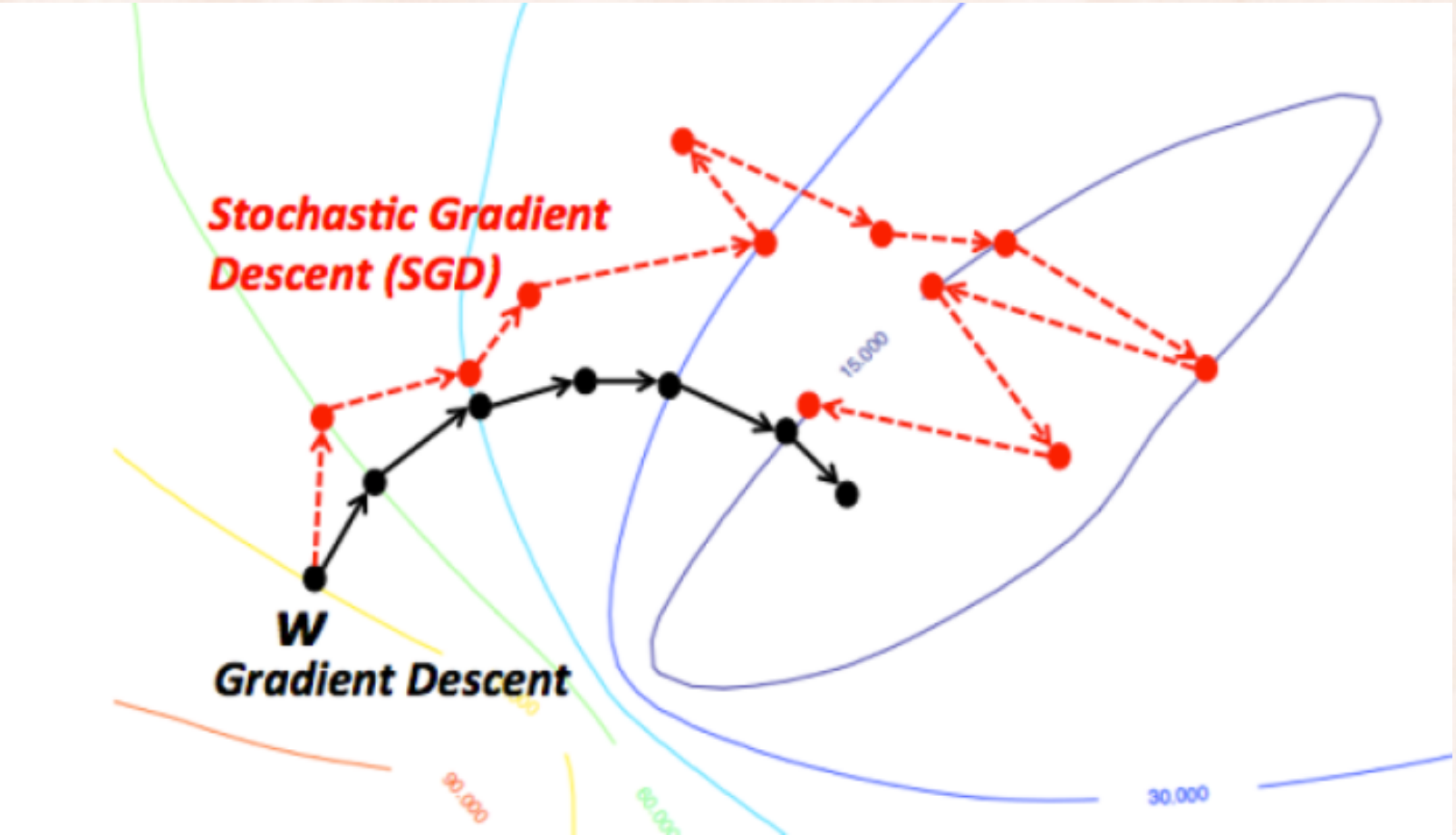
- Update parameters **w** after each example, sequentially:

  => the *least-mean-square* (LMS) algorithm.

Batch GD vs. Stochastic GD

- Accuracy:
- Time complexity:
- Memory complexity:
- Online learning:

Batch GD vs. Stochastic GD



Machine Learning: Logistic Regression

Lecture 04

Razvan C. Bunescu

School of Electrical Engineering and Computer Science

bunescu@ohio.edu

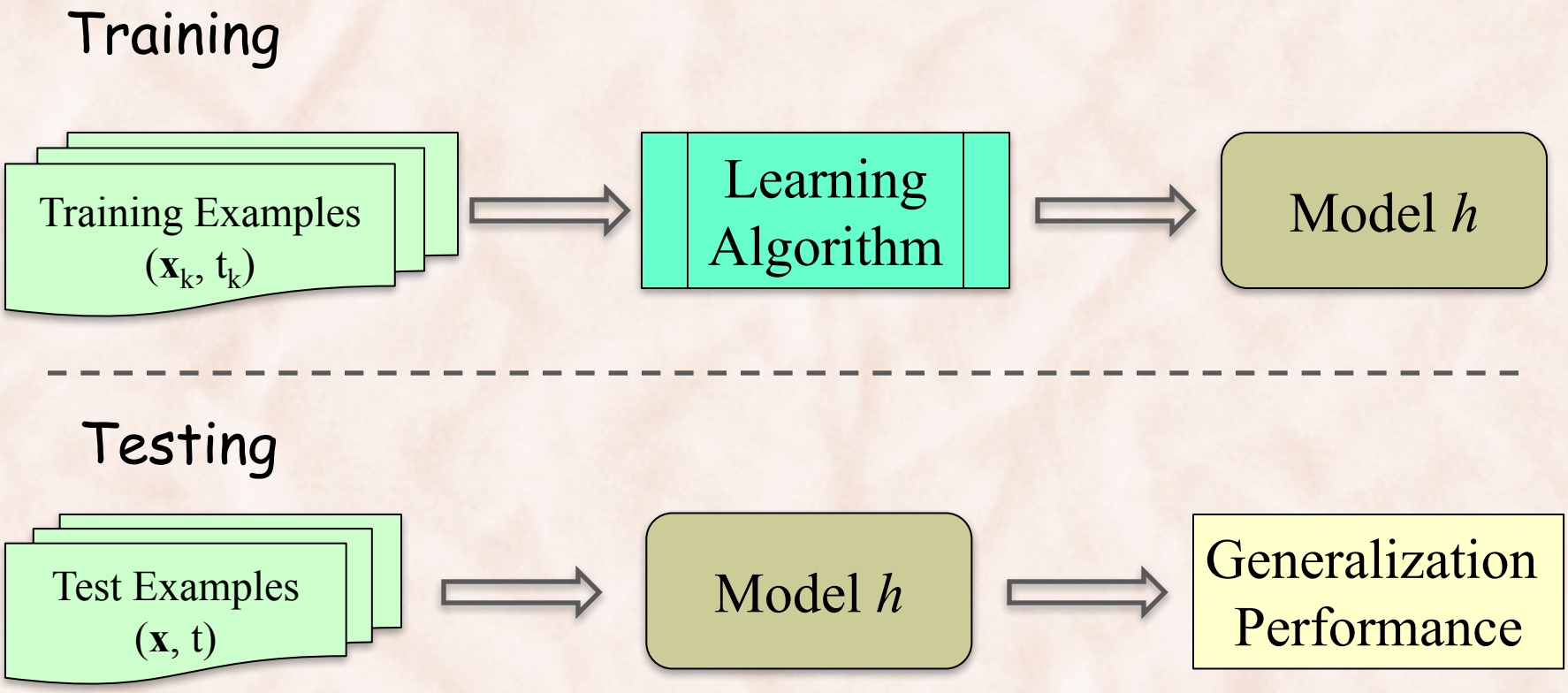
Supervised Learning

- **Task** = learn an (unkown) function $t : X \rightarrow T$ that maps input instances $\mathbf{x} \in X$ to output targets $t(\mathbf{x}) \in T$:
  - **Classification**:
    - The output $t(\mathbf{x}) \in T$ is one of a finite set of discrete categories.
  - **Regression**:
    - The output $t(\mathbf{x}) \in T$ is continuous, or has a continuous component.

- Target function $t(\mathbf{x})$ is known (only) through (noisy) set of training examples:

$$(\mathbf{x}_1,t_1), (\mathbf{x}_2,t_2), \ldots (\mathbf{x}_n,t_n)$$

Supervised Learning

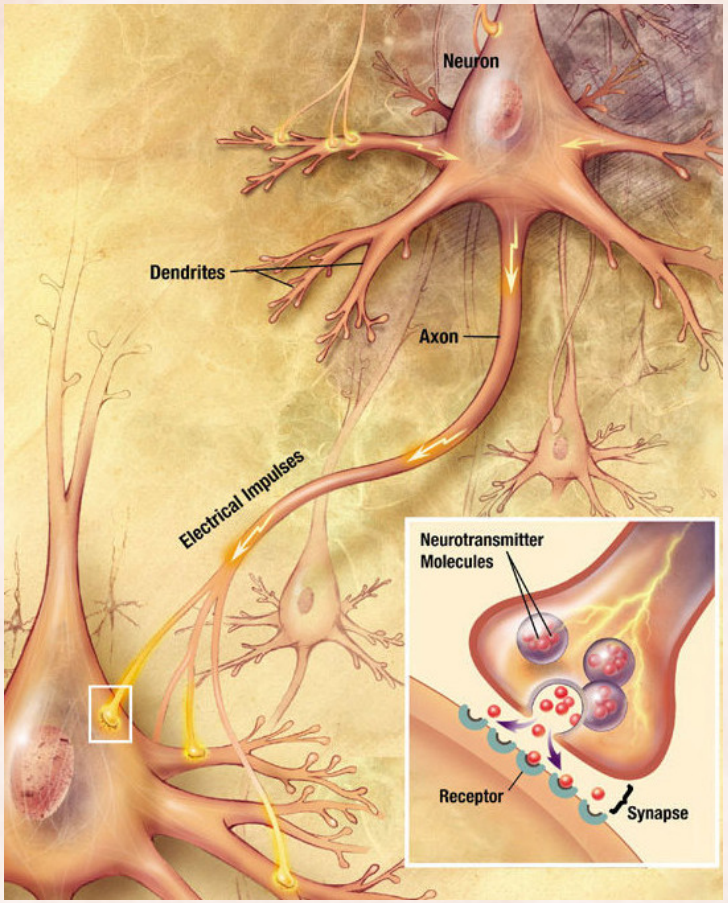


Parametric Approaches to Supervised Learning

- **Task** = build a function $h(\mathbf{x})$ such that:
  - h matches t well on the training data:
    => h is able to fit data that it has seen.
  - h also matches t well on test data:
    => h is able to **generalize to unseen data**.

- **Task** = choose h from a "nice" *class of functions* that depend on a vector of parameters $\mathbf{w}$:
  - $h(\mathbf{x}) \equiv h_{\mathbf{w}}(\mathbf{x}) \equiv h(\mathbf{w},\mathbf{x})$
  - **what classes of functions are "nice"?**

Neurons



Soma is the central part of the neuron:
- *where the input signals are combined.*

Dendrites are cellular extensions:
- *where majority of the input occurs.*

Axon is a fine, long projection:
- *carries nerve signals to other neurons.*

Synapses are molecular structures between axon terminals and other neurons:
- *where the communication takes place.*

Neuron Models

https://www.research.ibm.com/software/IBMResearch/multimedia/IJCNN2013.neuron-model.pdf

Year	Model Name	Reference
1907	Integrate and fire	[13]
1943	McCulloch and Pitts	[11]
1952	Hodgkin-Huxley	[12]
1958	Perceptron	[14]
1961	Fitzhugh-Nagumo	[15]
1965	Leaky integrate-and-fire	[16]
1981	Morris-Lecar	[17]
1986	Quadratic integrate-and-fire	[18]
1989	Hindmarsh-Rose	[19]
1998	Time-varying integrate-and-fire model	[20]
1999	Wilson Polynomial	[21]
2000	Integrate-and-fire or burst	[22]
2001	Resonate-and-fire	[23]
2003	Izhikevich	[24]
2003	Exponential integrate-and-fire	[25]
2004	Generalized integrate-and-fire	[26]
2005	Adaptive exponential integrate-and-fire	[27]
2009	Mihalas-Neibur	[28]

Spiking/LIF Neuron Function

http://ee.princeton.edu/research/prucnal/sites/default/files/06497478.pdf

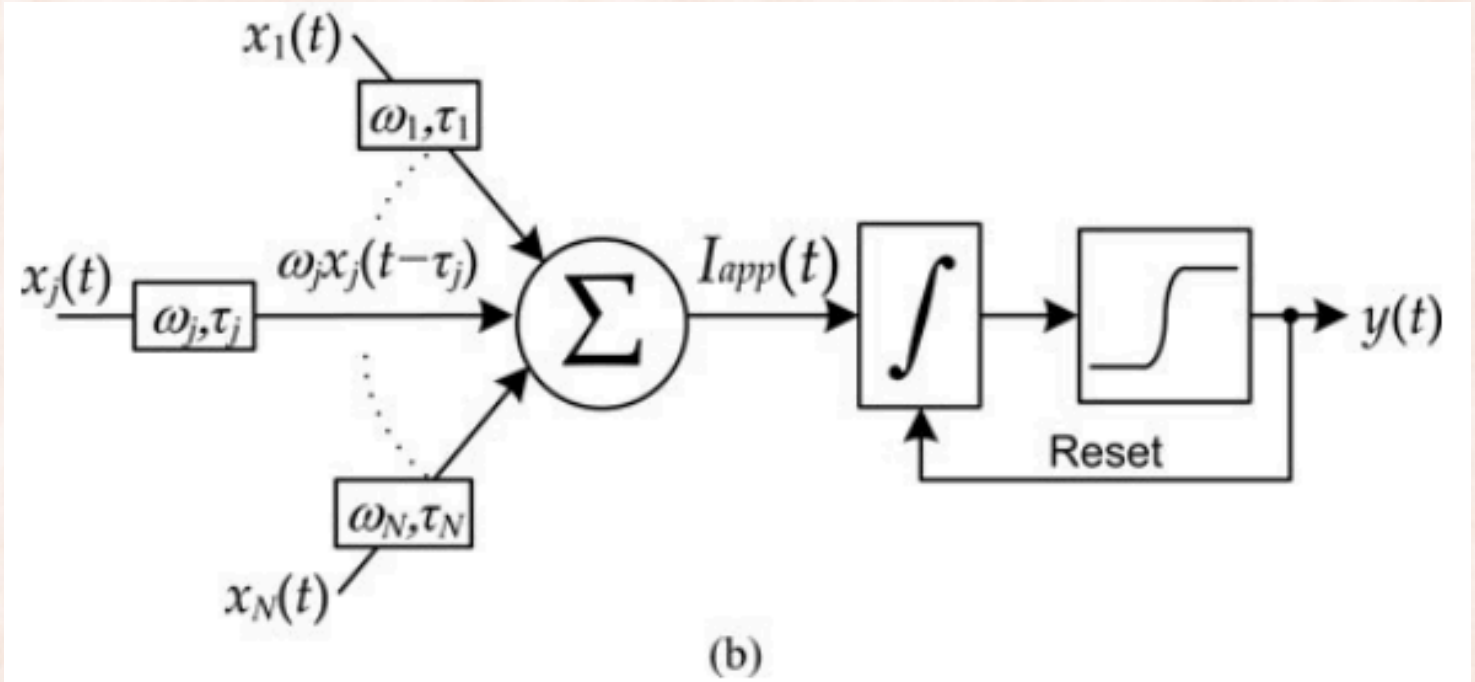


Fig. 2. (a) Illustration and (b) functional description of a leaky integrate-and-fire neuron. Weighted and delayed input signals are summed into the input current $I_{\mathrm{app}}(t)$, which travel to the soma and perturb the internal state variable, the voltage V. Since V is hysteric, the soma performs integration and then applies a threshold to make a spike or no-spike decision. After a spike is released, the voltage V is reset to a value V_{reset}. The resulting spike is sent to other neurons in the network.

Neuron Models

https://www.research.ibm.com/software/IBMResearch/multimedia/IJCNN2013.neuron-model.pdf

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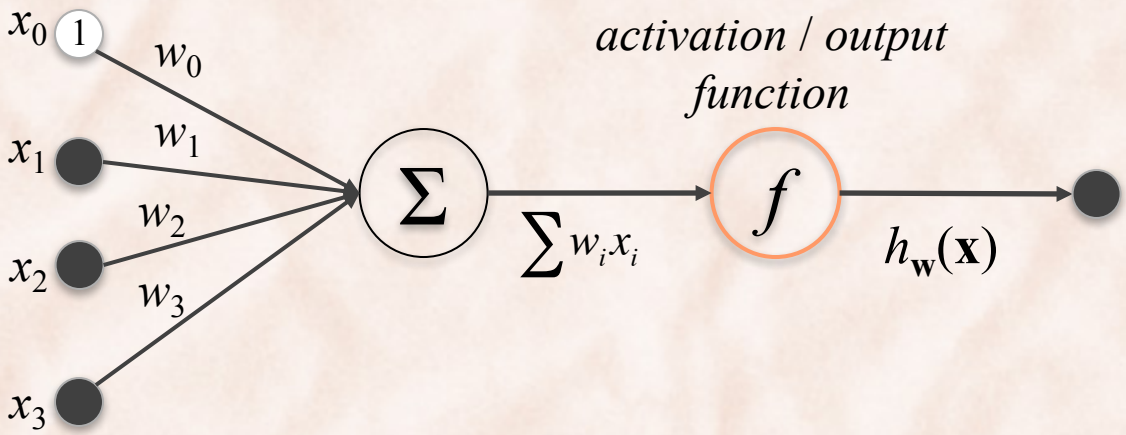
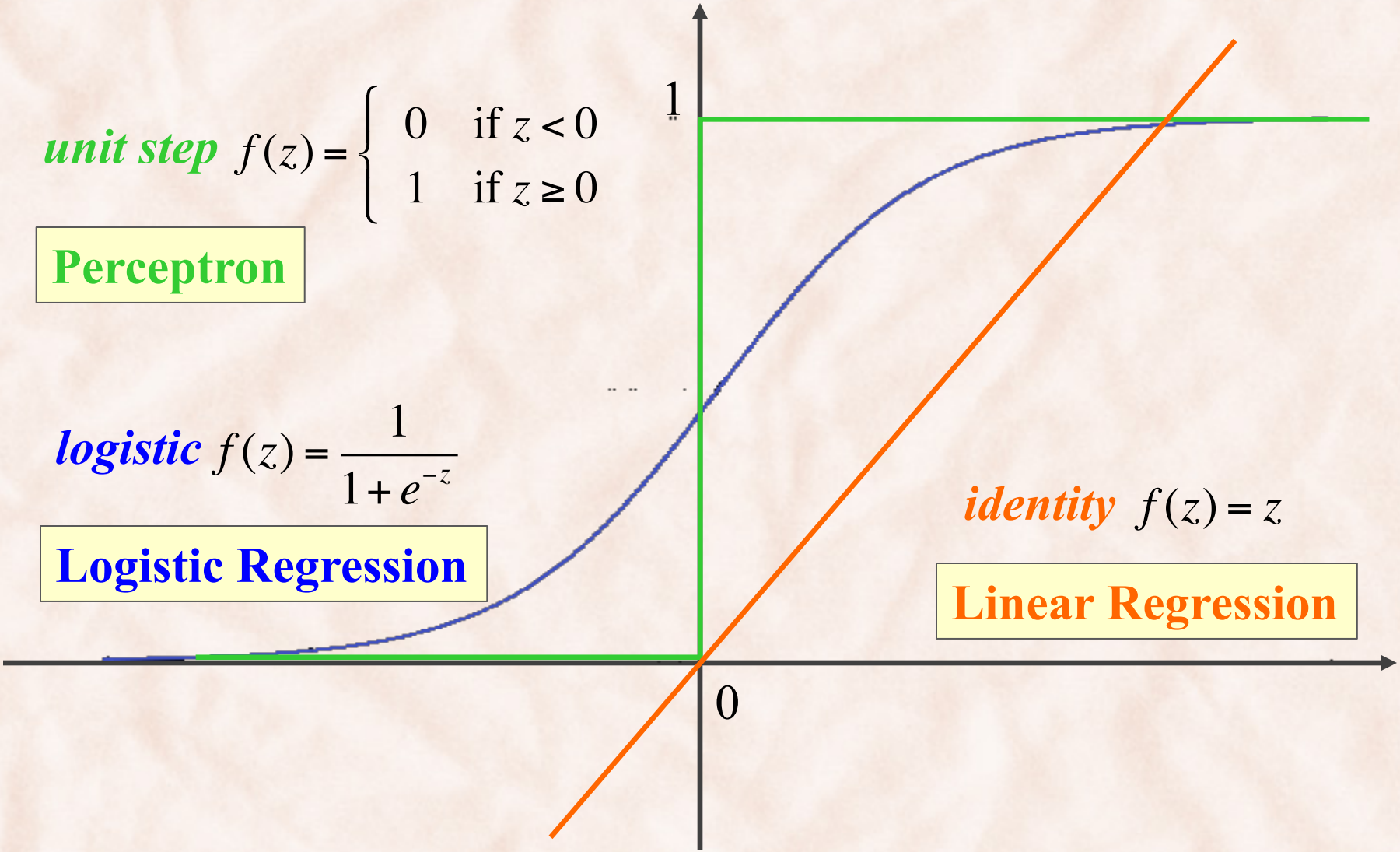
McCulloch-Pitts Neuron Function

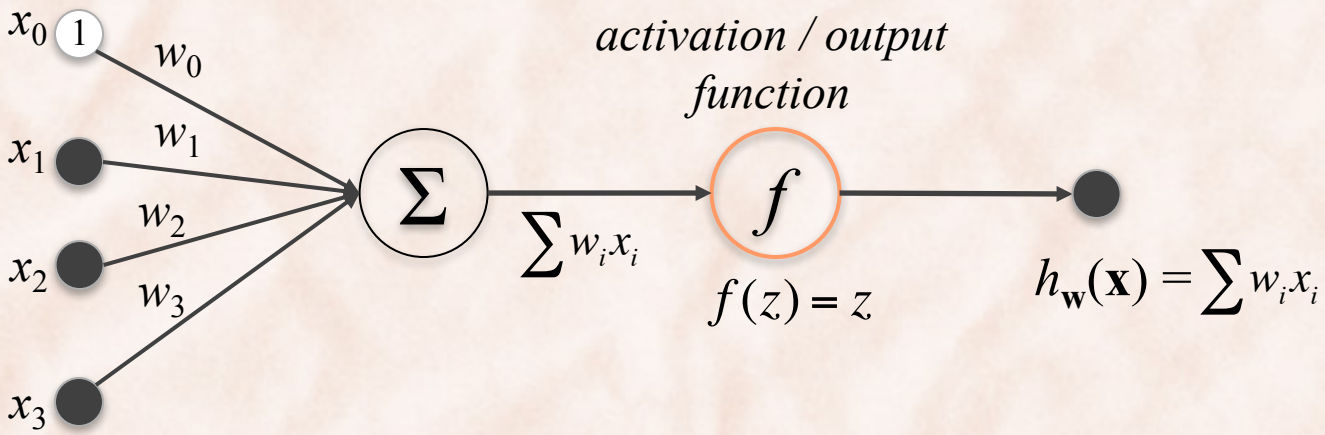


- Algebraic interpretation:
  - The output of the neuron is a **linear combination** of inputs from other neurons, **rescaled by** the synaptic **weights**.
    - weights w_i correspond to the synaptic weights (activating or inhibiting).
    - summation corresponds to combination of signals in the soma.
  - It is often transformed through an **activation / output function**.

Activation Functions



Linear Regression

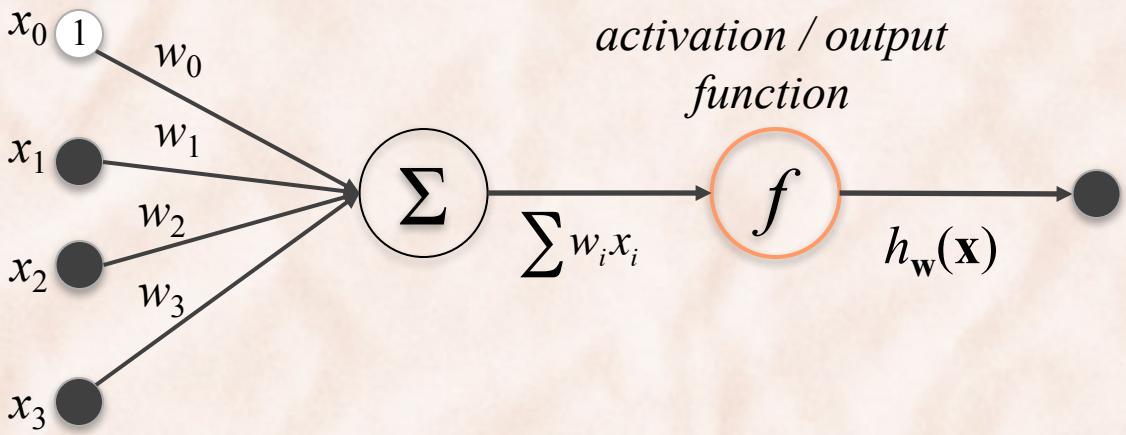


- Polynomial curve fitting is Linear Regression:

  $\mathbf{x} = \varphi(x) = [1, x, x^2, ..., x^M]^T$

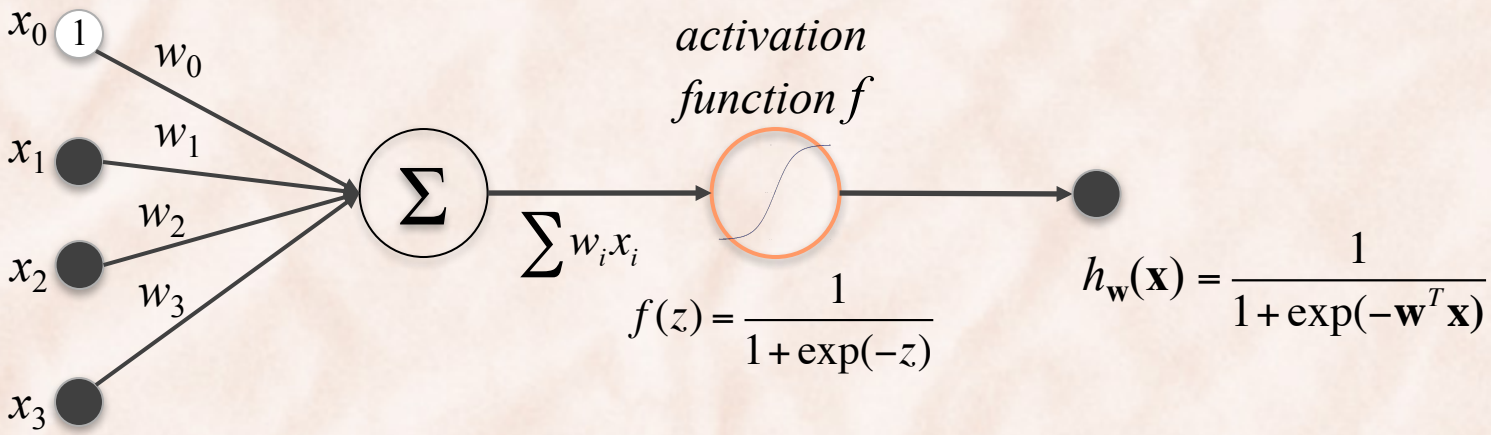
  $h(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$

McCulloch-Pitts Neuron Function



- Algebraic interpretation:
  - The output of the neuron is a **linear combination** of inputs from other neurons, **rescaled by** the synaptic **weights**.
    - weights w_i correspond to the synaptic weights (activating or inhibiting).
    - summation corresponds to combination of signals in the soma.
  - It is often transformed through a monotonic **activation / output function**.

Logistic Regression



- Training set is $(\mathbf{x}_1,t_1)$, $(\mathbf{x}_2,t_2)$, … $(\mathbf{x}_n,t_n)$.

  $\mathbf{x} = [1, x_1, x_2, ..., x_k]^T$

  $h(\mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x})$

- Can be used for both classification and regression:
  - Classification: T = $\{C_1, C_2\}$ = {1, 0}.
  - Regression: T = [0, 1] (i.e. output needs to be normalized).

Logistic Regression for Binary Classification

- Model output can be interpreted as **posterior class probabilities**:

$$p(C_1 \mid \mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x}) = \frac{1}{1+\exp(-\mathbf{w}^T\mathbf{x}))}$$

$$p(C_2 \mid \mathbf{x}) = 1-\sigma(\mathbf{w}^T\mathbf{x}) = \frac{\exp(-\mathbf{w}^T\mathbf{x})}{1+\exp(-\mathbf{w}^T\mathbf{x})}$$

- How do we train a logistic regression model?
  - What **error/cost function** to minimize?

Logistic Regression Learning

- Learning = finding the "right" parameters $\mathbf{w}^T = [w_0, w_1, \ldots, w_k]$
  - Find $\mathbf{w}$ that minimizes an *error function* $E(\mathbf{w})$ which measures the misfit between $h(\mathbf{x}_n, \mathbf{w})$ and t_n.
  - Expect that $h(\mathbf{x}, \mathbf{w})$ performing well on training examples $\mathbf{x}_n \Rightarrow$ $h(\mathbf{x}, \mathbf{w})$ will perform well on arbitrary test examples $\mathbf{x} \in X$.

- **Least Squares** error function?

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{h(\mathbf{x}_n, \mathbf{w}) - t_n\}^2$$

  - Differentiable => can use gradient descent ✓
  - Non-convex => not guaranteed to find the global optimum ✗

Maximum Likelihood

Training set is $D = \{\langle \mathbf{x}_n, t_n \rangle \mid t_n \in \{0,1\}, n \in 1\ldots N\}$

Let $h_n = p(C_1 \mid \mathbf{x}_n) \Leftrightarrow h_n = p(t_n = 1 \mid \mathbf{x}_n) = \sigma(\mathbf{w}^T \mathbf{x}_n)$

Maximum Likelihood (ML) principle: find parameters that maximize the likelihood of the labels.

- The likelihood function is $p(\mathbf{t} \mid \mathbf{w}) = \prod_{n=1}^{N} h_n^{t_n} (1 - h_n)^{(1-t_n)}$

- The negative log-likelihood (cross entropy) error function:

$$E(\mathbf{w}) = -\ln p(\mathbf{t} \mid \mathbf{x}) = -\sum_{n=1}^{N} \{t_n \ln h_n + (1 - t_n) \ln(1 - h_n)\}$$

Maximum Likelihood Learning for Logistic Regression

- The ML solution is:

$$\mathbf{w}_{ML} = \arg\max_{\mathbf{w}} p(\mathbf{t} \mid \mathbf{w}) = \arg\min_{\mathbf{w}} E(\mathbf{w})$$

convex in $\mathbf{w}$

- ML solution is given by $\nabla E(\mathbf{w}) = 0$.
  - Cannot solve analytically => solve numerically with gradient based methods: (stochastic) gradient descent, conjugate gradient, L-BFGS, etc.
  - Gradient is (prove it):

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (h_n - t_n)\mathbf{x}_n^T$$

Regularized Logistic Regression

- Use a Gaussian prior over the parameters:

$$\mathbf{w} = [w_0, w_1, \ldots, w_M]^{\mathrm{T}}$$

$$p(\mathbf{w}) = N(\mathbf{0}, \alpha^{-1}\mathbf{I}) = \left(\frac{\alpha}{2\pi}\right)^{(M+1)/2} \exp\left\{-\frac{\alpha}{2}\mathbf{w}^T\mathbf{w}\right\}$$

- Bayes' Theorem:

$$p(\mathbf{w}\,|\,\mathbf{t}) = \frac{p(\mathbf{t}\,|\,\mathbf{w})p(\mathbf{w})}{p(\mathbf{t})} \propto p(\mathbf{t}\,|\,\mathbf{w})p(\mathbf{w})$$

- MAP solution:

$$\mathbf{w}_{MAP} = \arg\max_{\mathbf{w}} p(\mathbf{w}\,|\,\mathbf{t})$$

Regularized Logistic Regression

- MAP solution:

$$\mathbf{w}_{MAP} = \arg\max_{\mathbf{w}} p(\mathbf{w}\,|\,\mathbf{t}) = \arg\max_{\mathbf{w}} p(\mathbf{t}\,|\,\mathbf{w})p(\mathbf{w})$$

$$= \arg\min_{\mathbf{w}} -\ln p(\mathbf{t}\,|\,\mathbf{w})p(\mathbf{w})$$

$$= \arg\min_{\mathbf{w}} -\ln p(\mathbf{t}\,|\,\mathbf{w}) - \ln p(\mathbf{w})$$

$$= \arg\min_{\mathbf{w}} E_D(\mathbf{w}) - \ln p(\mathbf{w})$$

$$= \arg\min_{\mathbf{w}} E_D(\mathbf{w}) + \frac{\alpha}{2}\mathbf{w}^T\mathbf{w} \qquad = \arg\min_{\mathbf{w}} E_D(\mathbf{w}) + E_{\mathbf{w}}(\mathbf{w})$$

$$E_D(\mathbf{w}) = -\sum_{n=1}^{N}\{t_n \ln y_n + (1-t_n)\ln(1-y_n)\}$$ ----------> *data term*

$$E_{\mathbf{w}}(\mathbf{w}) = \frac{\alpha}{2}\mathbf{w}^T\mathbf{w}$$ ----------> *regularization term*

Regularized Logistic Regression

- MAP solution:

$$\mathbf{w}_{MAP} = \arg\min_{\mathbf{w}} E_D(\mathbf{w}) + E_{\mathbf{w}}(\mathbf{w})$$

still convex in $\mathbf{w}$

- ML solution is given by $\nabla E(\mathbf{w}) = 0$.

$$\nabla E(\mathbf{w}) = \nabla E_D(\mathbf{w}) + \nabla E_{\mathbf{w}}(\mathbf{w}) = \sum_{n=1}^{N} (h_n - t_n)\mathbf{x}_n^T + \alpha \mathbf{w}^T$$

where $h_n = \sigma(\mathbf{w}^T \mathbf{x}_n)$

- Cannot solve analytically => solve numerically:
  - (stochastic) gradient descent [PRML 3.1.3], Newton Raphson iterative optimization [PRML 4.3.3], conjugate gradient, LBFGS.

Softmax Regression = Logistic Regression for Multiclass Classification

- Multiclass classification:

  $T = \{C_1, C_2, ..., C_K\} = \{1, 2, ..., K\}$.

- Training set is $(\mathbf{x}_1,t_1)$, $(\mathbf{x}_2,t_2)$, … $(\mathbf{x}_n,t_n)$.

  $\mathbf{x} = [1, x_1, x_2, ..., x_M]$

  $t_1, t_2, \ldots t_n \in \{1, 2, ..., K\}$

- One weight vector per class [PRML 4.3.4]:

$$p(C_k \mid \mathbf{x}) = \frac{\exp(\mathbf{w}_k^T \mathbf{x}))}{\sum_j \exp(\mathbf{w}_j^T \mathbf{x})}$$

Softmax Regression (K ≥ 2)

- Inference:

$$C_* = \arg\max_{C_k} p(C_k \mid \mathbf{x})$$

$$= \arg\max_{C_k} \frac{\exp(\mathbf{w}_k^T \mathbf{x})}{\sum_j \exp(\mathbf{w}_j^T \mathbf{x})}$$

$Z(\mathbf{x})$ *a normalization constant*

$$= \arg\max_{C_k} \exp(\mathbf{w}_k^T \mathbf{x})$$

$$= \arg\max_{C_k} \mathbf{w}_k^T \mathbf{x}$$

- Training using:
  - Maximum Likelihood (ML)
  - Maximum A Posteriori (MAP) with a Gaussian prior on $\mathbf{w}$.

Softmax Regression

- The **negative log-likelihood** error function is:

$$E_D(\mathbf{w}) = -\frac{1}{N}\ln\prod_{n=1}^{N} p(t_n \mid \mathbf{x}_n)$$

$$= -\frac{1}{N}\sum_{n=1}^{N}\ln\frac{\exp(\mathbf{w}_{t_n}^T\mathbf{x}_n)}{Z(\mathbf{x}_n)}$$

$$= -\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K}\delta_k(t_n)\ln\frac{\exp(\mathbf{w}_k^T\mathbf{x}_n)}{Z(\mathbf{x}_n)}$$

convex in $\mathbf{w}$

where $\delta_t(x) = \begin{cases} 1 & x = t \\ 0 & x \neq t \end{cases}$ is the *Kronecker delta* function.

Softmax Regression

- The ML solution is:

$$\mathbf{w}_{ML} = \arg\min_{\mathbf{w}} E_D(\mathbf{w})$$

- The **gradient** is (prove it):

$$\nabla_{\mathbf{w}_k} E_D(\mathbf{w}) = -\frac{1}{N}\sum_{n=1}^{N}\left(\delta_k(t_n) - p(C_k \mid \mathbf{x}_n)\right)\mathbf{x}_n$$

$$= -\frac{1}{N}\sum_{n=1}^{N}\left(\delta_k(t_n) - \frac{\exp(\mathbf{w}_k^T\mathbf{x}_n)}{Z(\mathbf{x}_n)}\right)\mathbf{x}_n$$

$$\nabla E_D(\mathbf{w}) = \left[\nabla_{\mathbf{w}_1}^T E_D(\mathbf{w}), \nabla_{\mathbf{w}_2}^T E_D(\mathbf{w}), \ldots, \nabla_{\mathbf{w}_K}^T E_D(\mathbf{w})\right]^T$$

Regularized Softmax Regression

- The new **cost** function is:

$$E(\mathbf{w}) = E_D(\mathbf{w}) + E_{\mathbf{w}}(\mathbf{w})$$

$$= -\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K}\delta_k(t_n)\ln\frac{\exp(\mathbf{w}_k^T\mathbf{x}_n)}{Z(\mathbf{x}_n)} + \frac{\alpha}{2}\sum_{k=1}^{K}\mathbf{w}_k^T\mathbf{w}_k$$

- The new **gradient** is (prove it):

$$\nabla_{\mathbf{w}_k} E(\mathbf{w}) = -\frac{1}{N}\sum_{n=1}^{N}\left(\delta_k(t_n) - p(C_k \mid \mathbf{x}_n)\right)\mathbf{x}_n^T + \alpha\mathbf{w}_k^T$$

Softmax Regression

- ML solution is given by $\nabla E_D(\mathbf{w}) = 0$.
  - Cannot solve analytically.
  - Solve numerically, by pluging [*cost*, *gradient*] = [$E_D(\mathbf{w})$, $\nabla E_D(\mathbf{w})$] values into general convex solvers:
    - L-BFGS
    - Newton methods
    - conjugate gradient
    - (stochastic / minibatch) gradient-based methods.
      - gradient descent (with / without momentum).
      - AdaGrad, AdaDelta
      - RMSProp
      - ADAM, ...

Implementation

- Need to compute [*cost*, ***gradient***]:
  - $cost = -\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K}\delta_k(t_n)\ln p(C_k \mid \mathbf{x}_n) + \frac{\alpha}{2}\sum_{k=1}^{K}\mathbf{w}_k^T\mathbf{w}_k$
  - $gradient_k = -\frac{1}{N}\sum_{n=1}^{N}\left(\delta_k(t_n) - p(C_k \mid \mathbf{x}_n)\right)\mathbf{x}_n^T + \alpha\mathbf{w}_k^T$

=> need to compute, for $k = 1, ..., K$:

- $output\ \ p(C_k \mid \mathbf{x}_n) = \frac{\exp(\mathbf{w}_k^T\mathbf{x}_n))}{\sum_j \exp(\mathbf{w}_j^T\mathbf{x}_n)}$

Overflow when $\mathbf{w}_k{}^T\mathbf{x}_n$ are too large.

Implementation: Preventing Overflows

- Subtract from each product $\mathbf{w}_k{}^{\mathrm{T}}\mathbf{x}_n$ the maximum product:

$$c = \max_{1 \le k \le K} \mathbf{w}_k^T \mathbf{x}_n$$

$$p(C_k \mid \mathbf{x}_n) = \frac{\exp(\mathbf{w}_k^T \mathbf{x}_n - c))}{\sum_j \exp(\mathbf{w}_j^T \mathbf{x}_n - c)}$$

Implementation: Gradient Checking

- Want to minimize $J(\theta)$, where θ is a scalar.

- Mathematical definition of derivative:

$$\frac{d}{d\theta}J(\theta) = \lim_{\varepsilon \to \infty} \frac{J(\theta+\varepsilon) - J(\theta-\varepsilon)}{2\varepsilon}$$

- Numerical approximation of derivative:

$$\frac{d}{d\theta}J(\theta) \approx \frac{J(\theta+\varepsilon) - J(\theta-\varepsilon)}{2\varepsilon}$$ where $\varepsilon = 0.0001$

Implementation: Gradient Checking

- If $\boldsymbol{\theta}$ is a vector of parameters $\boldsymbol{\theta}_i$,
  - Compute numerical derivative with respect to each $\boldsymbol{\theta}_i$.
  - Aggregate all derivatives into numerical gradient $G_{\text{num}}(\boldsymbol{\theta})$.

- Compare numerical gradient $G_{\text{num}}(\boldsymbol{\theta})$ with implementation of gradient $G_{\text{imp}}(\boldsymbol{\theta})$:

$$\frac{\left\| G_{num}(\boldsymbol{\theta}) - G_{imp}(\boldsymbol{\theta}) \right\|}{\left\| G_{num}(\boldsymbol{\theta}) + G_{imp}(\boldsymbol{\theta}) \right\|} \leq 10^{-6}$$

Machine Learning: Fisher's Linear Discriminant

Lecture 05

Razvan C. Bunescu

School of Electrical Engineering and Computer Science

bunescu@ohio.edu

Supervised Learning

- **Task** = learn an (unkown) function $t : X \rightarrow T$ that maps input instances $\mathbf{x} \in X$ to output targets $t(\mathbf{x}) \in T$:
  - **Classification**:
    - The output $t(\mathbf{x}) \in T$ is one of a finite set of discrete categories.
  - **Regression**:
    - The output $t(\mathbf{x}) \in T$ is continuous, or has a continuous component.

- Target function $t(\mathbf{x})$ is known (only) through (noisy) set of training examples:

$$(\mathbf{x}_1,t_1), (\mathbf{x}_2,t_2), \ldots (\mathbf{x}_n,t_n)$$

Three Parametric Approaches to Classification

1) Discriminant Functions: construct $f: \mathrm{X} \rightarrow \mathrm{T}$ that directly assigns a vector $\mathbf{x}$ to a specific class C_k.
   - Inference and decision combined into a single learning problem.
   - *Linear Discriminant*: the decision surface is a hyperplane in X:
     - Fisher 's Linear Discriminant
     - Perceptron
     - Support Vector Machines

Three Parametric Approaches to Classification

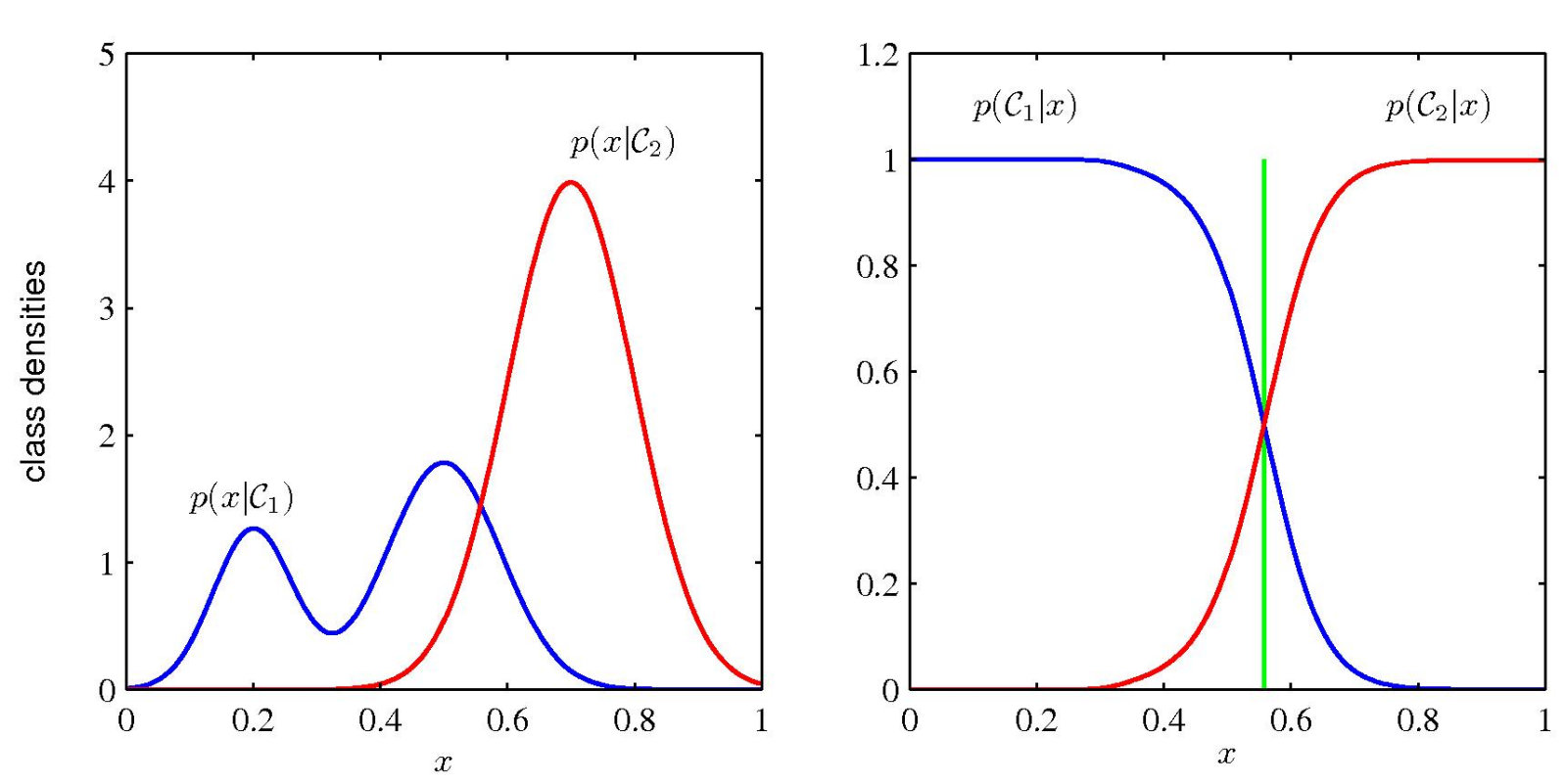
2) Probabilistic Discriminative Models: directly model the posterior class probabilities $p(C_k \mid \mathbf{x})$.
   - Inference and decision are separate.
   - Less data needed to estimate $p(C_k \mid \mathbf{x})$ than $p(\mathbf{x} \mid C_k)$.
   - Can accommodate many overlapping features.
     - Logistic Regression
     - Conditional Random Fields

Three Parametric Approaches to Classification

3) Probabilistic Generative Models:

- Model class-conditional $p(\mathbf{x} \mid C_k)$ as well as the priors $p(C_k)$, then use Bayes's theorem to find $p(C_k \mid \mathbf{x})$.
  - or model $p(\mathbf{x}, C_k)$ directly, then marginalize to obtain the posterior probabilities $p(C_k \mid \mathbf{x})$.
- Inference and decision are separate.
- Can use $p(\mathbf{x})$ for *outlier* or *novelty detection*.
- Need to model dependencies between features.
  - Naïve Bayes.
  - Hidden Markov Models.

Generative vs. Discriminative



Left-hand mode has no effect on posterior class probabilities.

Linear Discriminant Functions: Two classes ($K = 2$)

- Use a linear function of the input vector:

$$y(\mathbf{x}) = \mathbf{w}^T \varphi(\mathbf{x}) + w_0$$

weight vector

bias = – threshold

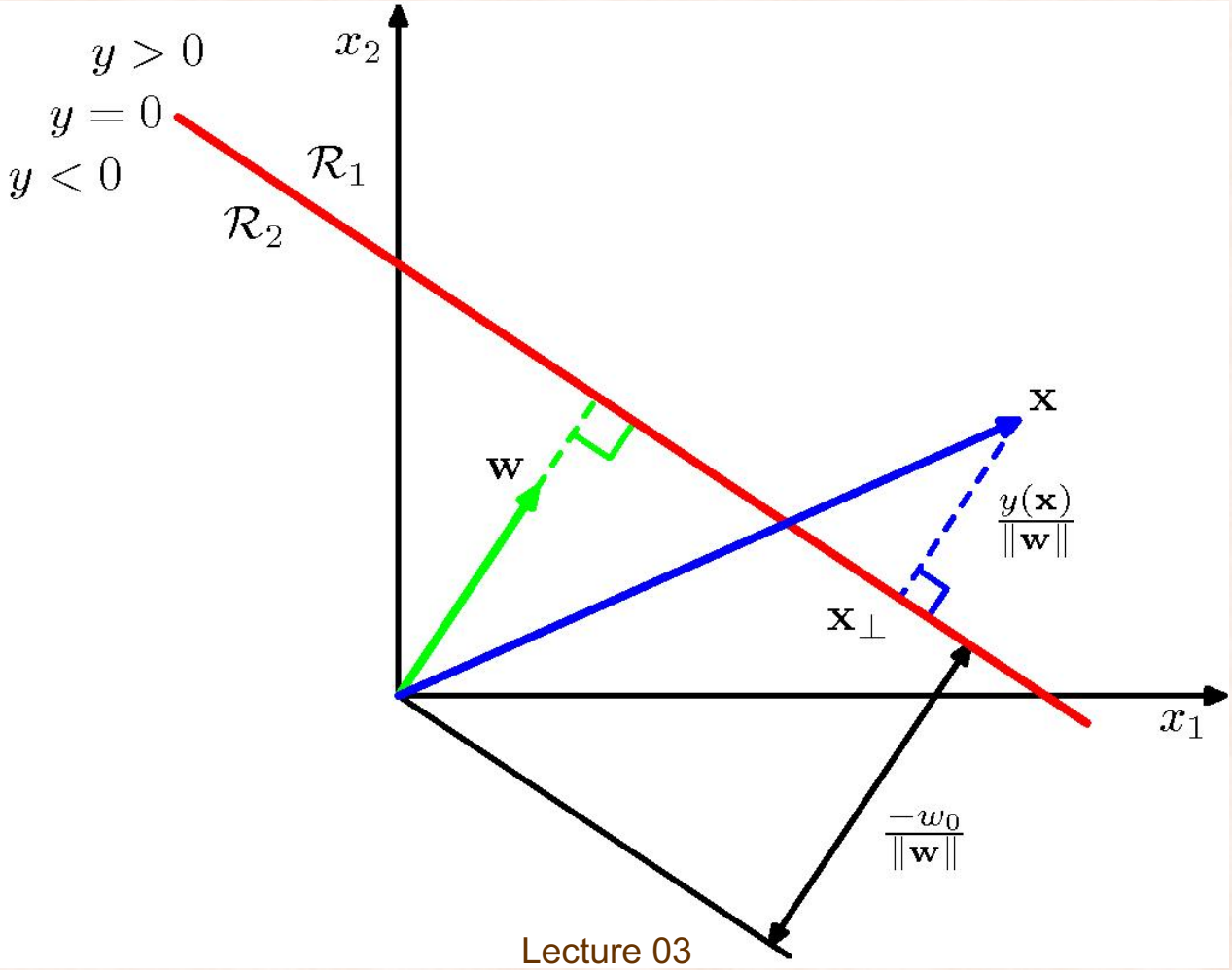
- Decision:

  $\mathbf{x} \in C_1$ if $y(\mathbf{x}) \geq 0$, otherwise $\mathbf{x} \in C_2$.

  $\Rightarrow$ decision boundary is hyperplane $y(\mathbf{x}) = 0$.

- Properties:
  - $\mathbf{w}$ is orthogonal to vectors lying within the decision surface.
  - w_0 controls the location of the decision hyperplane.

Linear Discriminant Functions: Two Classes ($K = 2$)



Linear Discriminant Functions: Multiple Classes (K > 2)

1) Train K or K–1 *one-versus-the-rest* classifiers.
2) Train K(K–1)/2 *one-versus-one* classifiers.

3) Train K linear functions:

$$y_k(\mathbf{x}) = \mathbf{w}_k^T \varphi(\mathbf{x}) + w_{k0}$$

- Decision:

$\mathbf{x} \in \mathrm{C_k}$ if $y_k(\mathbf{x}) > y_j(\mathbf{x})$, for all $j \neq k$.

$\Rightarrow$ decision boundary between classes C_k and C_j is hyperplane defined by $y_k(\mathbf{x}) = y_j(\mathbf{x})$ i.e. $(\mathbf{w}_k - \mathbf{w}_j)^T \varphi(\mathbf{x}) + (w_{k0} - w_{j0}) = 0$

$\Rightarrow$ same geometrical properties as in binary case.

Linear Discriminant Functions: Multiple Classes (K > 2)

4) More general ranking approach:

$$y(\mathbf{x}) = \arg\max_{t \in T} \mathbf{w}^T \varphi(\mathbf{x}, t) \quad \text{where} \quad T = \{c_1, c_2 ..., c_K\}$$

- It subsumes the approach with K separate linear functions.

- Useful when T is very large (e.g. exponential in the size of input $\mathbf{x}$), assuming inference can be done efficiently.

Linear Discriminant Functions: Two Classes (K = 2)

- What algorithms can be used to learn $y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\varphi(\mathbf{x}) + w_0$?

  Assume a training dataset of $N = N_1 + N_2$ examples in C_1 and C_2.

  - Fisher's Linear Discriminant
  - Perceptron:
    - Voted/Averaged Perceptron
    - Kernel Perceptron
  - Support Vector Machines:
    - Linear
    - Kernel

Fisher's Linear Discriminant

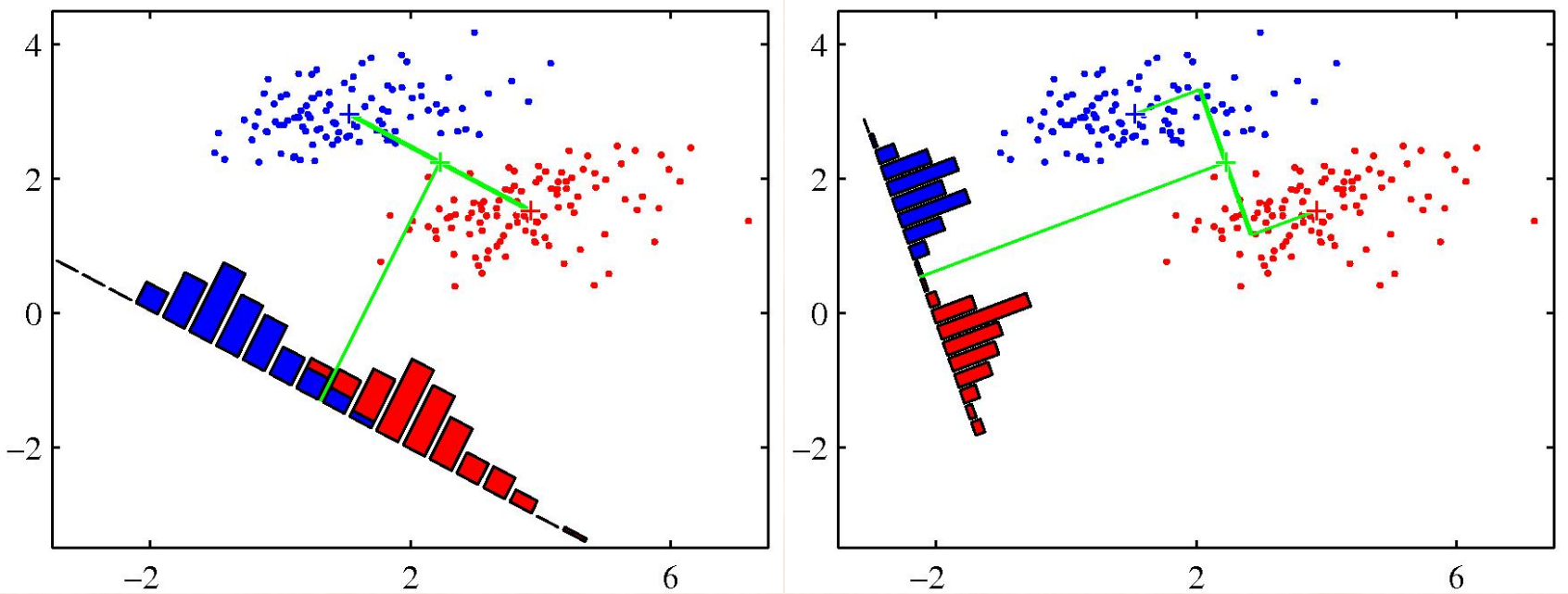
- Discriminant function $y(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0$ can be interpreted as follows:
  1. Project D-dimensional $\mathbf{x}$ down to one dimension $\Rightarrow \mathbf{w}^T\mathbf{x}$
  2. Use a threshold $-w_0$ to classify $\mathbf{x} \Rightarrow$

     $\mathbf{x} \in C_1$, if $\mathbf{w}^T\mathbf{x} \geq -w_0$

     $\mathbf{x} \in C_2$, otherwise.

- Fisher's idea:
  - Maximize the **between-class separation** of projected dataset.
  - Minimize the **within-class variance** of projected dataset.

Fisher's Linear Discriminant



Line joining the class means vs. Line inferred with Fisher's criterion.

Fisher's Linear Discriminant

1) Measure of the separation between the classes is the *between class variance*:

$$\left.\begin{aligned}\mathbf{m}_1 &= \frac{1}{N_1}\sum_{n\in C_1}\mathbf{x}_n \\ \mathbf{m}_2 &= \frac{1}{N_2}\sum_{n\in C_2}\mathbf{x}_n\end{aligned}\right\} \Rightarrow m_2 - m_1 = \mathbf{w}^T(\mathbf{m}_2 - \mathbf{m}_1) \Rightarrow \boxed{(m_2 - m_1)^2}$$

Fisher's Linear Discriminant

2) Measure of the *within-class variance*:

$$\left.\begin{aligned} s_1^2 &= \sum_{n \in C_1} (\mathbf{w}^T \mathbf{x}_n - m_1)^2 \\ s_2^2 &= \sum_{n \in C_2} (\mathbf{w}^T \mathbf{x}_n - m_2)^2 \end{aligned}\right\} \Rightarrow \boxed{s_1^2 + s_2^2}$$

Fisher's Linear Discriminant

- Maximize the between-class separation and minimize the within-class variance $\Rightarrow$ Fisher's criterion:

$$\mathbf{w}^* = \arg\max_{\mathbf{w}} J(\mathbf{w}) \quad \text{, where } J(\mathbf{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2}$$

- The objective function can be rewritten as:

$$J(\mathbf{w}) = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$$

where

$$\mathbf{S}_B = (\mathbf{m}_2 - \mathbf{m}_1)(\mathbf{m}_2 - \mathbf{m}_1)^T$$

$$\mathbf{S}_W = \sum_{n \in C_1} (\mathbf{x}_n - \mathbf{m}_1)(\mathbf{x}_n - \mathbf{m}_1)^T + \sum_{n \in C_2} (\mathbf{x}_n - \mathbf{m}_2)(\mathbf{x}_n - \mathbf{m}_2)^T$$

Fisher's Linear Discriminant

- Optimization formulation:

$$\mathbf{w}^* = \arg\max_{\mathbf{w}} J(\mathbf{w}) = \arg\max_{\mathbf{w}} \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$$

- Solution:

$$\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}} = 0 \Rightarrow (\mathbf{w}^T \mathbf{S}_W \mathbf{w}) \mathbf{S}_B \mathbf{w} = (\mathbf{w}^T \mathbf{S}_B \mathbf{w}) \mathbf{S}_W \mathbf{w}$$

$$\Rightarrow \mathbf{S}_B \mathbf{w} = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}} \mathbf{S}_W \mathbf{w} \Rightarrow \boxed{\mathbf{S}_B \mathbf{w} = \lambda \mathbf{S}_W \mathbf{w}}$$

generalized eigenvalue problem

- If $\mathbf{S}_W$ is nonsingular:

$$\Rightarrow \boxed{\mathbf{S}_W^{-1} \mathbf{S}_B \mathbf{w} = \lambda \mathbf{w}}$$

conventional eigenvalue problem

Fisher's Linear Discriminant

- No need to solve the eigenvalue problem:

  $\mathbf{S}_B\mathbf{w} = (\mathbf{m}_2 - \mathbf{m}_1)(\mathbf{m}_2 - \mathbf{m}_1)^T\mathbf{w}$ is a vector in the direction $(\mathbf{m}_2 - \mathbf{m}_1)$

- The norm of $\mathbf{w}$ is immaterial, only its direction is important.

  $\Rightarrow$ can take

  $$\mathbf{w} = \mathrm{S}_W^{-1}(\mathbf{m}_2 - \mathbf{m}_1)$$

- How to find w_0:
  - Assume $p(\mathbf{w}^T\mathbf{x}|C_1)$ and $p(\mathbf{w}^T\mathbf{x}|C_2)$ are Gaussians.
  - Estimate means and variances using maximum likelihood.
  - Use decision theory to find $\mathbf{w}_0$ i.e. $p(-\mathbf{w}_0|C_1) = p(-\mathbf{w}_0|C_2)$

Supplementary Reading

- PRML Section 1.4 (The Curse of Dimensionality).
- PRML Section 1.5 (Decision Theory).
- PRML Section 4 (Linear Models for Classification):
  - 4.1.1 to 4.1.4.

Machine Learning: The Perceptron

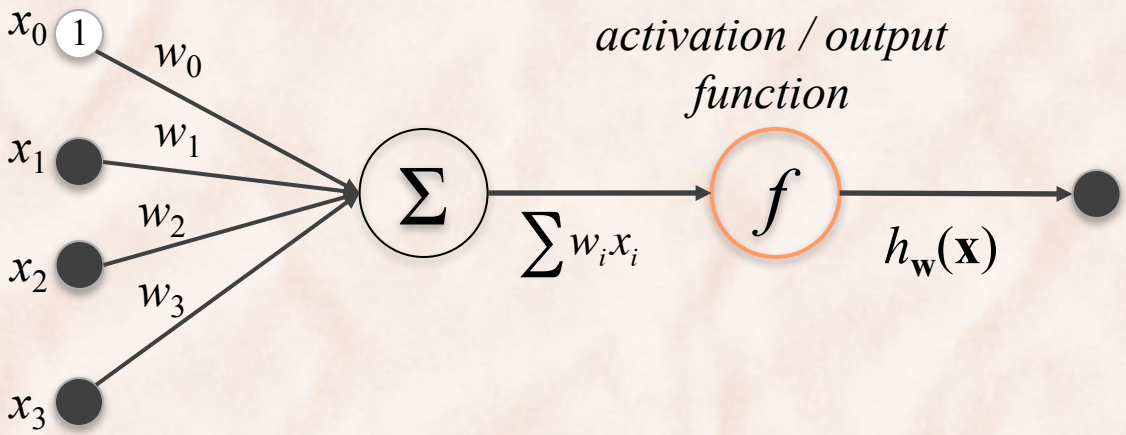
Lecture 06

Razvan C. Bunescu

School of Electrical Engineering and Computer Science

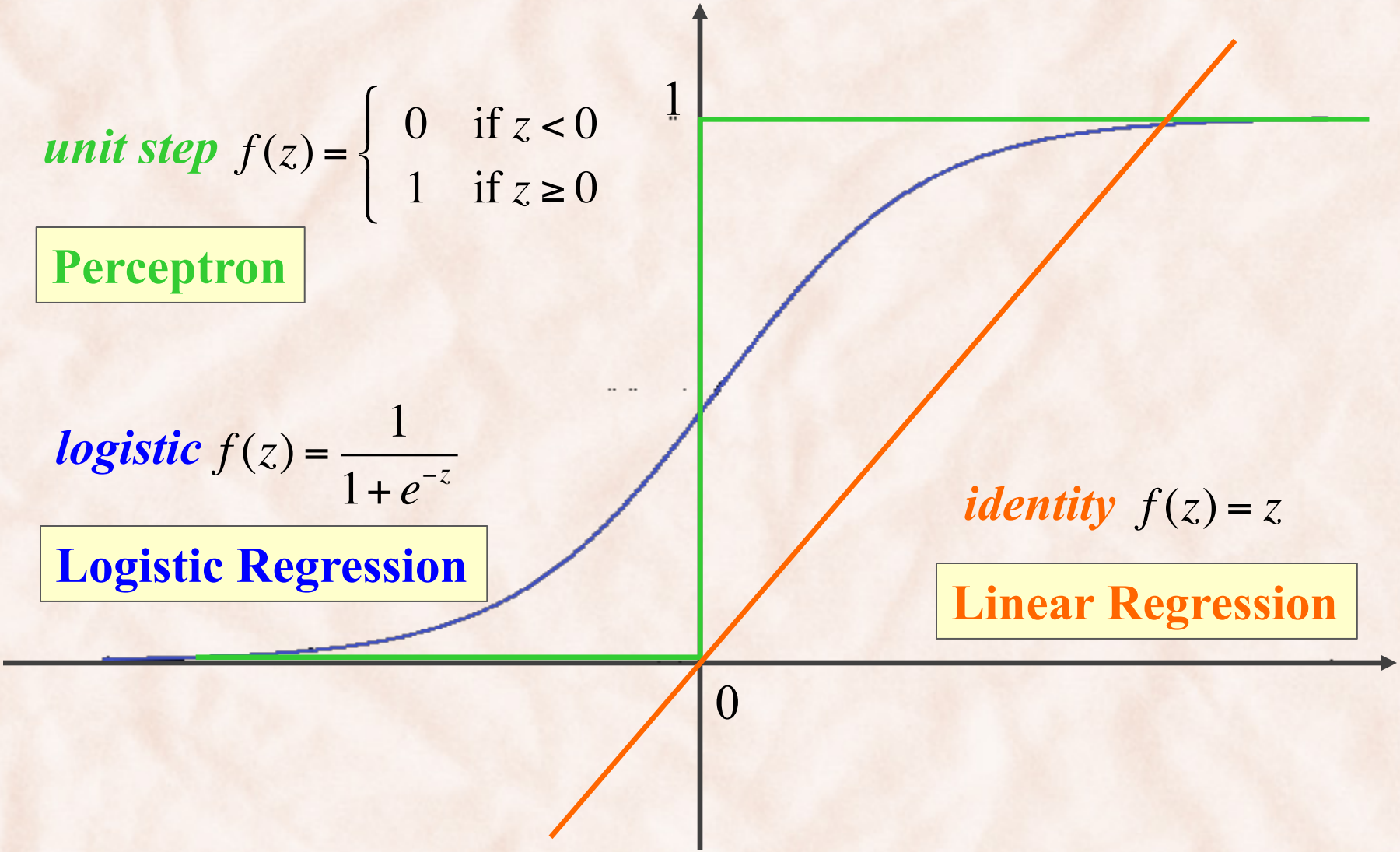
bunescu@ohio.edu

McCulloch-Pitts Neuron Function

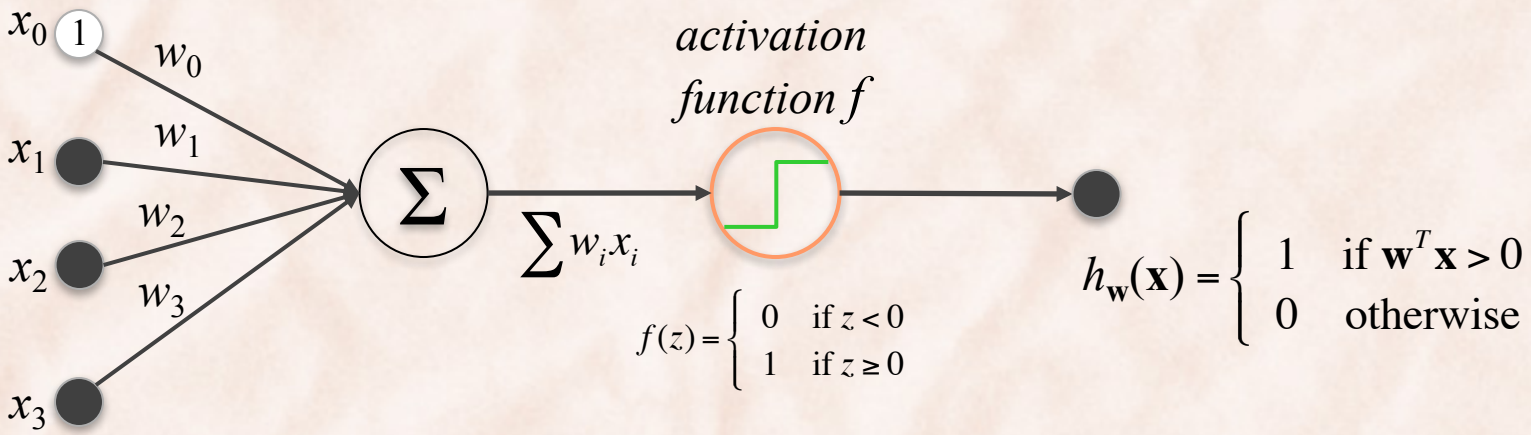


- Algebraic interpretation:
  - The output of the neuron is a **linear combination** of inputs from other neurons, **rescaled by** the synaptic **weights**.
    - weights w_i correspond to the synaptic weights (activating or inhibiting).
    - summation corresponds to combination of signals in the soma.
  - It is often transformed through a monotonic **activation function**.

Activation Functions



Perceptron



- Assume classes $T = \{c_1, c_2\} = \{1, 0\}$.
- Training set is $(\mathbf{x}_1,t_1), (\mathbf{x}_2,t_2), \ldots (\mathbf{x}_n,t_n)$.

  $\mathbf{x} = [1, x_1, x_2, \ldots, x_k]^T$

  $h(\mathbf{x}) = step(\mathbf{w}^T\mathbf{x})$

Perceptron Learning

- Learning = finding the "right" parameters $\mathbf{w}^T = [w_0, w_1, \ldots, w_k]$
  - Find $\mathbf{w}$ that minimizes an *error function* $E(\mathbf{w})$ which measures the misfit between $h(\mathbf{x}_n, \mathbf{w})$ and t_n.
  - Expect that $h(\mathbf{x},\mathbf{w})$ performing well on training examples $x_n \Rightarrow h(x,\mathbf{w})$ will perform well on arbitrary test examples $\mathbf{x} \in X$.

- **Least Squares** error function?

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{h(\mathbf{x}_n, \mathbf{w}) - t_n\}^2$$

# of mistakes

Least Squares vs. Perceptron Criterion

- **Least Squares** => cost is # of misclassified patterns:
  - Piecewise constant function of **w** with discontinuities.
  - Cannot find closed form solution for **w** that minimizes cost.
  - Cannot use gradient methods (gradient zero almost everywhere).

- **Perceptron Criterion**:
  - Set labels to be +1 and − 1. Want $\mathbf{w}^{\mathrm{T}}\mathbf{x}_n > 0$ for $t_n = 1$, and $\mathbf{w}^{\mathrm{T}}\mathbf{x}_n < 0$ for $t_n = -1$.
    - $\Rightarrow$ would like to have $\mathbf{w}^{\mathrm{T}}\mathbf{x}_n t_n > 0$ for all patterns.
    - $\Rightarrow$ want to minimize $-\mathbf{w}^{\mathrm{T}}\mathbf{x}_n t_n$ for all missclassified patterns M.

$$\Rightarrow \text{minimize } E_p(\mathbf{w}) = -\sum_{n \in M} \mathbf{w}^T \mathbf{x}_n t_n$$

Stochastic Gradient Descent

- **Perceptron Criterion**:

$$\text{minimize } E_p(\mathbf{w}) = -\sum_{n \in M} \mathbf{w}^T \mathbf{x}_n t_n$$

- Update parameters **w** sequentially **after each mistake**:

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_P(\mathbf{w}^{(\tau)}, \mathbf{x}_n)$$

$$= \mathbf{w}^{(\tau)} + \eta \mathbf{x}_n t_n$$

- The magnitude of **w** is inconsequential => set $\eta = 1$.

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} + \mathbf{x}_n t_n$$

The Perceptron Algorithm: Two Classes

1. **initialize** parameters $\mathbf{w} = 0$
2. **for** $n = 1 \ldots \mathrm{N}$
3. $\quad h_n = sgn(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n)$
4. $\quad$ **if** $h_{\mathrm{n}} \neq t_n$ **then**
5. $\quad\quad \mathbf{w} = \mathbf{w} + t_n\mathbf{x}_n$

Repeat:
a) until convergence.
b) for a number of epochs E.

Theorem [Rosenblatt, 1962]:

If the training dataset is linearly separable, the perceptron learning algorithm is guaranteed to find a solution in a finite number of steps.

- see Theorem 1 (Block, Novikoff) in [Freund & Schapire, 1999].

Averaged Perceptron: Two Classes

1. **initialize** parameters $\mathbf{w} = 0$, $\tau = 1$, $\overline{\mathbf{w}} = 0$
2. **for** $n = 1 \ldots \mathrm{N}$
3. $\quad h_n = sgn(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n)$
4. $\quad$ **if** $h_n \neq t_n$ **then**
5. $\quad\quad \mathbf{w} = \mathbf{w} + t_n\mathbf{x}_n$
6. $\quad \overline{\mathbf{w}} = \overline{\mathbf{w}} + \mathbf{w}$
7. $\quad \tau = \tau + 1$
8. **return** $\overline{\mathbf{w}} / \tau$

Repeat:
a) until convergence.
b) for a number of epochs E.

During testing: $\mathrm{h}(\mathbf{x}) = sgn(\overline{\mathbf{w}}^T\mathbf{x})$

The Perceptron Algorithm: Two Classes

1. **initialize** parameters $\mathbf{w} = 0$
2. **for** $n = 1 \ldots N$
3. $\quad h_n = sgn(\mathbf{w}^T \mathbf{x}_n)$
4. $\quad$ **if** $h_n \neq t_n$ **then**
5. $\quad\quad \mathbf{w} = \mathbf{w} + t_n \mathbf{x}_n$

Repeat:
a) until convergence.
b) for a number of epochs E.

Loop invariant: $\mathbf{w}$ is a weighted sum of training vectors:

$$\mathbf{w} = \sum_n \alpha_n t_n \mathbf{x}_n \quad \Rightarrow \quad \mathbf{w}^T \mathbf{x} = \sum_n \alpha_n t_n \mathbf{x}_n^T \mathbf{x}$$

Kernel Perceptron: Two Classes

1. **define** $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} = \sum_n \alpha_n t_n \mathbf{x}_n^T\mathbf{x} = \sum_n \alpha_n t_n K(\mathbf{x}_n, \mathbf{x})$
2. **initialize** dual parameters $\alpha_n = 0$
3. **for** $n = 1 \ldots N$
4. $\quad h_n = sgn\, f(\mathbf{x}_n)$
5. $\quad$ **if** $h_n \neq t_n$ **then**
6. $\quad\quad \alpha_n = \alpha_n + 1$

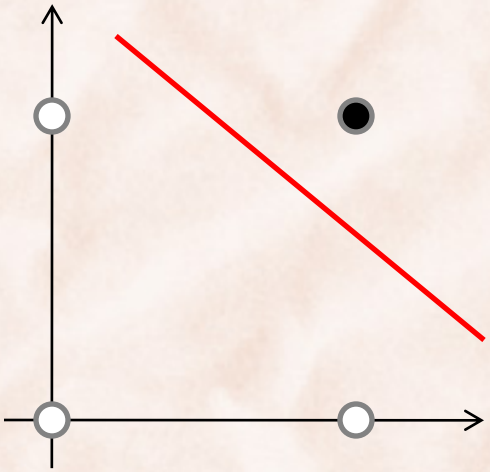
During testing: $h(\mathbf{x}) = sgn\, f(\mathbf{x})$

Kernel Perceptron: Two Classes

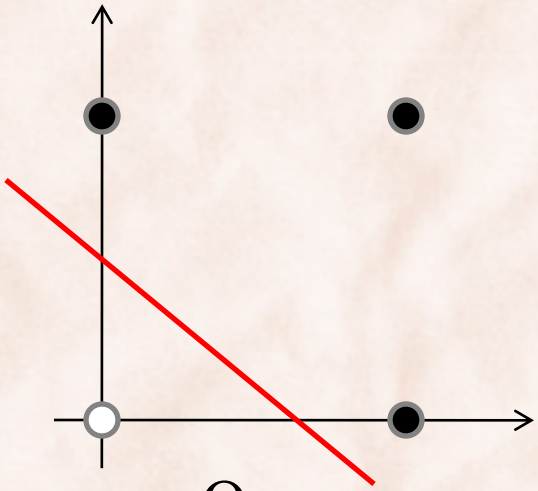
1. **define** $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} = \sum_n \alpha_n \mathbf{x}_n^T\mathbf{x} = \sum_n \alpha_n K(\mathbf{x}_n, \mathbf{x})$
2. **initialize** dual parameters $\alpha_n = 0$
3. **for** $n = 1 \ldots \mathrm{N}$
4. $\quad h_n = sgn\, f(\mathbf{x}_n)$
5. $\quad$ **if** $h_n \neq t_n$ **then**
6. $\quad\quad \alpha_n = \alpha_n + t_n$

During testing: $h(\mathbf{x}) = sgn\, f(\mathbf{x})$

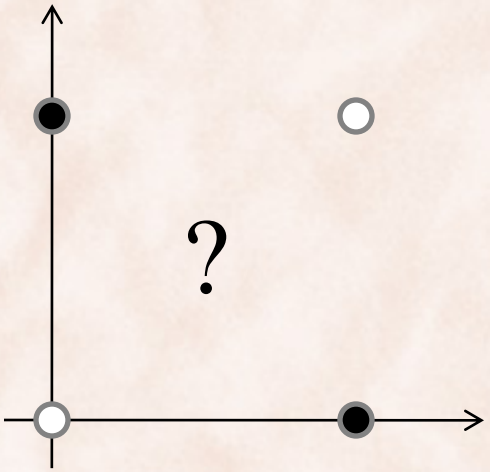
The Perceptron vs. Boolean Functions



And



Or



Xor

$$\left.\begin{aligned}\varphi(\mathbf{x}) &= [1, x_1, x_2]^T \\ \mathbf{w} &= [w_0, w_1, w_2]^T\end{aligned}\right\} \Rightarrow \mathbf{w}^T\varphi(\mathbf{x}) = [w_1, w_2]^T[x_1, x_2] + w_0$$

Perceptron with Quadratic Kernel

- Discriminant function:

$$f(\mathbf{x}) = \sum_i \alpha_i t_i \varphi(\mathbf{x}_i)^T \varphi(\mathbf{x}) = \sum_i \alpha_i t_i K(\mathbf{x}_i, \mathbf{x})$$

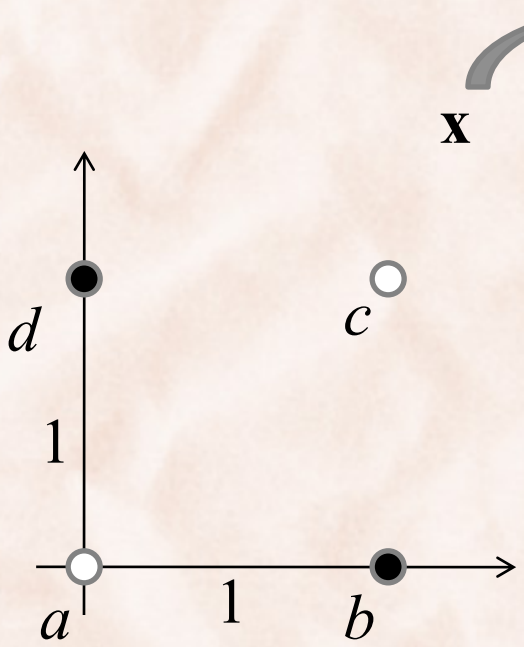
- Quadratic kernel:

$$K(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^T \mathbf{y})^2 = (x_1 y_1 + x_2 y_2)^2$$

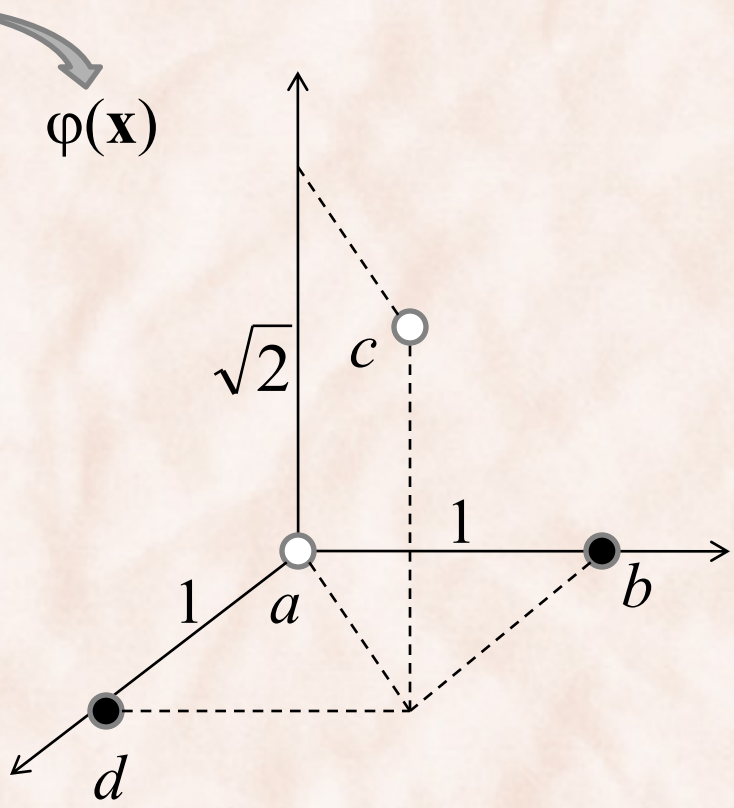
$\Rightarrow$ corresponding feature space $\varphi(\mathbf{x}) = ?$

conjunctions of two atomic features

Perceptron with Quadratic Kernel



Linear kernel $K(\mathbf{x},\mathbf{y}) = \mathbf{x}^T\mathbf{y}$



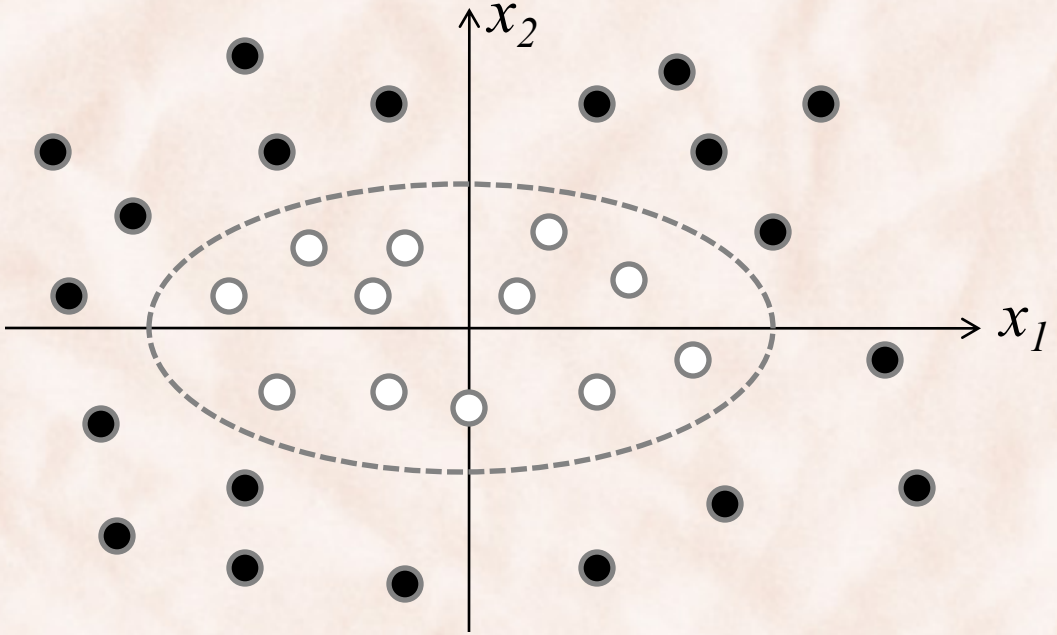
Quadratic kernel $K(\mathbf{x},\mathbf{y}) = (\mathbf{x}^T\mathbf{y})^2$

Quadratic Kernels

- Circles, hyperbolas, and ellipses as separating surfaces:

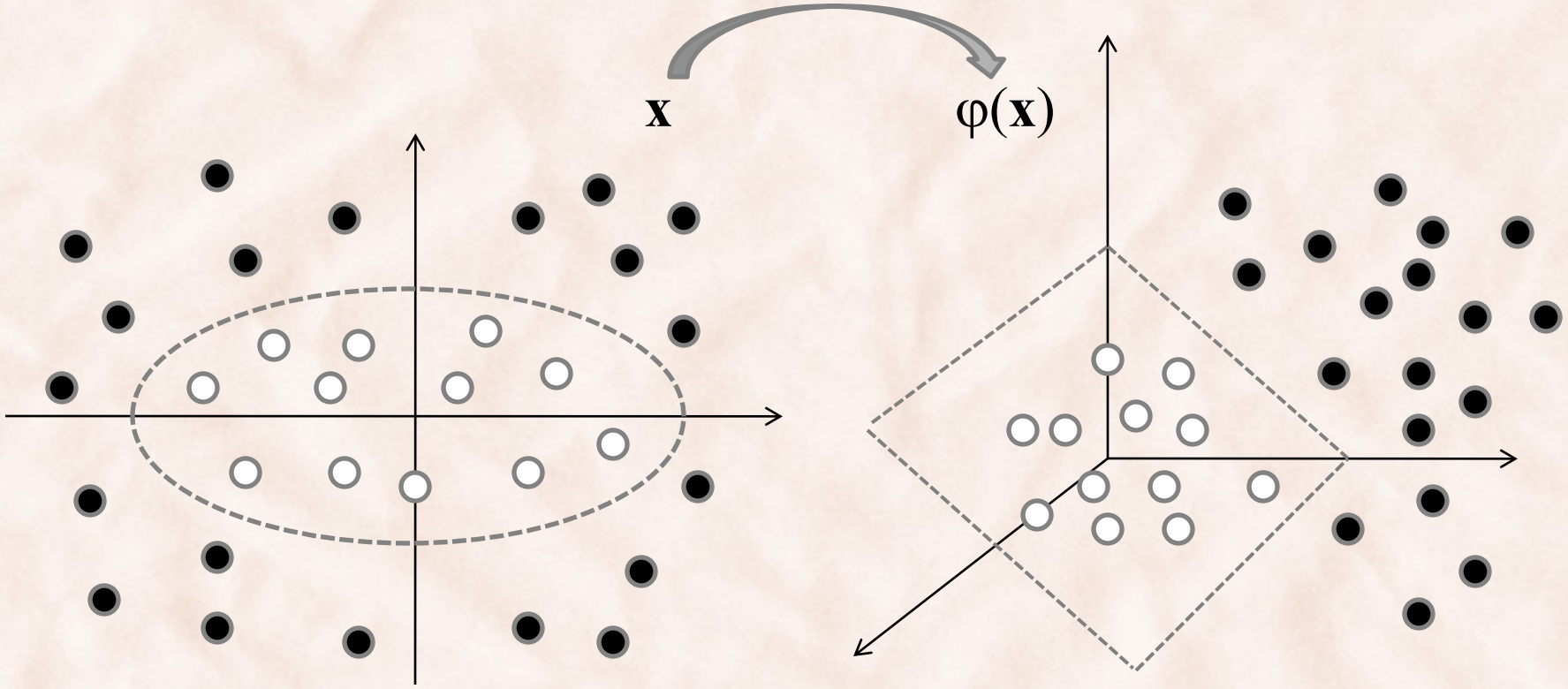
$$K(\mathbf{x},\mathbf{y}) = (1+\mathbf{x}^T\mathbf{y})^2 = \varphi(x)^T\varphi(y)$$

$$\varphi(x) = [1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, \sqrt{2}x_1x_2, x_2^2]^T$$



Quadratic Kernels

$$K(\mathbf{x},\mathbf{y}) = (\mathbf{x}^T\mathbf{y})^2 = \varphi(\mathbf{x})^T\varphi(\mathbf{y})$$



Explicit Features vs. Kernels

- Explicitly enumerating features can be prohibitive:
  - 1,000 basic features for $\mathbf{x}^T\mathbf{y}$ => 500,500 quadratic features for $(\mathbf{x}^T\mathbf{y})^2$
  - Much worse for higher order features.

- Solution:
  - Do not compute the feature vectors, compute kernels instead (i.e. compute dot products between implicit feature vectors).
    - $(\mathbf{x}^T\mathbf{y})^2$ takes 1001 multiplications.
    - $\varphi(\mathbf{x})^T \varphi(\mathbf{y})$ in feature space takes 500,500 multiplications.

Kernel Functions

- Definition:

  A function $k : \mathrm{X} \times \mathrm{X} \rightarrow \mathrm{R}$ is a kernel function if there exists a feature mapping $\varphi : \mathrm{X} \rightarrow \mathrm{R}^n$ such that:

  $$k(\mathbf{x},\mathbf{y}) = \varphi(\mathbf{x})^{\mathrm{T}}\varphi(\mathbf{y})$$

- Theorem:

  $k : \mathrm{X} \times \mathrm{X} \rightarrow \mathrm{R}$ is a valid kernel $\Leftrightarrow$ the Gram matrix K whose elements are given by $k(\mathbf{x}_n,\mathbf{x}_m)$ is positive semidefinite for all possible choices of the set $\{\mathbf{x}_n\}$.

Techniques for Constructing Kernels

Given valid kernels $k_1(\mathbf{x}, \mathbf{x}')$ and $k_2(\mathbf{x}, \mathbf{x}')$, the following new kernels will also be valid:

$$
\begin{aligned}
k(\mathbf{x}, \mathbf{x}') &= c k_1(\mathbf{x}, \mathbf{x}') && (6.13)\\
k(\mathbf{x}, \mathbf{x}') &= f(\mathbf{x}) k_1(\mathbf{x}, \mathbf{x}') f(\mathbf{x}') && (6.14)\\
k(\mathbf{x}, \mathbf{x}') &= q\left(k_1(\mathbf{x}, \mathbf{x}')\right) && (6.15)\\
k(\mathbf{x}, \mathbf{x}') &= \exp\left(k_1(\mathbf{x}, \mathbf{x}')\right) && (6.16)\\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}') && (6.17)\\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') k_2(\mathbf{x}, \mathbf{x}') && (6.18)\\
k(\mathbf{x}, \mathbf{x}') &= k_3\left(\boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}')\right) && (6.19)\\
k(\mathbf{x}, \mathbf{x}') &= \mathbf{x}^{\mathrm{T}} \mathbf{A} \mathbf{x}' && (6.20)\\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}'_a) + k_b(\mathbf{x}_b, \mathbf{x}'_b) && (6.21)\\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}'_a) k_b(\mathbf{x}_b, \mathbf{x}'_b) && (6.22)
\end{aligned}
$$

where $c > 0$ is a constant, $f(\cdot)$ is any function, $q(\cdot)$ is a polynomial with nonnegative coefficients, $\boldsymbol{\phi}(\mathbf{x})$ is a function from $\mathbf{x}$ to $\mathbb{R}^M$, $k_3(\cdot, \cdot)$ is a valid kernel in $\mathbb{R}^M$, $\mathbf{A}$ is a symmetric positive semidefinite matrix, $\mathbf{x}_a$ and $\mathbf{x}_b$ are variables (not necessarily disjoint) with $\mathbf{x} = (\mathbf{x}_a, \mathbf{x}_b)$, and k_a and k_b are valid kernel functions over their respective spaces.

Kernel Examples

- Linear kernel: $K(\mathbf{x}, \mathbf{y}) = \mathbf{x}^T \mathbf{y}$
- Quadratic kernel: $K(\mathbf{x}, \mathbf{y}) = (c + \mathbf{x}^T \mathbf{y})^2$
  - contains constant, linear terms and terms of order two (c > 0).
- Polynomial kernel: $K(\mathbf{x}, \mathbf{y}) = (c + \mathbf{x}^T \mathbf{y})^M$
  - contains all terms up to degree M (c > 0).
- Gaussian kernel: $K(\mathbf{x}, \mathbf{y}) = \exp(-\|\mathbf{x} - \mathbf{y}\|^2 / 2\sigma^2)$
  - corresponding feature space has infinite dimensionality.

Kernels over Discrete Structures

- Subsequence Kernels [Lodhi et al., JMLR 2002]:
  - Σ is a finite alphabet (set of symbols).
  - $\mathbf{x},\mathbf{y} \in \Sigma^*$ are two sequences of symbols with lengths $|\mathbf{x}|$ and $|\mathbf{y}|$
  - $k(\mathbf{x},\mathbf{y})$ is defined as the number of common substrings of length n.
  - $k(\mathbf{x},\mathbf{y})$ can be computed in $O(n|\mathbf{x}||\mathbf{y}|)$ time complexity.

- Tree Kernels [Collins and Duffy, NIPS 2001]:
  - T_1 and T_2 are two trees with N_1 and N_2 nodes respectively.
  - $k(T_1, T_2)$ is defined as the nummber of common subtrees.
  - $k(T_1, T_2)$ can be computed in $O(N_1 N_2)$ time complexity.
  - in practice, time is linear in the size of the trees.

Supplementary Reading

- PRML Chapter 6:
  - Section 6.1 on dual representations for linear regression models.
  - Section 6.2 on techniques for constructing new kernels.

The Perceptron Algorithm: K classes

1. **initialize** parameters $\mathbf{w} = 0$
2. **for** $i = 1 \ldots n$
3. $\quad y_i = \arg\max_{t \in T} \mathbf{w}^T \varphi(\mathbf{x}_i, t)$
4. $\quad$ **if** $y_i \neq t_i$ **then**
5. $\quad\quad \mathbf{w} = \mathbf{w} + \varphi(\mathbf{x}_i, t_i) - \varphi(\mathbf{x}_i, y_i)$

Repeat:
a) until convergence.
b) for a number of epochs E.

During testing:

$$t^* = \arg\max_{t \in T} \mathbf{w}^T \phi(\mathbf{x}, t)$$

Averaged Perceptron: K classes

1. **initialize** parameters $\mathbf{w} = 0$, $\tau = 1$, $\overline{\mathbf{w}} = 0$
2. **for** $i = 1 \ldots n$
3. $\quad y_i = \arg\max_{t \in T} \mathbf{w}^T \varphi(\mathbf{x}_i, t)$
4. $\quad$ **if** $y_i \neq t_i$ **then**
5. $\quad\quad \mathbf{w} = \mathbf{w} + \varphi(\mathbf{x}_i, t_i) - \varphi(\mathbf{x}_i, y_i)$
6. $\quad \overline{\mathbf{w}} = \overline{\mathbf{w}} + \mathbf{w}$
7. $\quad \tau = \tau + 1$
8. **return** $\overline{\mathbf{w}} / \tau$

Repeat:
a) until convergence.
b) for a number of epochs E.

During testing: $t^* = \arg\max_{t \in T} \overline{\mathbf{w}}^T \varphi(\mathbf{x}, t)$

The Perceptron Algorithm: K classes

1. **initialize** parameters $\mathbf{w} = 0$
2. **for** $i = 1 \ldots n$
3. $\quad c_j = \arg\max_{t \in T} \mathbf{w}^T \varphi(\mathbf{x}_i, t)$
4. $\quad$ **if** $c_j \neq t_i$ **then**
5. $\quad\quad \mathbf{w} = \mathbf{w} + \varphi(\mathbf{x}_i, t_i) - \varphi(\mathbf{x}_i, c_j)$

Repeat:
a) until convergence.
b) for a number of epochs E.

Loop invariant: $\mathbf{w}$ is a weighted sum of training vectors:

$$\mathbf{w} = \sum_{i,j} \alpha_{ij} (\phi(\mathbf{x}_i, t_i) - \phi(\mathbf{x}_i, c_j))$$

$$\Rightarrow \quad \mathbf{w}^T \phi(\mathbf{x}, t) = \sum_{i,j} \alpha_{ij} (\phi(\mathbf{x}_i, t_i)^T \phi(\mathbf{x}, t) - \phi(\mathbf{x}_i, c_j)^T \phi(\mathbf{x}, t))$$

Kernel Perceptron: K classes

1. **define** $f(\mathbf{x},t) = \sum_{i,j} \alpha_{ij} (\phi(\mathbf{x}_i, t_i)^T \phi(\mathbf{x},t) - \phi(\mathbf{x}_i, c_j)^T \phi(\mathbf{x},t))$
2. **initialize** dual parameters $\alpha_{ij} = 0$
3. **for** $i = 1 \ldots n$
4. $\quad c_j = \arg\max_{t \in T} f(\mathbf{x}_i, t)$
5. $\quad$ **if** $y_i \neq t_i$ **then**
6. $\quad\quad \alpha_{ij} = \alpha_{ij} + 1$

Repeat:
a) until convergence.
b) for a number of epochs E.

During testing:

$$t^* = \arg\max_{t \in T} f(\mathbf{x},t)$$

Kernel Perceptron: K classes

- Discriminant function:

$$f(\mathbf{x},t) = \sum_{i,j} \alpha_{i,j} (\phi(\mathbf{x}_i, t_i)^T \phi(\mathbf{x},t) - \phi(\mathbf{x}_i, c_j)^T \phi(\mathbf{x},t))$$

$$= \sum_{i,j} \alpha_{ij} (K(\mathbf{x}_i, t_i, \mathbf{x}, t) - K(\mathbf{x}_i, c_j, \mathbf{x}, t))$$

where:

$$K(\mathbf{x}_i, t_i, \mathbf{x}, t) = \varphi^T(\mathbf{x}_i, t_i)\varphi(\mathbf{x}, t)$$

$$K(\mathbf{x}_i, y_i, \mathbf{x}, t) = \phi^T(\mathbf{x}_i, y_i)\phi(\mathbf{x}, t)$$

Machine Learning: Support Vector Machines

Lecture 07

Razvan C. Bunescu

School of Electrical Engineering and Computer Science

bunescu@ohio.edu

Max-Margin Classifiers: Separable Case

- Linear model for binary classification:

$$y(\mathbf{x}) = \mathbf{w}^T \varphi(\mathbf{x}) + b$$

- Training examples:

$$(\mathbf{x}_1, t_1),\ (\mathbf{x}_2, t_2),\ \ldots\ (\mathbf{x}_N, t_N),\ \text{where } t_n \in \{+1, -1\}$$

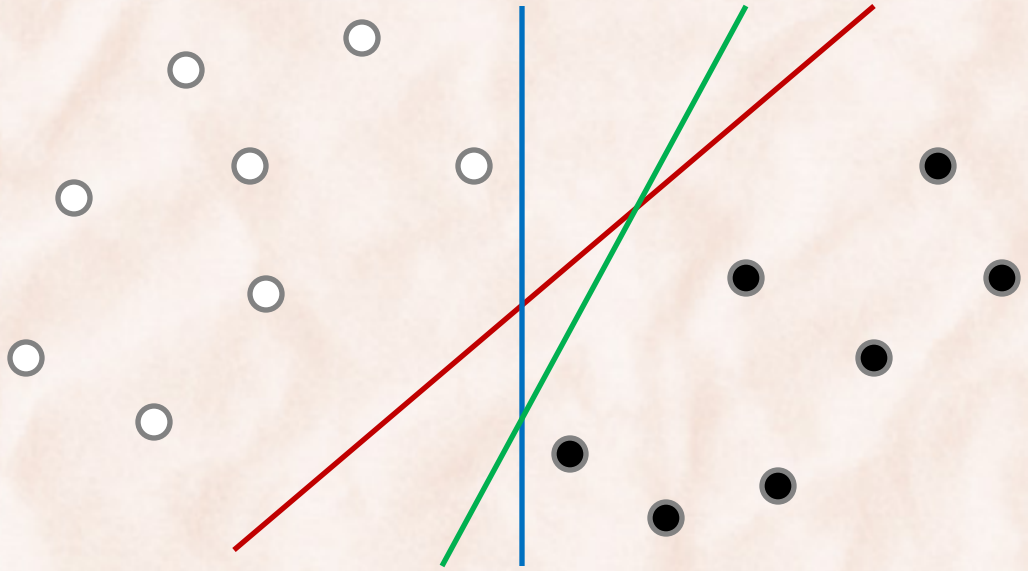
- Assume training data is linearly separable:

$$t_n y(x_n) > 0\,,\ \text{for all}\ 1 \le n \le N$$

$\Rightarrow$ perceptron solution depends on:

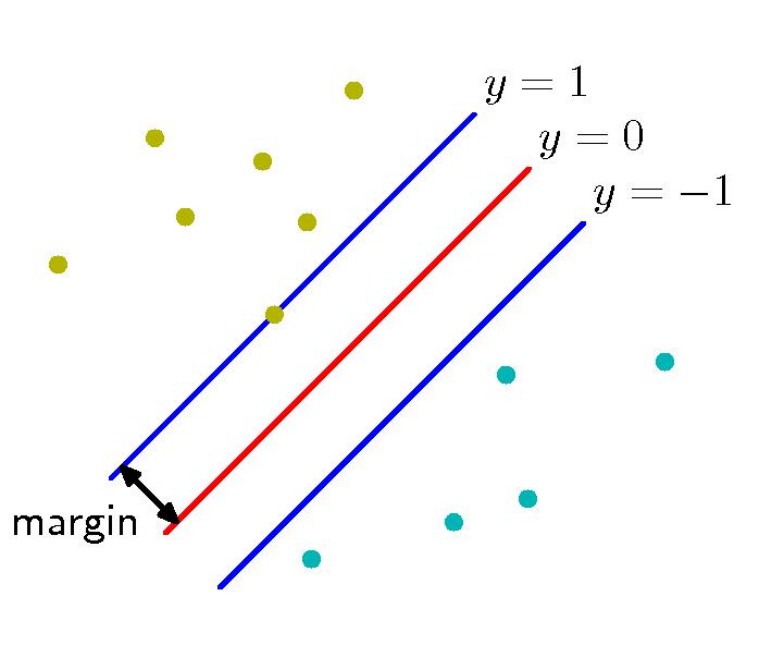
- initial values of **w** and b.
- order of processing of data points.

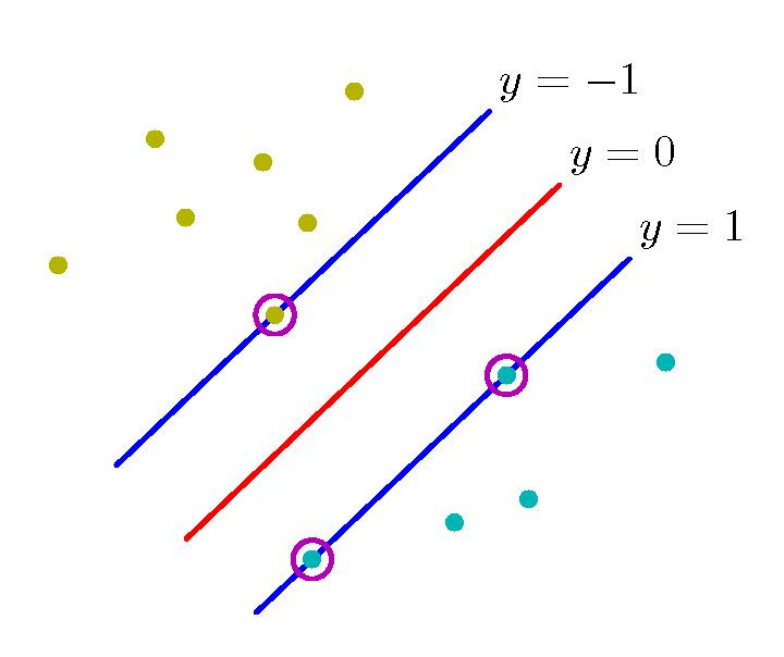
Maximum Margin Classifiers



- Which hyperplane has the smallest generalization error?
  - The one that maximizes the margin [Computational Learning Theory]
    - margin = the distance between the decision boundary and the closest sample.

Maximum Margin Classifiers





- The distance between a point $\mathbf{x}_n$ and a hyperplane $y(\mathbf{x})=0$ is:

$$\frac{|y(\mathbf{x}_n)|}{\|\mathbf{w}\|} = \frac{t_n y(\mathbf{x}_n)}{\|\mathbf{w}\|} = \frac{t_n(\mathbf{w}^T\varphi(\mathbf{x}_n)+b)}{\|\mathbf{w}\|}$$

Maximum Margin Classifiers

- Margin = the distance between hyperplane $y(\mathbf{x})=0$ and closest sample:

$$\min_n \left[\frac{t_n(\mathbf{w}^T\varphi(\mathbf{x}_n)+b)}{\|\mathbf{w}\|} \right]$$

- Find parameters $\mathbf{w}$ and b that maximize the margin:

$$\arg\max_{\mathbf{w},b} \left\{ \frac{1}{\|\mathbf{w}\|} \min_n \left[t_n(\mathbf{w}^T\varphi(\mathbf{x}_n)+b) \right] \right\}$$

- Rescaling $\mathbf{w}$ and b does not change distances to the hyperplane:

$\Rightarrow$ for the closest point(s), set $t_n(\mathbf{w}^T\varphi(\mathbf{x}_n)+b)=1$

$$\Rightarrow t_n(\mathbf{w}^T\varphi(\mathbf{x}_n)+b) \geq 1, \quad \forall n \in \{1,\ldots,N\}$$

Max-Margin: Quadratic Optimization

- Constrained optimization problem:

minimize:

$$J(\mathbf{w}, b) = \frac{1}{2}\|\mathbf{w}\|^2$$

subject to:

$$t_n(\mathbf{w}^T\varphi(\mathbf{x}_n) + b) \geq 1, \quad \forall n \in \{1, \ldots, N\}$$

- Solved using the technique of Lagrange Multipliers.

Convex Optimization

- Convex optimization problem in standard form (primal):

minimize:

$$f_0(\mathbf{x})$$

subject to:

$$f_i(\mathbf{x}) \le 0, \quad i = 1, \ldots, m$$

$$h_i(\mathbf{x}) = 0, \quad i = 1, \ldots, p$$

solution **x***

  - $f_i : \mathrm{R}^n \to \mathrm{R}$ are all **convex functions**, for $i = 0, \ldots, m$
  - $h_i : \mathrm{R}^n \to \mathrm{R}$ are all **afine functions** , for $i = 0, \ldots, p$ (e.g. $h_i(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{b}$)

Lagrange Multipliers

- Define Lagrangian function $L_P : \mathrm{R}^n \times \mathrm{R}^m \times \mathrm{R}^p \to \mathrm{R}$:

$$L_P(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\upsilon}) = f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) + \sum_{i=1}^{p} \upsilon_i h_i(x)$$

- $\lambda_i \geq 0$, and v_i are the *Lagrange multipliers*.

- Define Lagrange dual function $L_D : \mathrm{R}^m \times \mathrm{R}^p \to \mathrm{R}$:

$$L_D(\boldsymbol{\lambda}, \boldsymbol{\upsilon}) = \inf_{\mathbf{x}} L_P(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\upsilon})$$

Convex Optimization

- Lagrange Dual Problem:

maximize:

$$L_D(\boldsymbol{\lambda}, \boldsymbol{\upsilon})$$

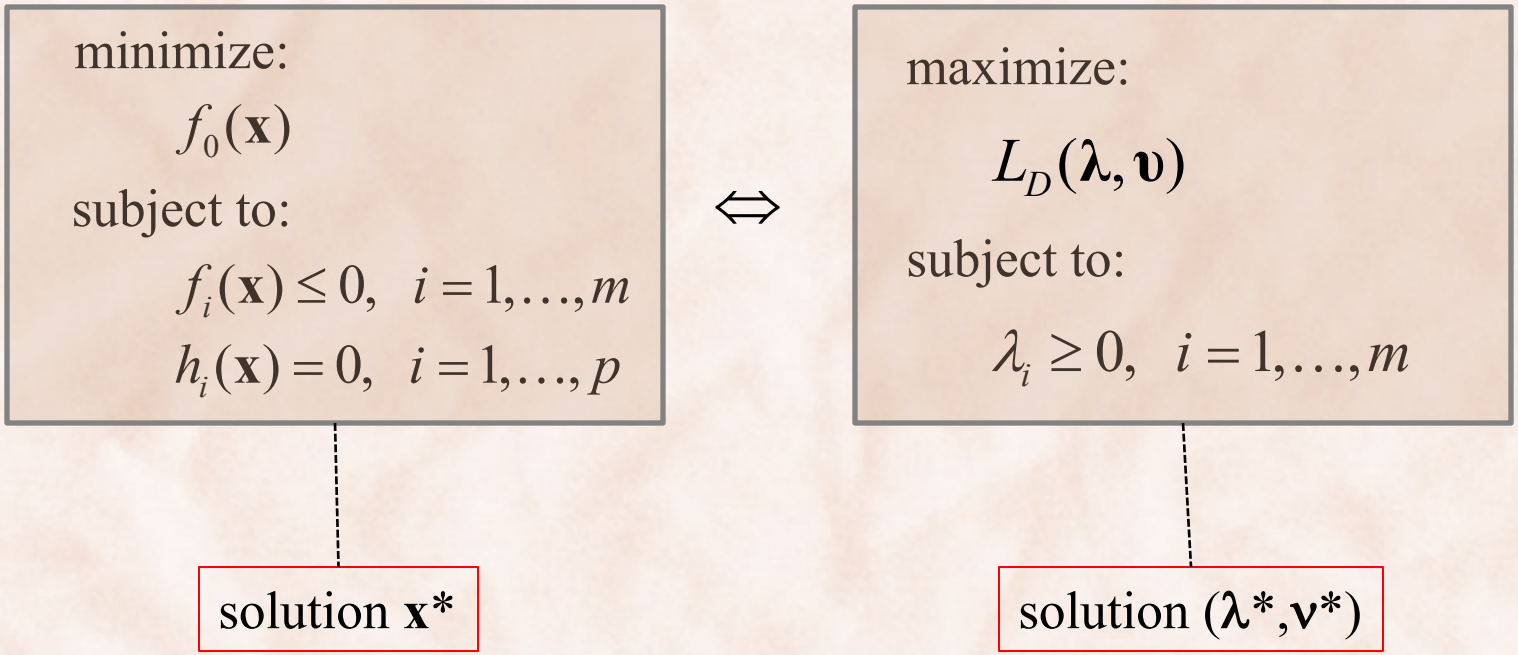
subject to:

$$\lambda_i \geq 0, \quad i = 1, \ldots, m$$

solution $(\boldsymbol{\lambda}^*, \boldsymbol{\nu}^*)$

$$L_D(\boldsymbol{\lambda}, \boldsymbol{\upsilon}) = \inf_{\mathbf{x}} L_P(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\upsilon})$$

Strong Duality



- Optimum for primal problem = optimum for dual problem:

$$f_0(\mathbf{x}^*) = L_D(\boldsymbol{\lambda}^*, \boldsymbol{\upsilon}^*)$$

Karush–Kuhn–Tucker (KKT) conditions

Assume ($\mathbf{x}$, $\boldsymbol{\lambda}$, $\boldsymbol{\nu}$) are the primal & dual solutions. Then ($\mathbf{x}$, $\boldsymbol{\lambda}$, $\boldsymbol{\nu}$) satisfy the following constraints:

1. primal constraints: $\begin{cases} f_i(\mathbf{x}) \le 0, \ i = 1,\ldots,m \\ h_i(\mathbf{x}) = 0, \ i = 1,\ldots,p \end{cases}$
2. dual constraints: $\lambda_i \ge 0, \quad i = 1,\ldots,m$
3. complementary slackness: $\lambda_i f_i(\mathbf{x}) = 0, \quad i = 1,\ldots,m$
4. gradient of Lagrangian with respect to $\mathbf{x}$ vanishes:

$$\nabla L_P(\mathbf{x}) = \nabla f_0(x) + \sum_{i=1}^{m} \lambda_i \nabla f_i(x) + \sum_{i=1}^{p} \upsilon_i \nabla h_i(x) = 0$$

Max-Margin: Quadratic Optimization

- Constrained optimization problem:

minimize:

$$J(\mathbf{w}, b) = \frac{1}{2}\|\mathbf{w}\|^2$$

subject to:

$$t_n(\mathbf{w}^T\varphi(\mathbf{x}_n) + b) \geq 1, \quad \forall n \in \{1, \ldots, N\}$$

- Let's solve it using the technique of Lagrange Multipliers.

Max-Margin: Quadratic Optimization

- Lagrangian function:

$$L_P(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} \alpha_n \left\{ t_n(\mathbf{w}^T \varphi(x_n) + b) - 1 \right\}$$

  - $\alpha_n \geq 0$ are the *Lagrangian multipliers*.

- Lagrangian dual function:

$$L_D(\boldsymbol{\alpha}) = \inf_{\mathbf{w},b} L_P(\mathbf{w}, b, \boldsymbol{\alpha})$$

- Solve:

$$\left.\begin{aligned} \frac{\partial L_P}{\partial \mathbf{w}} &= 0 \\ \frac{\partial L_P}{\partial b} &= 0 \end{aligned}\right\} \Rightarrow \begin{cases} \mathbf{w} = \sum_{n=1}^{N} \alpha_n t_n \varphi(x_n) \\ \sum_{n=1}^{N} \alpha_n t_n = 0 \end{cases}$$

Max-Margin: Quadratic Optimization

- Dual representation:

maximize:

$$L_D(\boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m)$$

subject to:

$$\alpha_n \geq 0, \quad n = 1, \ldots, N$$

$$\sum_{n=1}^{N} \alpha_n t_n = 0$$

- $k(\mathbf{x}_n, \mathbf{x}_m) = \varphi(\mathbf{x}_n)^T \varphi(\mathbf{x}_n)$ is the *kernel* function.

KKT conditions

1. primal constraints: $t_n y(x_n) - 1 \geq 0$
1. dual constraints: $\alpha_n \geq 0$
2. complementary slackness: $\alpha_n \left\{ t_n y(x_n) - 1 \right\} = 0$

$\Rightarrow$ for any data point, either $\alpha_n = 0$ or $t_n y(x_n) = 1$

S = $\{n \mid t_n y(x_n) = 1\}$ is the set of *support vectors*

Max-Margin Solution

- After solving the dual problem $\Rightarrow$ know α_n, for $n = 1 \ldots N$

$$\mathbf{w} = \sum_{n=1}^{N} \alpha_n t_n \varphi(x_n) = \sum_{m \in S} \alpha_m t_m \varphi(x_m)$$

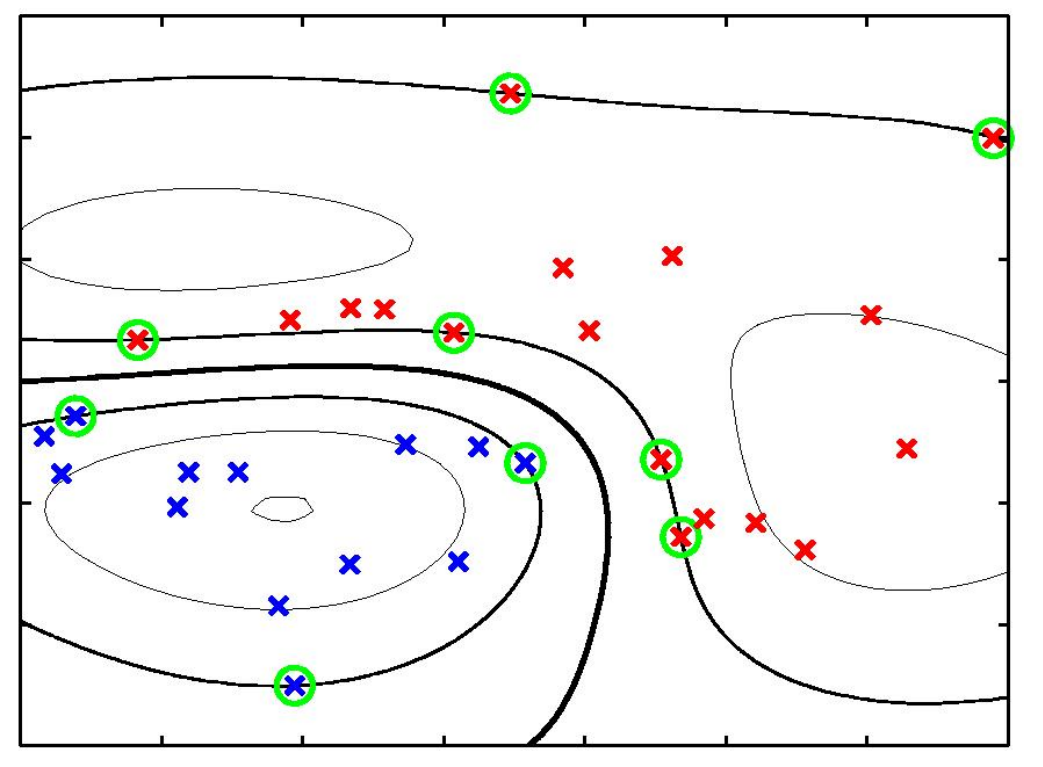
$$b = \frac{1}{|S|} \sum_{n \in S} \left(t_n - \sum_{m \in S} \alpha_m t_m k(\mathbf{x}_n, \mathbf{x}_m) \right)$$

- Linear discriminant function becomes:

$$y(x) = \sum_{m \in S} \alpha_m t_m k(x, x_m) + b$$

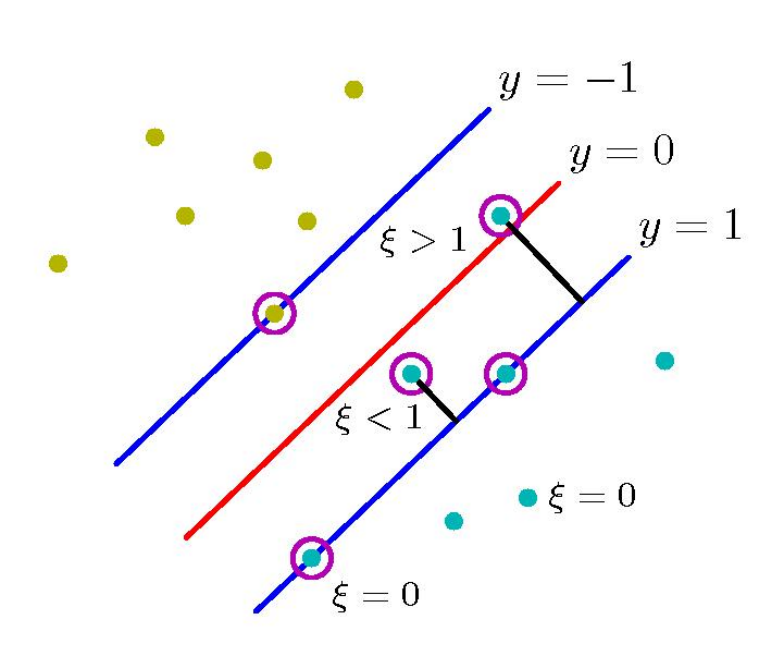
$\Rightarrow$ In both training and testing, examples are used only through the *kernel function*!

An SVM with Gaussian kernel



Max-Margin Classifiers: Non-Separable Case

- Allow data points to be on the wrong side of the margin boundary.
  - Penalty that increases with the distance from the boundary.



Max-Margin: Quadratic Optimization

- Optimization problem:

minimize:

$$J(\mathbf{w}, b) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n$$

subject to:

$$t_n(\mathbf{w}^T\varphi(\mathbf{x}_n) + b) \geq 1 - \xi_n, \quad \forall n \in \{1, \ldots, N\}$$
$$\xi_n \geq 0$$

- Solve it using the technique of Lagrange Multipliers.

Max-Margin: Quadratic Optimization

- Dual representation:

maximize:

$$L_D(\boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m)$$

subject to:

$$0 \le \alpha_n \le C, \quad n = 1, \ldots, N$$

$$\sum_{n=1}^{N} \alpha_n t_n = 0$$

- $k(\mathbf{x}_n, \mathbf{x}_m) = \varphi(\mathbf{x}_n)^T \varphi(\mathbf{x}_n)$ is the *kernel* function.

(Some of the) KKT conditions

1. primal constraints: $t_n y(x_n) - 1 + \xi_n \geq 0$

1. dual constraints: $0 \leq \alpha_n \leq C$

2. complementary slackness: $\alpha_n \left\{ t_n y(x_n) - 1 + \xi_n \right\} = 0$

$\Rightarrow$ for any data point, either $\alpha_n = 0$ or $t_n y(x_n) = 1 - \xi_n$

$S = \{n \mid t_n y(x_n) = 1 - \xi_n\}$ is the set of *support vectors*

$M = \{n \mid 0 < \alpha_n < \mathrm{C}\}$ is the set of SVs that lie on the margin.

Max-Margin Solution

- After solving the dual problem $\Rightarrow$ know α_n, for $n = 1 \ldots N$

$$\mathbf{w} = \sum_{n=1}^{N} \alpha_n t_n \varphi(x_n) = \sum_{m \in S} \alpha_m t_m \varphi(x_m)$$

$$b = \frac{1}{|M|} \sum_{n \in M} \left(t_n - \sum_{m \in S} \alpha_m t_m k(\mathbf{x}_n, \mathbf{x}_m) \right)$$

- Linear discriminant function becomes:

$$y(x) = \sum_{m \in S} \alpha_m t_m k(x, x_m) + b$$

$\Rightarrow$ In both training and testing, examples are used only through the *kernel function*!

Support Vector Machines

- Optimization problem:

minimize:

$$J(\mathbf{w},b)=\frac{1}{2}\|\mathbf{w}\|^2+C\sum_{n=1}^{N}\xi_n$$

subject to:

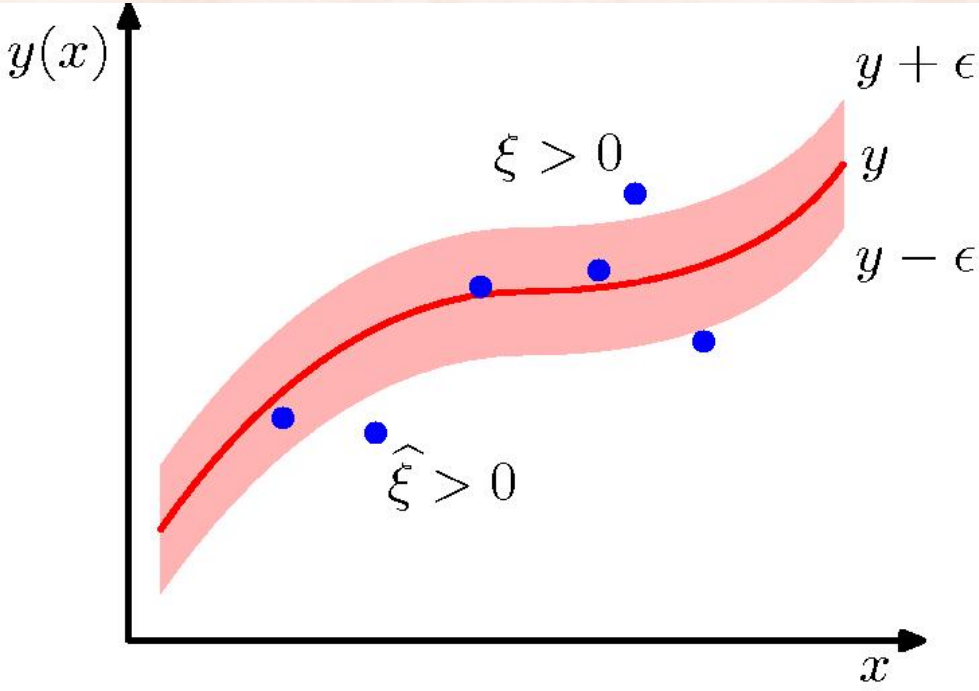
$$t_n(\mathbf{w}^T\varphi(\mathbf{x}_n)+b)\geq 1-\xi_n, \quad \forall n\in\{1,\ldots,N\}$$

$$\xi_n\geq 0$$

upper bound on the missclassification error on the training data.

SVMs for Regression

- Use an ε-insensitive error function ($\varepsilon > 0$) to obtain *sparse solutions*.
  - Penalty that increases with the distance from the ε-insensitive "tube".



SVMs for Regression: Quadratic Optimization

- Optimization problem:

minimize:

$$J(\mathbf{w},b)=\frac{1}{2}\|\mathbf{w}\|^2+C\sum_{n=1}^{N}(\xi_n+\hat{\xi}_n)$$

subject to:

$$t_n \le \mathbf{w}^T\varphi(\mathbf{x}_n)+b+\varepsilon+\xi_n$$

$$t_n \ge \mathbf{w}^T\varphi(\mathbf{x}_n)+b-\varepsilon-\hat{\xi}_n$$

$$\xi_n,\hat{\xi}_n \ge 0, \quad \forall n\in\{1,\ldots,N\}$$

- Solve it using the technique of Lagrange Multipliers.

SVMs for Regression: Sparse Solution

- After solving the dual problem $\Rightarrow$ know $\alpha_n, \hat{\alpha}_n$ for $n = 1 \ldots N$

$$\mathbf{w} = \sum_{n=1}^{N} (\alpha_n - \hat{\alpha}_n)\varphi(x_n) = \sum_{m \in S} (\alpha_m - \hat{\alpha}_m)\varphi(x_m)$$

- S is the set of *support vectors*:

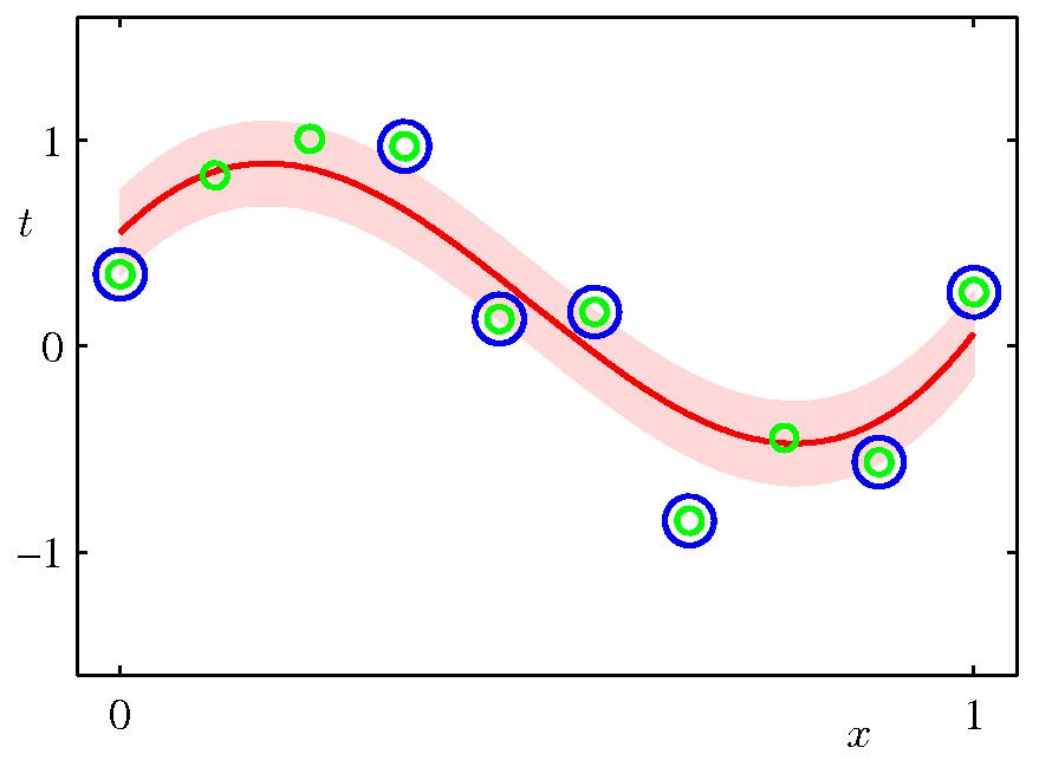
  i.e. points for which either $\alpha_n \neq 0$ or $\hat{\alpha}_n \neq 0$

  $\Rightarrow$ points that lie on the boundary of the ε-insensitive tube or outside the tube

$$y(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b = \sum_{m \in S} (\alpha_m - \hat{\alpha}_m) k(x, x_m) + b$$

$\Rightarrow$ In both training and testing, examples are used only through the *kernel function*!

SVMs for Regression: Sparse Solution



SVMs for Ranking [Joachims, KDD'02]

- Problem:
  - For a query q, a search engine returns a set of documents D.
  - Want to rank d_i higher than d_j if d_i is more relevant to q than d_j.

- Solution:
  - Learn a ranking function $f(q,d) = \mathbf{w}^T \varphi(q,d)$
  - Rank d_i higher than d_j if $f(q,d_i) \geq f(q,d_j) \Leftrightarrow \mathbf{w}^T \varphi(q,d_i) \geq \mathbf{w}^T \varphi(q,d_j)$
  - Training data:
    - Set $\{(q_k, d_i, d_j) \mid d_i$ ranked higher than d_j for query $q_k\}$.
    - Relative rankings obtained from clicktrough data.

SVMs for Ranking [Joachims, KDD'02]

- Optimization problem:

minimize:

$$J(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum \xi_{k,i,j}$$

subject to:

$$\mathbf{w}^T\varphi(q_k,d_i) \geq \mathbf{w}^T\varphi(q_k,d_i) + 1 - \xi_{k,i,j}$$

$$\xi_{k,i,j} \geq 0$$

$$\mathbf{w}^T\left(\varphi(q_k,d_i) - \varphi(q_k,d_i)\right) \geq 1 - \xi_{k,i,j}$$

$\Rightarrow$ equivalent with a classification problem

SVMs for Ranking [Joachims, KDD'02]

- After solving the quadratic problem:

$$\mathbf{w} = \sum_{k,l} \alpha_{k,l} \varphi(q_k, d_l)$$

$$\Rightarrow f(q,d) = \mathbf{w}^T \varphi(q,d)$$

$$= \sum_{k,l} \alpha_{k,l} \varphi^T(q_k, d_l) \varphi(q,d)$$

$$= \sum_{k,l} \alpha_{k,l} K(q_k, d_l, q, d)$$

$\Rightarrow$ In both training and testing, examples are used only through the *kernel function*!

Learning Scenarios for SVMs

- **Classification.**
- **Ranking.**
- **Regression.**
- Ordinal Regression.
- One Class Learning.
- Learning with Positive and Unlabeled examples.
- Transductive Learning.
- Semi-Supervised Learning.
- Multiple Instance Learning.

Practical Issues

- **Data Scaling**:
  - Between [-1,+1] or [0, 1].
  - Use same scaling factors in training and testing!
- **Parameter Tuning**:
  - Most SVM packages specify reasonable default values.
    - Tuning helps, especially with kernels that tend to overfit.
  - Grid search is simple and effective:
    - For RBF kernels, need to tune C and γ:
      - $C \in \{2^{-5}, 2^{-3}, ..., 2^{15}\}$, $\gamma \in \{2^{-15}, 2^{-13}, ..., 2^{3}\}$
- Read LibSVM's "A practical guide to SVM classification".

Conclusion

- SVMs were originally proposed by Boser, Guyon, and Vapnik in 1992.
- SVMs are currently among the best performers on a number of classification tasks ranging from text to genomic data.
- SVMs can be applied to complex data types, e.g. *graphs, trees, sequences*, by designing kernel functions for such data.
  - Also to probability distributions – "Learning from Distributions via Support Measure Machines" [Muandet et al., NIPS 2012]
- Kernel trick has been extended to other methods such as Perceptron, PCA, kNN, etc.
- Popular optimization algorithms for SVMs use decomposition to hill-climb over a subset of α_n's at a time, e.g. SMO [Platt '99].
  - But training and testing with linear SVMs are much faster.
- Read Lin's "Machine Learning Software: Design and Practical Use"

Machine Learning: k-Nearest Neighbors

Lecture 08

Razvan C. Bunescu

School of Electrical Engineering and Computer Science

bunescu@ohio.edu

Nonparametric Methods: k-Nearest Neighbors

Input:

- A training dataset $(\mathbf{x}_1, t_1), (\mathbf{x}_2, t_2), \ldots (\mathbf{x}_n, t_n)$.
- A test instance $\mathbf{x}$.

Output:

- Estimated class label $y(\mathbf{x})$.

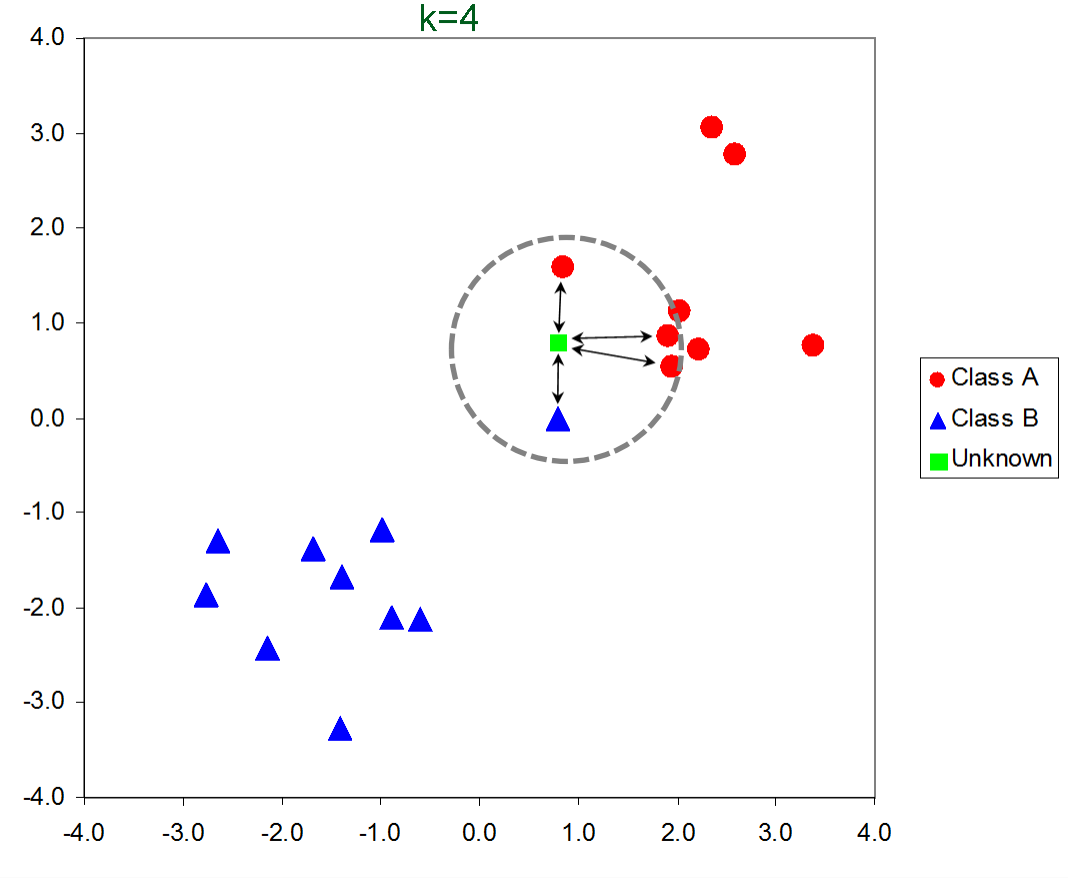
---

1. Find k instances $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k$ *nearest* to $\mathbf{x}$.
2. Let $y(x) = \arg\max_{t \in T} \sum_{i=1}^{k} \delta_t(t_i)$

where $\delta_t(x) = \begin{cases} 1 & x = t \\ 0 & x \neq t \end{cases}$ is the *Kronecker delta* function.

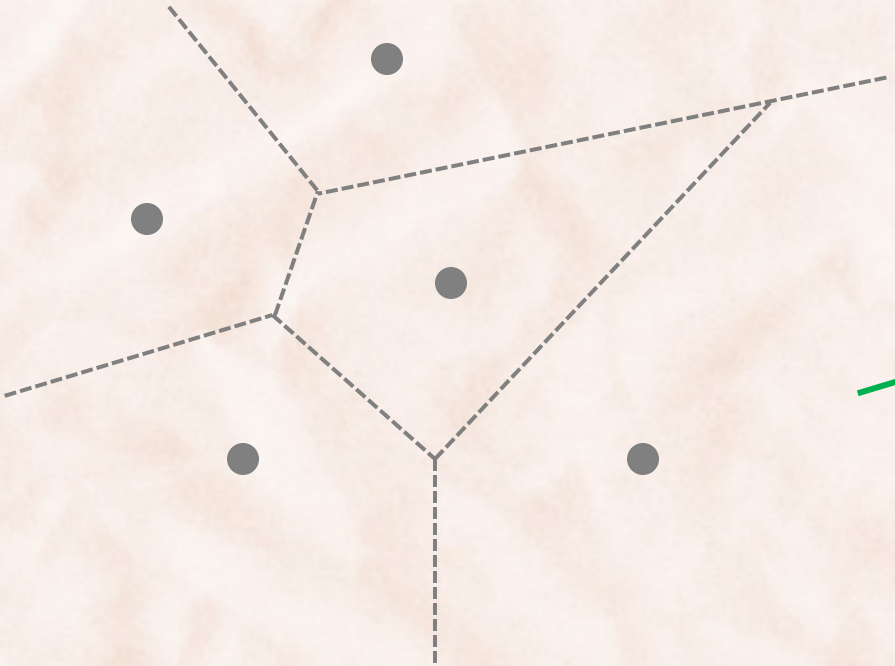
k-Nearest Neighbors (k-NN)

- Euclidean distance, $k = 4$

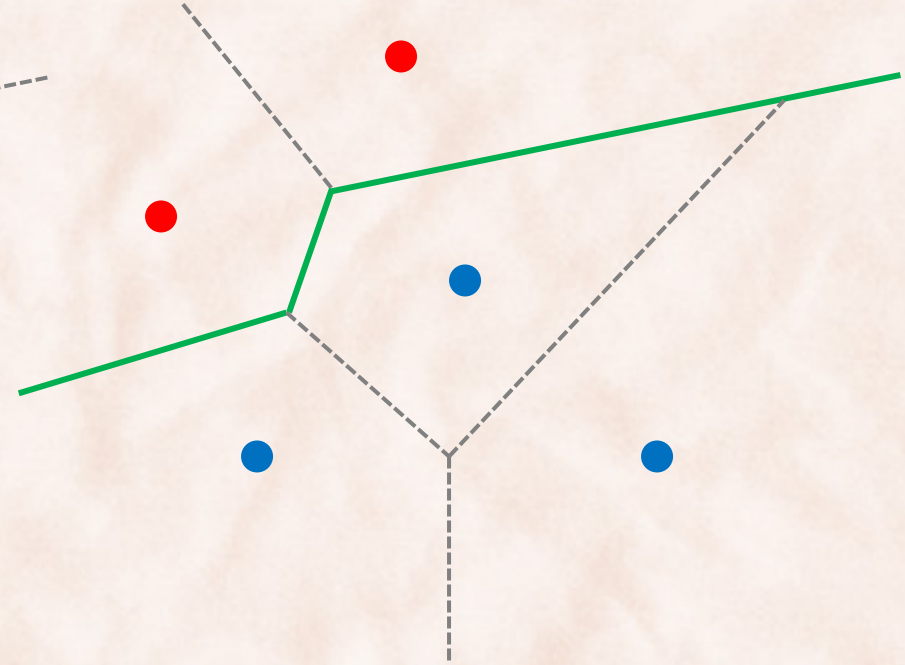


k-Nearest Neighbors (k-NN)

- Euclidian distance, k = 1.



Voronoi diagram



decision boundary

k-NN for Classification: Probabilistic Justification

- Assume a dataset with N_j points in class C_j.

  $\Rightarrow$ total number of points is $N = \sum_j N_j$

- Draw a sphere centered at $\mathbf{x}$ containing K points:
  - sphere has volume V.
  - sphere contains K_j points from class C_j.
- If V sufficiently small and K sufficiently large, we can estimate [2.5.1]:

$$p(\mathbf{x} \mid C_j) = \frac{K_j}{N_j V} \qquad p(\mathbf{x}) = \frac{K}{NV} \qquad p(C_j) = \frac{N_j}{N}$$

- Bayes' theorem $\Rightarrow p(C_j \mid \mathbf{x}) = \frac{K_j}{K}$ $\Rightarrow$ choose class C_j with most neighbors.

Distance Metrics

- Euclidean distance:

$$d(\mathbf{x},\mathbf{y}) = \|\mathbf{x}-\mathbf{y}\|_2 = \sqrt{(\mathbf{x}-\mathbf{y})^T(\mathbf{x}-\mathbf{y})}$$

- Hamming distance:

  # of (discrete) features that have different values in **x** and **y**.

- Mahalanobis distance:

(sample) covariance matrix

$$d(\mathbf{x},\mathbf{y}) = \sqrt{(\mathbf{x}-\mathbf{y})^T S^{-1}(\mathbf{x}-\mathbf{y})}$$

  - scale-invariant metric that normalizes for variance.
  - if $S = I \Rightarrow$ Euclidean distance.
  - if $S = diag(\sigma_1^{-2}, \sigma_2^{-2}, \ldots \sigma_K^{-2}) \Rightarrow$ *normalized* Euclidean distance.

Distance Metrics

- Cosine similarity:

$$d(\mathbf{x},\mathbf{y}) = 1 - \cos(\mathbf{x},\mathbf{y}) = 1 - \frac{\mathbf{x}^T\mathbf{y}}{\|\mathbf{x}\|\|\mathbf{y}\|}$$

  - used for text and other high-dimensional data.

- Levenshtein distance (Edit distance):
  - distance metric on strings (sequences of symbols).
  - min. # of basic edit operations that can transform one string into the other (delete, insert, substitute).

$$\left.\begin{array}{l}\mathbf{x} = \text{“athens”} \\ \mathbf{y} = \text{“hints”}\end{array}\right\} \Rightarrow d(\mathbf{x},\mathbf{y}) = 4$$

  - used in bioinformatics.

Efficient Indexing

- Linear searching for *k*-nearest neighbors is not efficient for large training sets:
  - O(N) time complexity.
- For Euclidean distance use a **kd-tree**:
  - instances stored at leaves of the tree.
  - internal nodes branch on threshold test on individual features.
  - expected time to find the nearest neighbor is O(log N)
- Indexing structures depend on distance function:
  - **inverted index** for text retrieval with cosine similarity.

k-NN and The Curse of Dimensionality

- Standard metrics weigh each feature equally:
  - Problematic when many features are irrelevant.

- One solution is to weigh each feature differently:
  - Use measure indicating ability to discriminate between classes, such as:
    - Information Gain, Chi-square Statistic
    - Pearson Correlation, Signal to Noise Ration, T test.
  - "Stretch" the axes:
    - lengthen for relevant features, shorten for irrelevant features.
  - Equivalent with Mahalanobis distance with diagonal covariance.

Distance-Weighted k-NN

For any test point **x**, weight each of the *k* neighbors according to their distance from **x**.

1. Find *k* instances $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k$ nearest to **x**.

2. Let $y(x) = \arg\max_{t \in T} \sum_{i=1}^{k} w_i \delta_t(t_i)$

   where $w_i = \|\mathbf{x} - \mathbf{x}_i\|^{-2}$ measures the similarity between **x** and $\mathbf{x}_i$

Kernel-based Distance-Weighted NN

For any test point **x**, weight all training instances according to their similarity with **x**.

---

1. Assume binary classification, T = {+1, –1}.

2. Compute weighted majority:

$$y(\mathbf{x}) = sign\left(\sum_{i=1}^{N} K(\mathbf{x}, \mathbf{x}_i) t_i\right)$$

Regression with k-Nearest Neighbor

Input:

- A training dataset $(\mathbf{x}_1, t_1), (\mathbf{x}_2, t_2), \ldots (\mathbf{x}_n, t_n)$.
- A test instance $\mathbf{x}$.

Output:

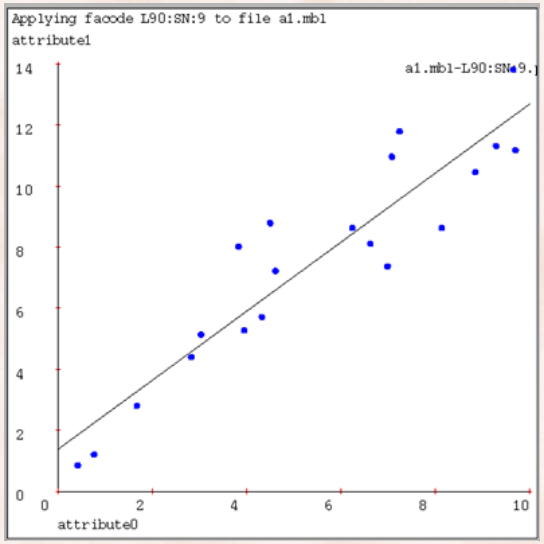
- Estimated function value $y(\mathbf{x})$.

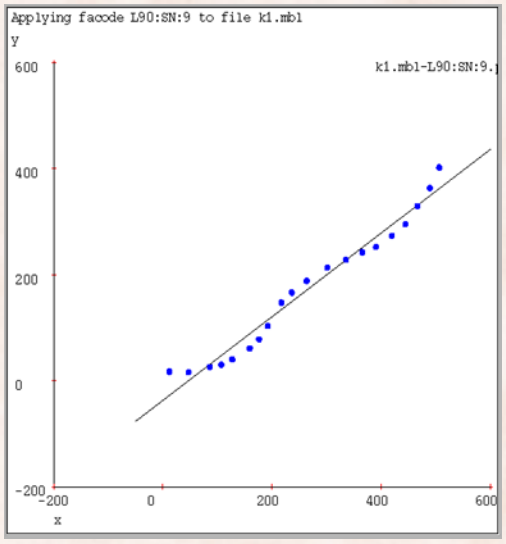
---

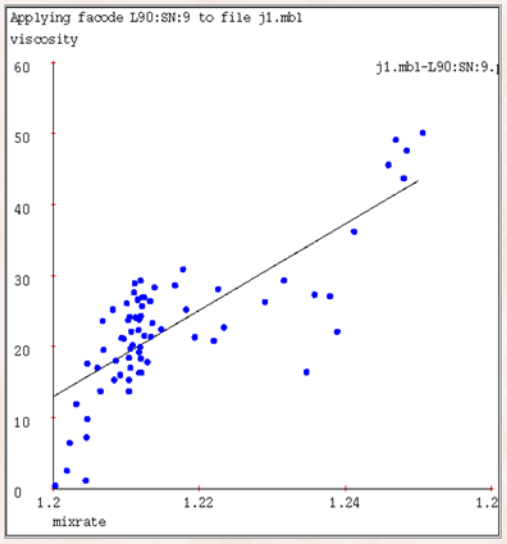
1. Find k instances $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k$ nearest to $\mathbf{x}$.
2. Let $y(x) = \frac{1}{k} \sum_{i=1}^{k} t_i$

3 Datasets & Linear Interpolation

[http://www.autonlab.org/tutorials/mbl08.pdf]

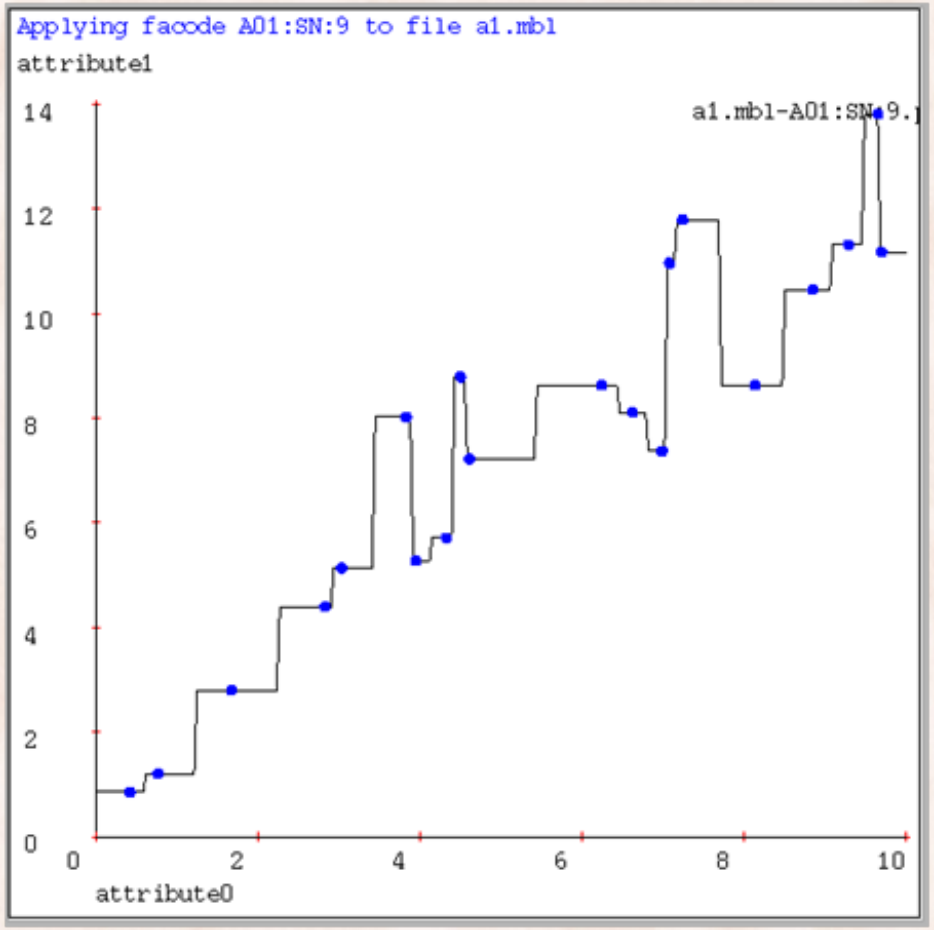




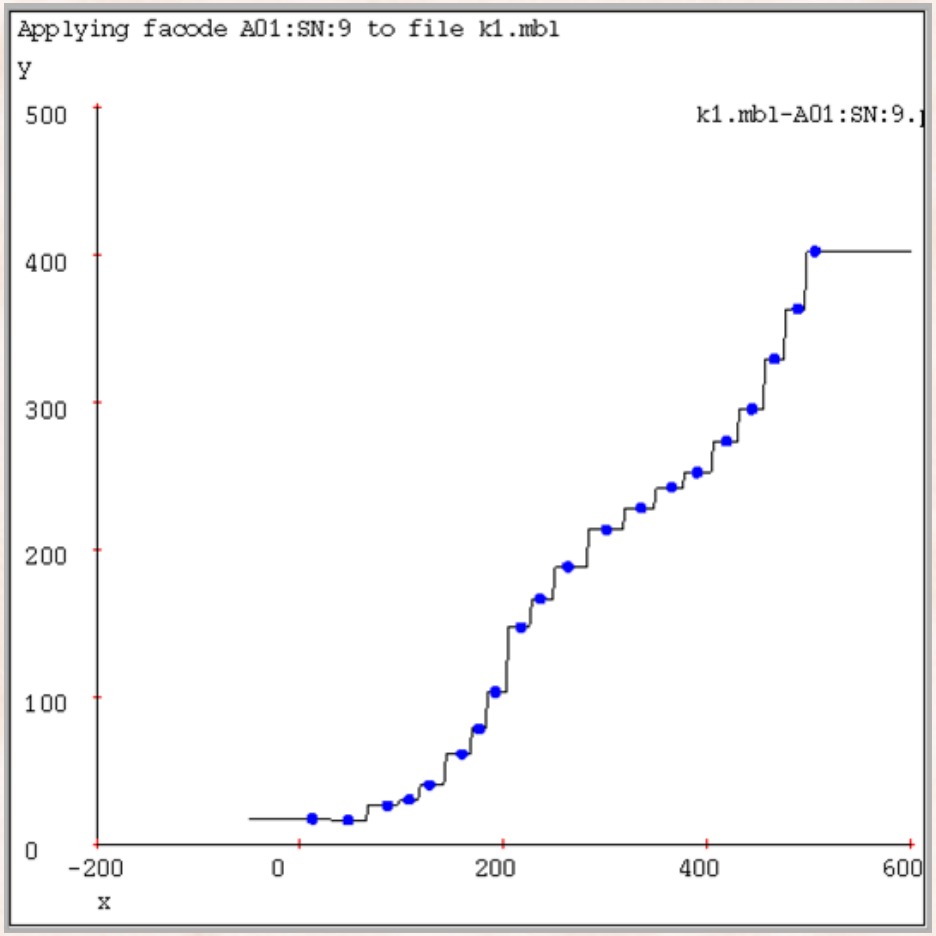


Linear interpolation does not always lead to good models of the data.

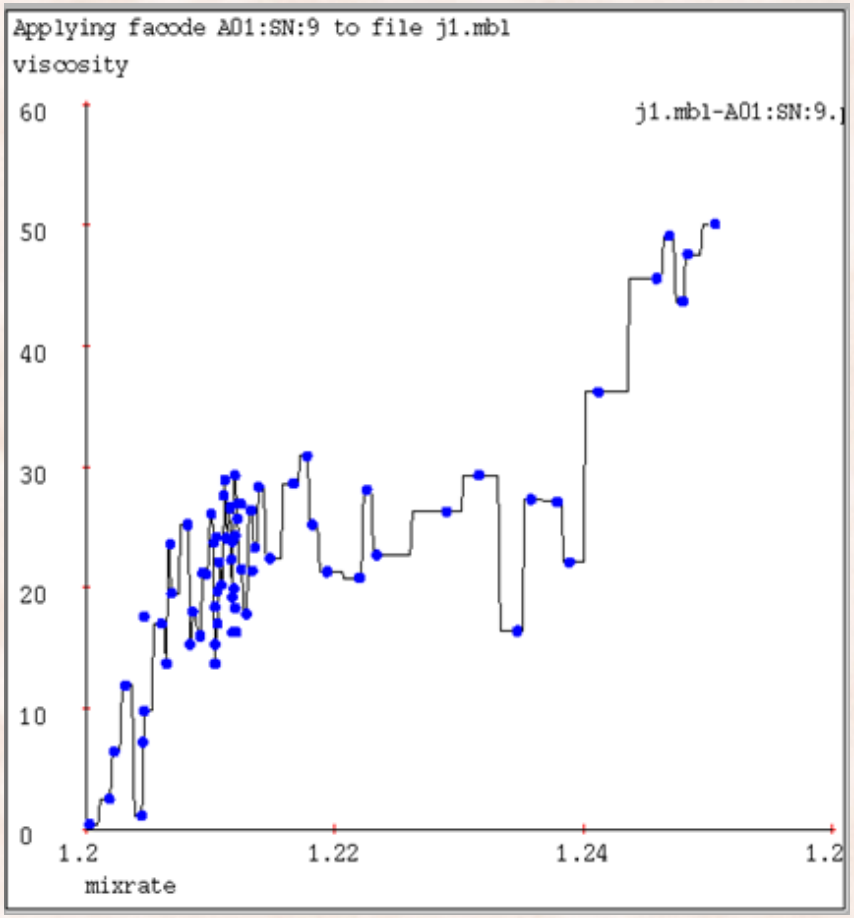
Regression with 1-Nearest Neighbor



Regression with 1-Nearest Neighbor



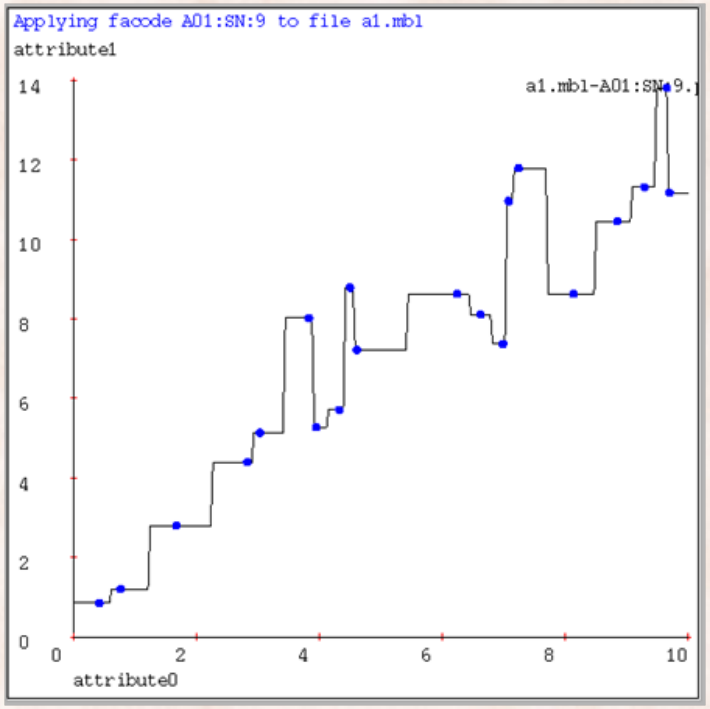
Regression with 1-Nearest Neighbor



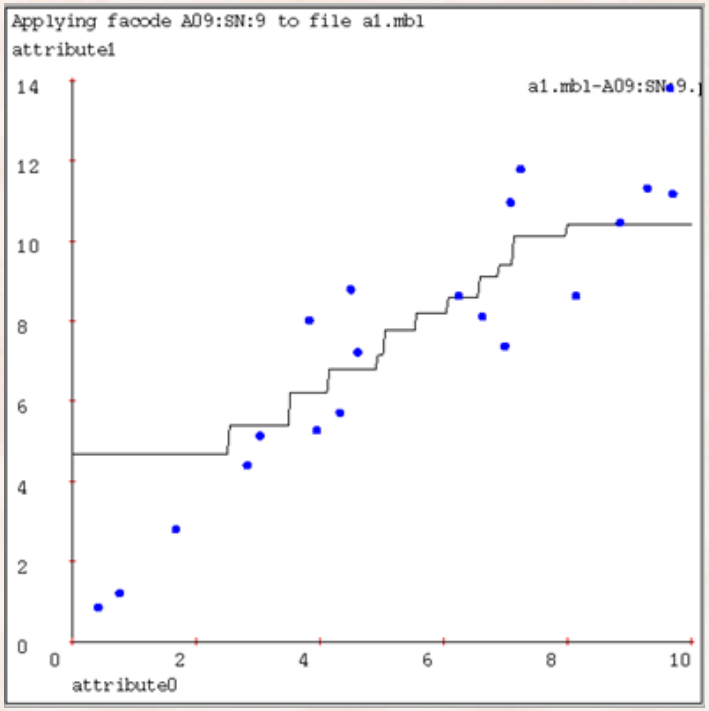
$\Rightarrow$ *1-NN has high variance*

Regression with 9-Nearest Neighbor

$k = 1$

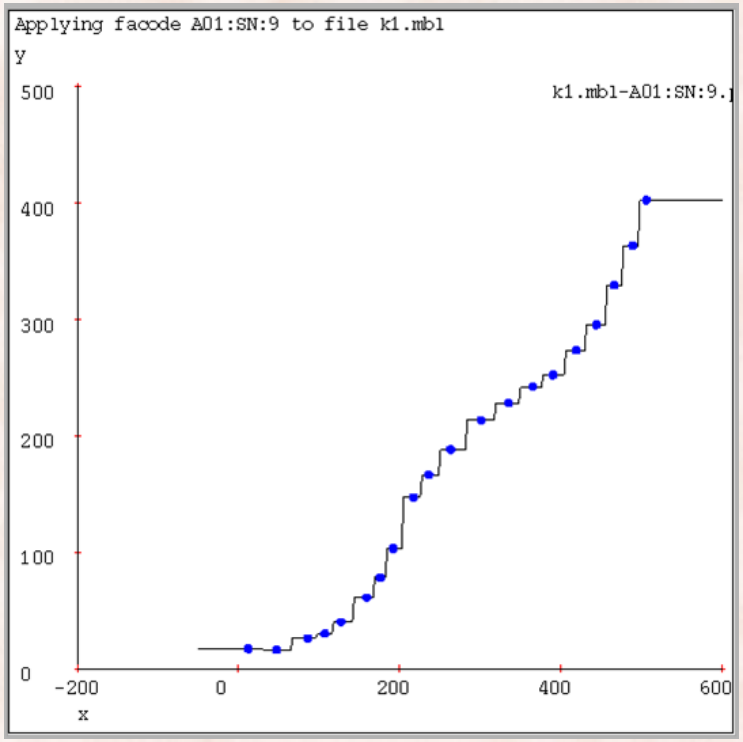


$k = 9$

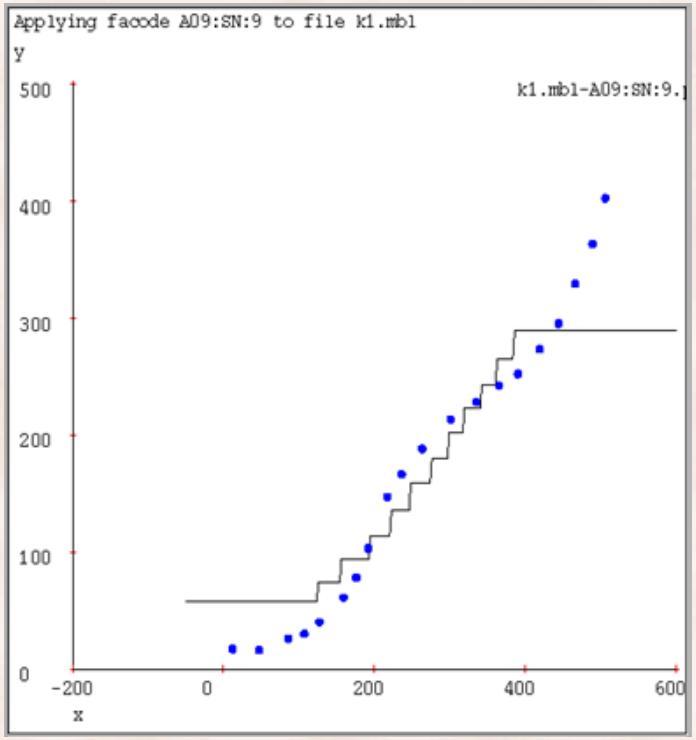


Regression with 9-Nearest Neighbor

$k = 1$

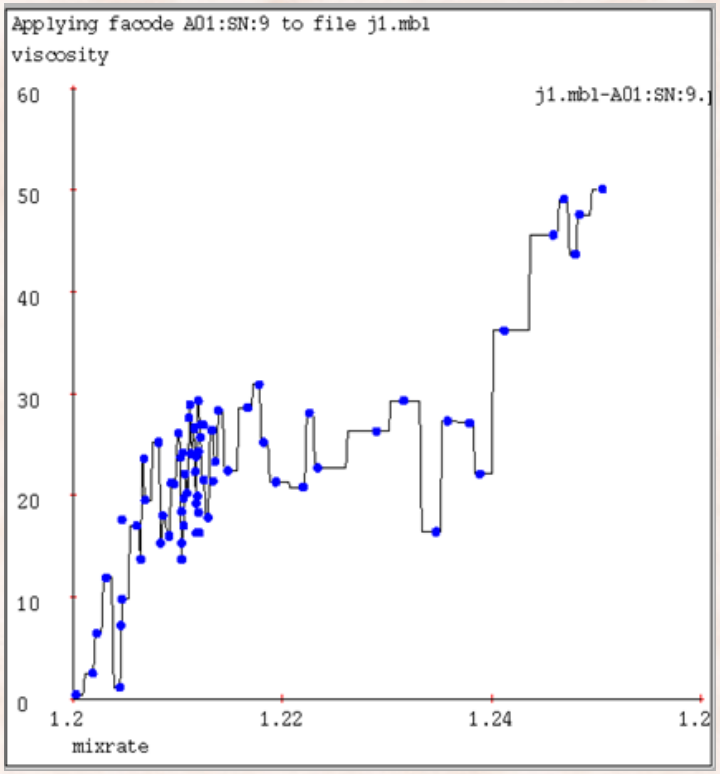


$k = 9$

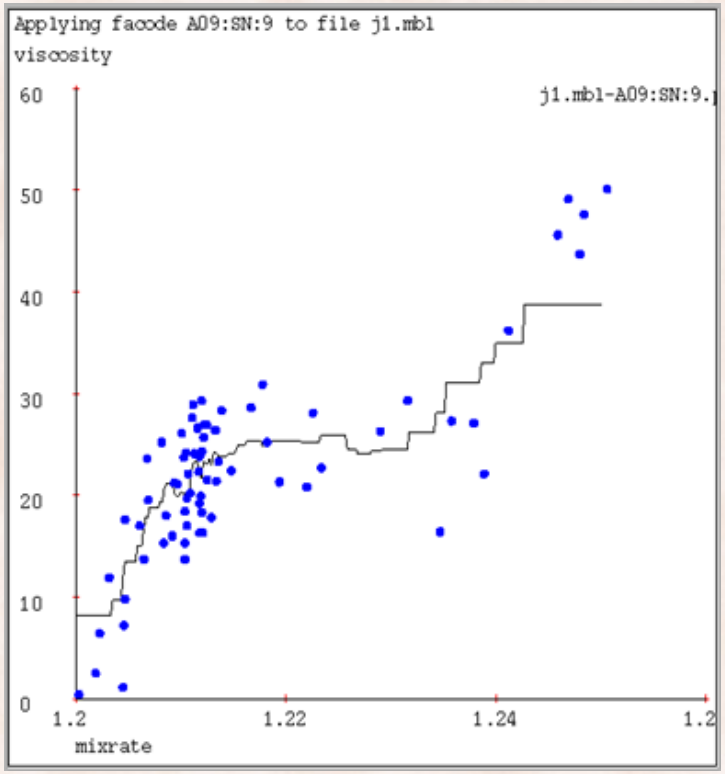


Regression with 9-Nearest Neighbor

$k = 1$



$k = 9$



Distance-Weighted k-NN for Regression

For any test point $\mathbf{x}$, weight each of the k neighbors according to their similarity with $\mathbf{x}$.

1. Find k instances $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k$ nearest to $\mathbf{x}$.

2. Let $$y(x) = \sum_{i=1}^{k} w_i t_i \Big/ \sum_{i=1}^{k} w_i$$

$$\text{where } w_i = \left\| \mathbf{x} - \mathbf{x}_i \right\|^{-2}$$

For $k = \mathrm{N} \Rightarrow$ Shepard's method [Shepard, ACM '68].

Kernel-based Distance Weighted NN Regression

For any test point **x**, weight all training instances according to their similarity with **x**.

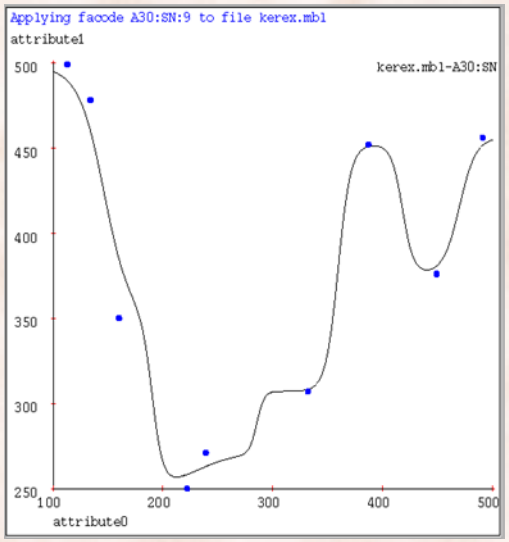
---

1. Return weighted average:

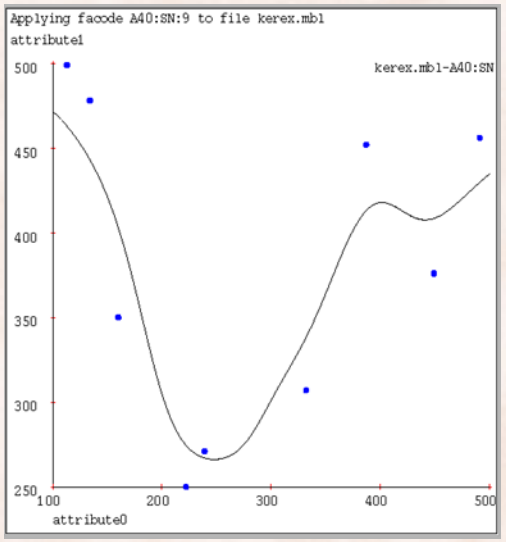
$$y(\mathbf{x}) = \frac{\sum_{i=1}^{N} K(\mathbf{x}, \mathbf{x}_i) t_i}{\sum_{i=1}^{N} K(\mathbf{x}, \mathbf{x}_i)}$$

NN Regression with Gaussian Kernel

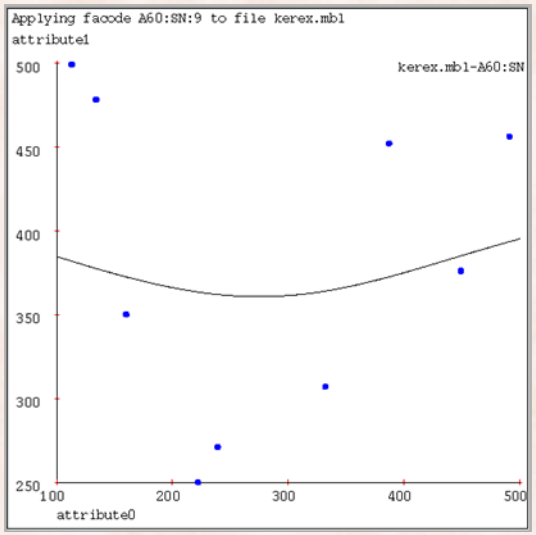
$2\sigma^2=10$



$2\sigma^2=20$



$2\sigma^2=80$

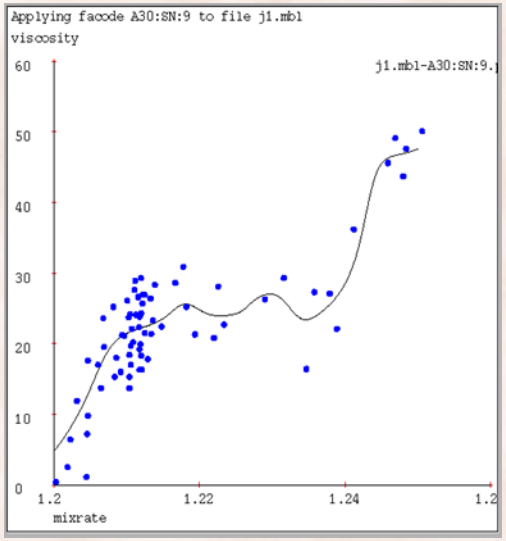


$$K(\mathbf{x},\mathbf{x}_i)=e^{-\frac{\|\mathbf{x}-\mathbf{x}_i\|^2}{2\sigma^2}}$$

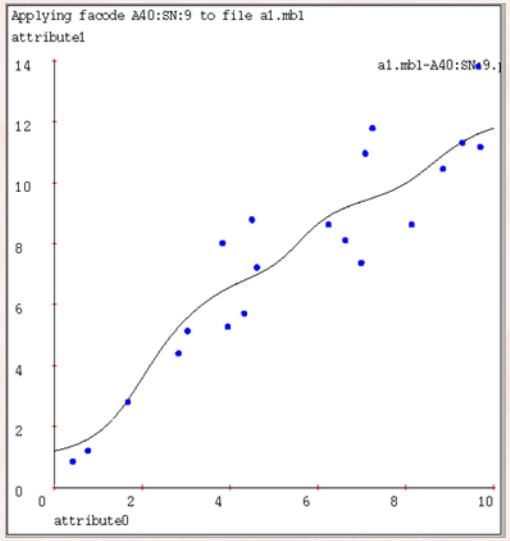
Increased kernel width means more influence from distant points.

NN Regression with Gaussian Kernel

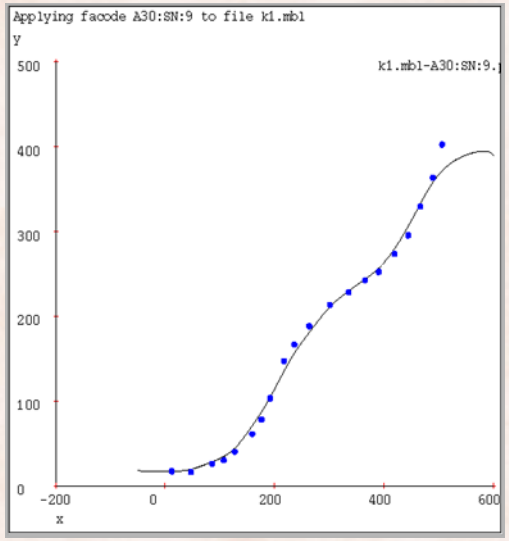
$2\sigma^2$=1/16 of x axis



$2\sigma^2$=1/32 of x axis



$2\sigma^2$=1/32 of x axis



$$K(\mathbf{x},\mathbf{x}_i) = e^{-\frac{\|\mathbf{x}-\mathbf{x}_i\|^2}{2\sigma^2}}$$

k-Nearest Neighbor Summary

- Training: memorize the training examples.
- Testing: compute distance/similarity with training examples.
- Trades decreased training time for increased test time.
- Use kernel trick to work in implicit high dimensional space.
- Needs feature selection when many irrelevant features.
- An Instance-Based Learning (IBL) algorithm:
  - Memory-based learning
  - Lazy learning
  - Exemplar-based
  - Case-based

Machine Learning: Feature Selection
CS 4900/5900

Lecture 08-1

Razvan C. Bunescu

School of Electrical Engineering and Computer Science

bunescu@ohio.edu

Feature Selection

- Datasets with thousands of features are common:
  - text documents
  - gene expression data
- Processing thousands of features during training & testing can be computationally infeasible.
- Many irrelevant features can lead to overfitting.

=> select most relevant features in order to obtain *faster*, *better* and *easier* to understand learning models.

Feature Selection: Methods

- **Wrapper method:**
  - uses a classifier to assess features or feature subsets.
- **Filter method:**
  - ranks features or feature subsets independently of the classifier.
- **Univariate method**:
  - considers one feature at a time.
- **Multivariate method:**
  - considers subsets of features together.

The Wrapper Method

Greedy Forward Selection:

- F is the set of all features.
- $S \subseteq F$ is the subset of selected features.

---

1. Start with no features in $S = \{\}$
2. For each feature f in $F - S$, train model with $S + \{f\}$
3. Add to S the best performing feature(s).
4. Repeat from 2 until:
   (a) performance does not improve, or
   (b) performance good enough.

The Wrapper Method

Greedy Backward Elimination:

- F is the set of all features.
- $S \subseteq F$ is the subset of selected features.

---

1. Start with all features in $S = F$
2. For each feature in S, train model without that feature.
3. Remove from S feature corresponding to best model.
4. Repeat from 2 until:
   (a) performance does not improve, or
   (b) performance good enough.

The Wrapper Method

- **Forward**: Greedily add features one (more) at a time.

  Efficiently Inducing Features of Conditional Random Fields"
  [McCallum, UAI'03]
- **Backward**: Greedily remove features one (more) at a time.

  Multiclass cancer diagnosis using tumor gene expression signatures"
  [Ramaswamy et al., PNAS'01]
- **Combined**: Two steps forward, one step back.

- Train multiple times ⇒ can be very time consuming!
  - Alternative: use external criteria to decide feature relevance ⇒ the Filter Method.

Recursive Feature Elimination with SVM

[Guyon et al., ML'03]

- An instance of Greedy Backward Elimination.

1. Let F = {1, 2, ..., K} be the set of features.
2. Let S = [] be the ranked set of features.
3. Repeat until F – S is empty:
   I. Train weight vector **w** using a linear SVM and F – S.
   II. Find feature f in F – S with minimum $|\mathbf{w}_f|$.
   III. Append f to S.
4. Return S.

The Filter Method

1. Rank all features using a measure of correlation with the label.
2. Select top *k* features to use in the model.

- Measures of correlation between feature X and label Y:
  - Mutual Information
  - Chi-square Statistic

  } *nominal features & label*

  - Pearson Correlation Coefficient
  - Signal-to-Noise Ratio
  - T-test

Mutual Information

- Independence:

$$P(X,Y) = P(X)P(Y)$$

- Measure of dependence:

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

$$= KL(p(X,Y) \,\|\, p(X)p(Y))$$

  - It is 0 when X and Y are independent.
  - It is maximum when X=Y.

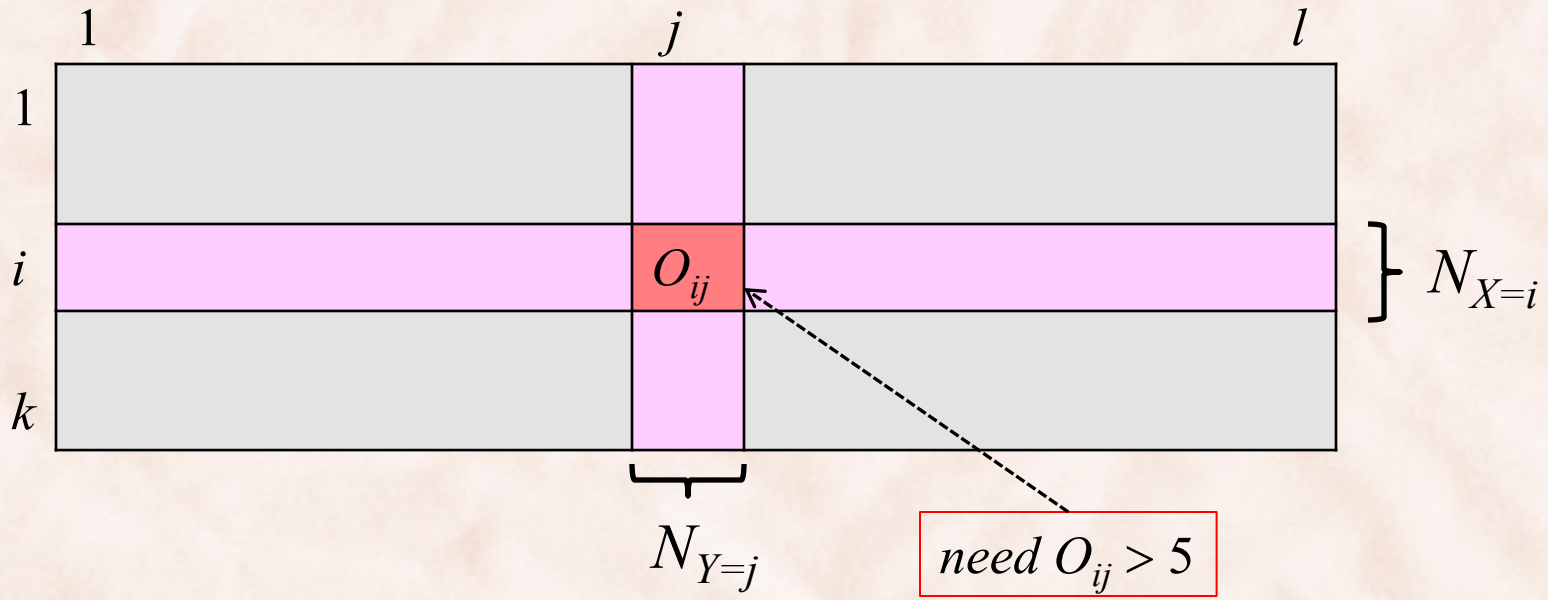
Mutual Information

- Problems:
  - Works only with nominal features & labels ⇒ discretization.
  - Biased toward high arity features ⇒ normalization.
  - May choose redundant features.
  - Features may become relevant in the context of other ⇒ use conditional MI [Fleuret, JMLR '04].
- Other measures:
  - Chi square (χ^2).
  - Log-likelihood Ratio (LLR).
- Comparison between MI, χ^2, and LLR in [Dunning, CL'98]

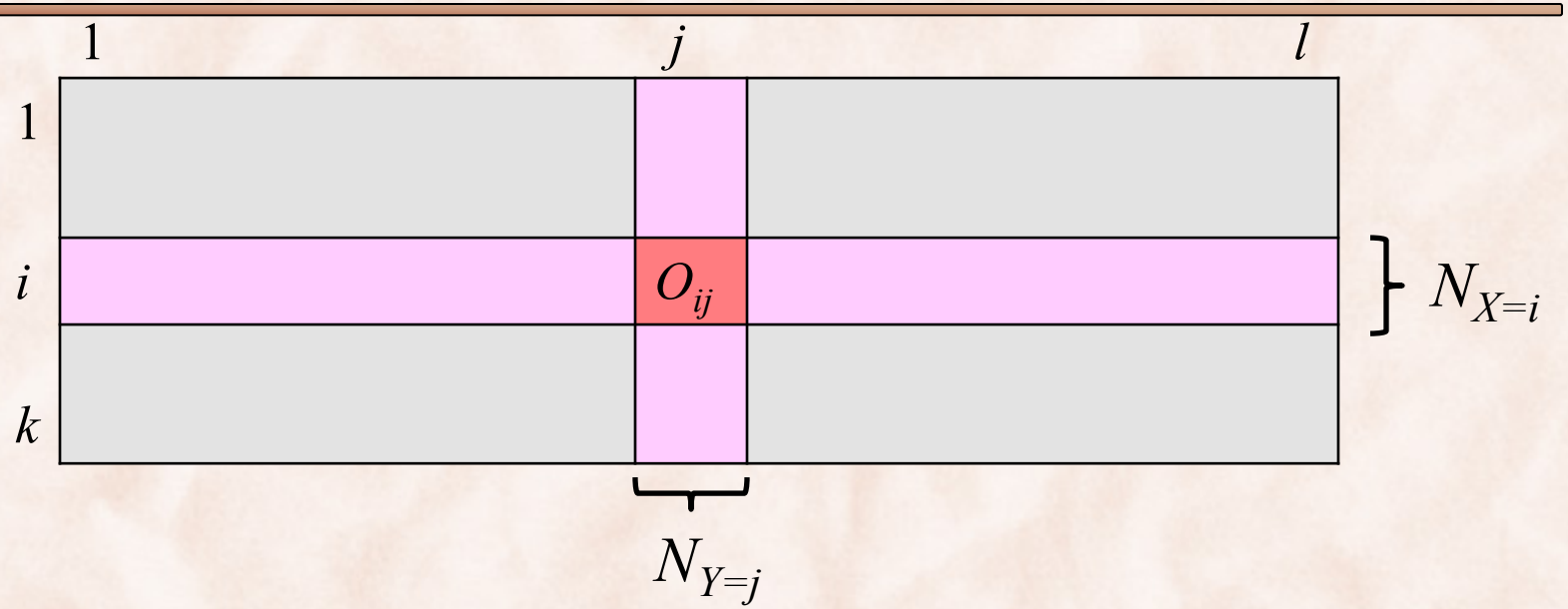
  "Accurate methods for the statistics of surprise and coincidence"

Chi Square (χ^2) Test of Independence

- N training examples (observations).
- X is a discrete feature with k possible values.
- Y is a label with l possible values.
- Create k-by-l contingency table with cells for every feature-label combination.



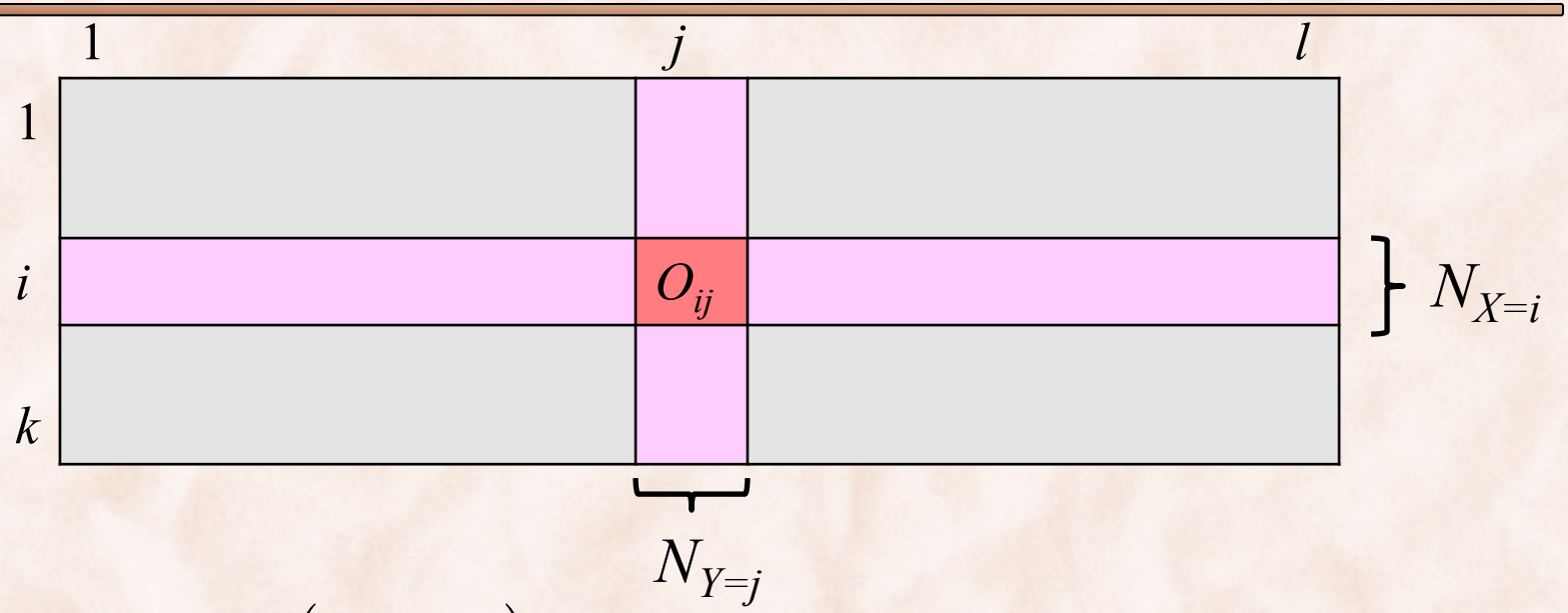
Chi Square (χ^2) Test of Independence



- O_{ij} is the observed count for $X=i$ & $Y=j$.
- E_{ij} is the expected value for $X=i$ & $Y=j$, assuming X,Y are independent.

$$E_{ij} = \frac{N_{X=i} \times N_{Y=j}}{N} = \frac{\left(\sum_{c=1}^{l} O_{ic}\right) \times \left(\sum_{r=1}^{k} O_{rj}\right)}{N}$$

Chi Square (χ^2) Test of Independence



$$X^2 = \sum_{i=1}^{k}\sum_{j=1}^{l}\frac{(O_{ij}-E_{ij})^2}{E_{ij}}$$

asymptotically distributed as χ^2 with $(k\text{-}1)(l\text{-}1)$ degrees of freedom if X,Y are independent.

Use X^2 test value to rank features X with respect to label Y.

Pearson Correlation Coefficient

- Feature X and label Y are two random variables.
- Population correlation coefficient (*linear dependence*):

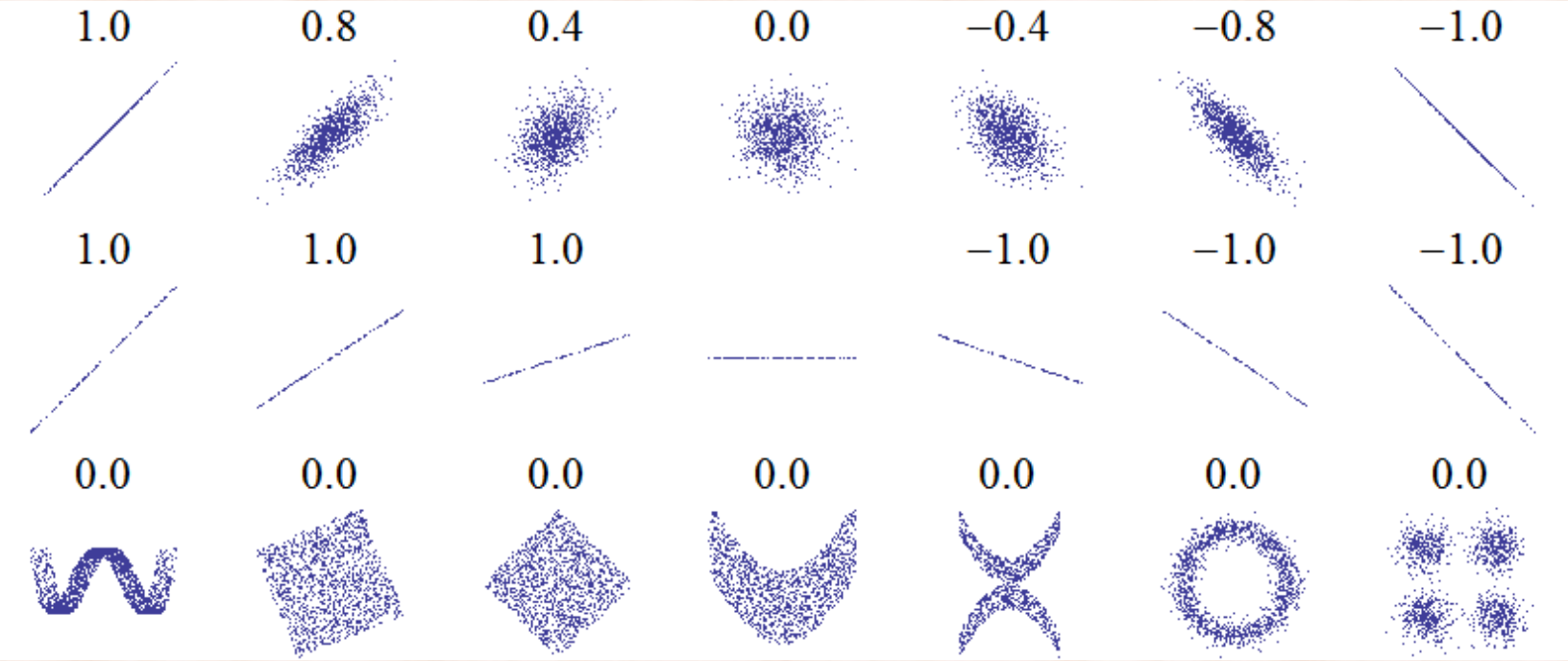
$$\rho(X,Y) = \frac{E[(X-\mu_X)(Y-\mu_Y)]}{\sigma_X \sigma_Y}$$

- Sample correlation coefficient:

$$\rho(X,Y) = \frac{\sum_{i=1}^{n}(X_i-\bar{X})(Y_i-\bar{Y})}{\sqrt{\sum_{i=1}^{n}(X_i-\bar{X})^2}\sqrt{\sum_{i=1}^{n}(Y_i-\bar{Y})^2}}$$

- Values always between $[-1,+1]$
  - when linearly dependent $+1$, -1, when independent 0.

Pearson Correlation Coefficient

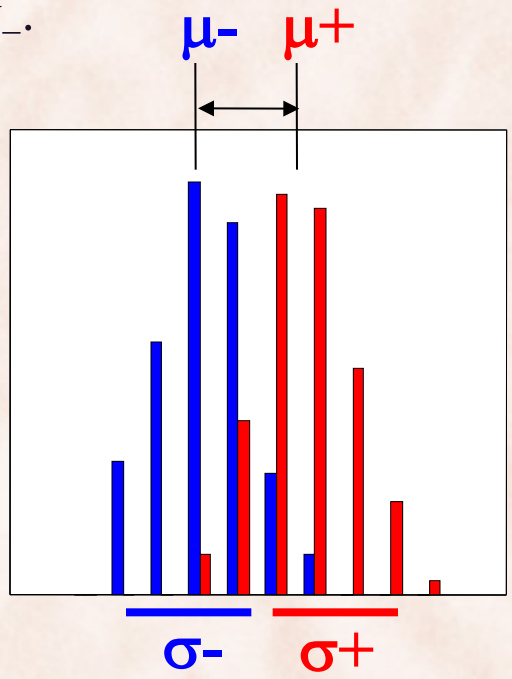


Signal-to-Noise Ratio (S2N)

- Feature X and label Y are two random variables:
  - Y is binary, $Y \in \{y_+, y_-\}$
- Let μ_+, σ_+ be the sample μ, σ of X for which $Y = y_+$.
- Let μ_-, σ_- be the sample μ, σ of X for which $Y = y_-$.

$$\mu(X,Y) = \frac{|\mu_+ - \mu_-|}{\sigma_+ + \sigma_-}$$

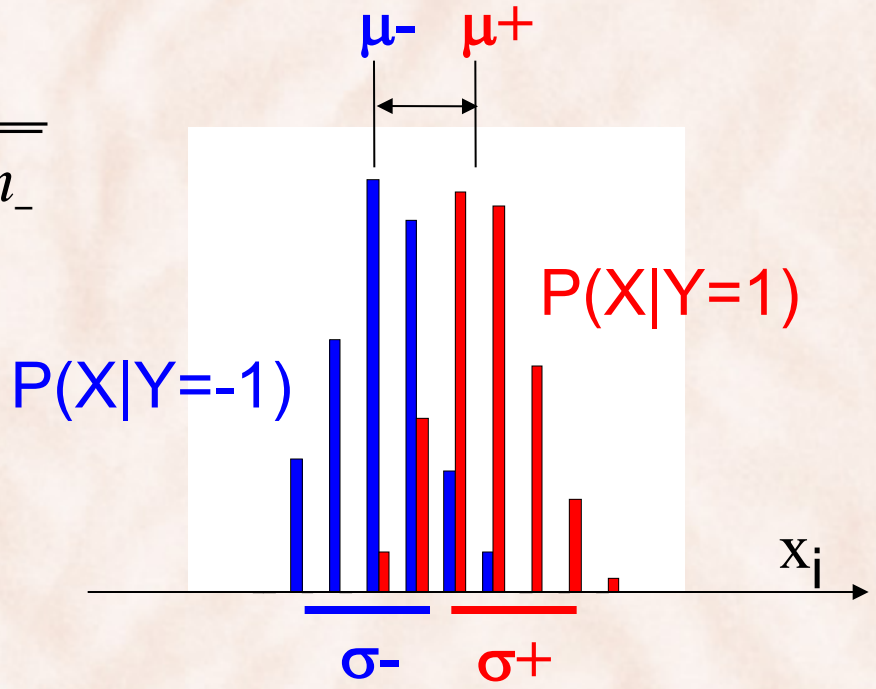
related to Fisher's criterion



Ranking Features with the T-test

- Let m_+ be the number of samples in class y_+.
- Let m_- be the number of sample in class y_- .

$$T(X,Y) = \frac{|\mu_+ - \mu_-|}{\sqrt{\sigma_+^2/m_+ + \sigma_-^2/m_-}}$$



Machine Learning: Naïve Bayes
CS 4900/5900

Lecture 09

Razvan C. Bunescu

School of Electrical Engineering and Computer Science

bunescu@ohio.edu

Three Parametric Approaches to Classification

1) Discriminant Functions: construct $f: \mathrm{X} \rightarrow \mathrm{T}$ that directly assigns a vector $\mathbf{x}$ to a specific class C_k.
   - Inference and decision combined into a single learning problem.
   - *Linear Discriminant*: the decision surface is a hyperplane in X:
     - Fisher 's Linear Discriminant
     - Perceptron
     - Support Vector Machines

Three Parametric Approaches to Classification

2) Probabilistic Discriminative Models: directly model the posterior class probabilities $p(C_k \mid \mathbf{x})$.
   - Inference and decision are separate.
   - Less data needed to estimate $p(C_k \mid \mathbf{x})$ than $p(\mathbf{x} \mid C_k)$.
   - Can accommodate many overlapping features.
     - Logistic Regression
     - Conditional Random Fields

Three Parametric Approaches to Classification

3) Probabilistic Generative Models:

- Model class-conditional $p(\mathbf{x} \mid C_k)$ as well as the priors $p(C_k)$, then use Bayes's theorem to find $p(C_k \mid \mathbf{x})$.
  - or model $p(\mathbf{x}, C_k)$ directly, then marginalize to obtain the posterior probabilities $p(C_k \mid \mathbf{x})$.
- Inference and decision are separate.
- Can use $p(\mathbf{x})$ for *outlier* or *novelty detection*.
- Need to model dependencies between features.
  - Naïve Bayes.
  - Hidden Markov Models.

Unbiased Learning of Generative Models

- Let $\mathbf{x} = [x_1, x_2, \ldots, x_M]^T$ be a feature vector with M features.
- Assume Boolean features:

  $\Rightarrow$ distribution $p(\mathbf{x} \mid C_k)$ is completely specified by a table of 2^M probabilities, of which $2^M - 1$ are independent.
- Assume binary classification:

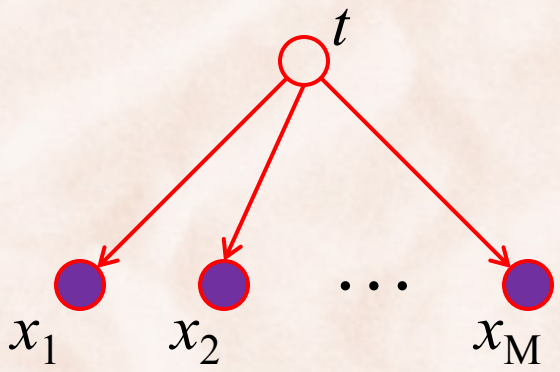
  $\Rightarrow$ need to estimate $2^M - 1$ parameters for each class

  $\Rightarrow$ total of $2(2^M - 1)$ independent parameters to estimate.

  – 30 features $\Rightarrow$ more than 2 billion parameters to estimate!

The Naïve Bayes Model

- Assume features are conditionally independent given the target output:



$$\Rightarrow p(\mathbf{x} \mid C_k) = \prod_{i=1}^{M} p(x_i \mid C_k)$$

- Assume binary classification & features:

  $\Rightarrow$ need to estimate only 2M parameters, a lot less than $2(2^{M}-1)$.

The Naïve Bayes Model: Inference

- Posterior distribution:

$$p(C_k \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid C_k)p(C_k)}{p(\mathbf{x})} \quad \text{, where } p(\mathbf{x}) = \sum_j p(\mathbf{x} \mid C_j)p(C_j)$$

$$= \frac{p(C_k)\prod_j p(x_j \mid C_k)}{p(\mathbf{x})}$$

- Inference ≡ find C_* to minimize missclassification rate:

$$C_* = \arg\max_{C_k} p(C_k \mid \mathbf{x})$$

$$= \arg\max_{C_k} p(C_k)\prod_j p(x_j \mid C_k)$$

The Naïve Bayes Model: Training

- Training ≡ estimate parameters $p(x_i|C_k)$ and $p(C_k)$.
- Maximum Likelihood (ML) estimation:

$$\hat{p}(x_i = v \mid t = C_k) = \frac{\sum_{(\mathbf{x},t)\in D} \delta_v(x_i)\delta_{C_k}(t)}{\sum_{(\mathbf{x},t)\in D} \delta_{C_k}(t)}$$

training examples in which $x_i = v$ and $t = C_k$

training examples in which $t = C_k$

$$\hat{p}(t = C_k) = \frac{\sum_{(\mathbf{x},t)\in D} \delta_{C_k}(t)}{|D|}$$

The Naïve Bayes Model: Training

- Maximum A-Posteriori (MAP) estimation:
  - assume a Dirichlet prior over the NB parameters, with equal-valued parameters.
  - assume x_i can take V values, label t can take K values.

$$\hat{p}(x_i = v \mid t = C_k) = \frac{\sum_{(\mathbf{x},t)\in D} \delta_v(x_i)\delta_{C_k}(t) + l}{\sum_{(\mathbf{x},t)\in D} \delta_{C_k}(t) + lV}$$

$\Leftrightarrow lV$ "hallucinated" examples spread evenly over all V values of x_i.

$$\hat{p}(t = C_k) = \frac{\sum_{(\mathbf{x},t)\in D} \delta_{C_k}(t) + l}{|D| + lK}$$

$l = 1 \Rightarrow$ *Laplace smoothing*

Text Categorization with Naïve Bayes

- Text categorization problems:
  - Spam filtering.
  - Targeted advertisement in Gmail.
  - Classification in multiple categories on news websites.

- Representation as one feature per word:

  $\Rightarrow$ each document is a very high dimensional feature vector.

- Most words are rare:
  - Zipf's law and heavy tail distribution.

  $\Rightarrow$ feature vectors are sparse.

Text Categorization with Naïve Bayes

- Generative model of documents:
  1) Generate document category by sampling from $p(C_k)$.
  2) Generate a document as a bag of words by repeatedly sampling with replacement from a vocabulary $V = \{w_1, w_2, \ldots, w_{|V|}\}$ based on $p(w_i \mid C_k)$.

- Inference with Naïve Bayes:
  - Input :
    - Document **x** with n words $v_1, v_2, \ldots v_n$.
  - Output:
    - Category $C_* = \arg\max_{C_k} p(C_k) \prod_{j=1}^{n} p(v_j \mid C_k)$

Text Categorization with Naïve Bayes

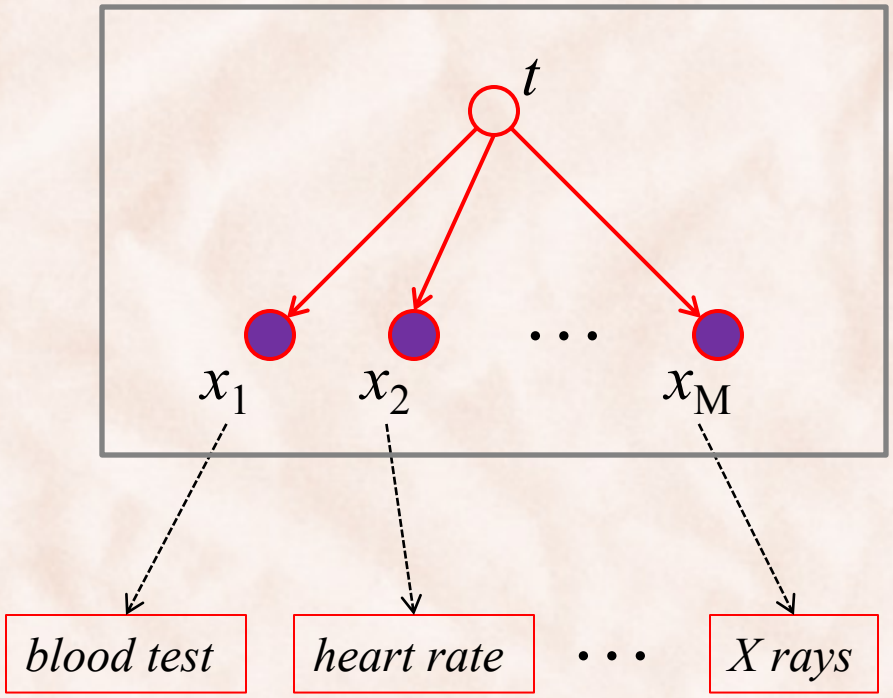
- Training with Naïve Bayes:
  - Input:
    - Dataset of training documents D with vocabulary V.
  - Output:
    - Parameters $p(C_k)$ and $p(w_i \mid C_k)$.

---

1. **for each** category C_k:
2. **let** D_k be the subset of documents in category C_k
3. **set** $p(C_k) = |D_k| / |D|$
4. **let** n_k be the total number of words in D_k
5. **for** each word $w_i \in$ V:
6. **let** n_{ki} be the number of occurrences of w_i in D_k
7. **set** $p(w_i \mid C_k) = (n_{ki}+1) / (n_k + |V|)$

Medical Diagnosis with Naïve Bayes

- Diagnose a disease T={*Yes*, *No*}, using information from various medical tests.



$$p(\mathbf{x} \mid C_k) = \prod_{i=1}^{M} p(x_i \mid C_k)$$

Medical tests may result in continuous values
$\Rightarrow$ need Naïve Bayes to work with *continuous features*.

Naïve Bayes with Continuous Features

- Assume $p(x_i \mid C_k)$ are Gaussian distributions $N(\mu_{ik}, \sigma_{ik})$.
- Training: use ML or MAP criteria to estimate μ_{ik}, σ_{ik}:

$$\hat{\mu}_{ik} = \frac{\sum_{(\mathbf{x},t)\in D} x_i \delta_{C_k}(t)}{\sum_{(\mathbf{x},t)\in D} \delta_{C_k}(t)} \qquad \hat{\sigma}_{ik}^2 = \frac{\sum_{(\mathbf{x},t)\in D} (x_i - \hat{\mu}_{ik})^2 \delta_{C_k}(t)}{\sum_{(\mathbf{x},t)\in D} \delta_{C_k}(t)}$$

- Inference:

$$C_* = \arg\max_{C_k} p(C_k \mid \mathbf{x}) = \arg\max_{C_k} p(C_k) \prod_i p(x_i \mid C_k)$$

Numerical Issues

- Multiplying lots of probabilities may results in underflow:
  - especially when many attributes (e.g. text categorization).

- Compute everything in *log space*:

$$p(\mathbf{x} \mid C_k) = \prod_{i=1}^{M} p(x_i \mid C_k) \Leftrightarrow \boxed{\ln p(\mathbf{x} \mid C_k) = \sum_{i=1}^{M} \ln p(x_i \mid C_k)}$$

$$C_* = \arg\max_{C_k} p(C_k \mid \mathbf{x}) \Leftrightarrow \boxed{C_* = \arg\max_{C_k} \ln p(C_k \mid \mathbf{x})}$$

$$= \arg\max_{C_k} \{\ln p(C_k) + \ln p(\mathbf{x} \mid C_k)\}$$

Naïve Bayes

- Often has good performance, despite strong independence assumptions:
  - quite competitive with other classification methods on UCI datasets.
- It does not produce accurate probability estimates when independence assumptions are violated:
  - the estimates are still useful for finding max-probability class.
- Does not focus on completely fitting the data $\Rightarrow$ resilient to noise.

Probabilistic Generative Models: Binary Classification (K = 2)

- Model class-conditional $p(\mathbf{x}\,|C_1)$, $p(\mathbf{x}\,|C_2)$ as well as the priors $p(C_1)$, $p(C_2)$, then use Bayes's theorem to find $p(C_1\,|\,\mathbf{x})$, $p(C_2\,|\,\mathbf{x})$:

$$p(C_1\,|\,\mathbf{x}) = \frac{p(\mathbf{x}\,|\,C_1)p(C_1)}{p(\mathbf{x}\,|\,C_1)p(C_1) + p(\mathbf{x}\,|\,C_2)p(C_2)}$$

$$= \sigma(a(\mathbf{x}))$$

logistic sigmoid

where $\sigma(a) = \dfrac{1}{1+\exp(-a)}$

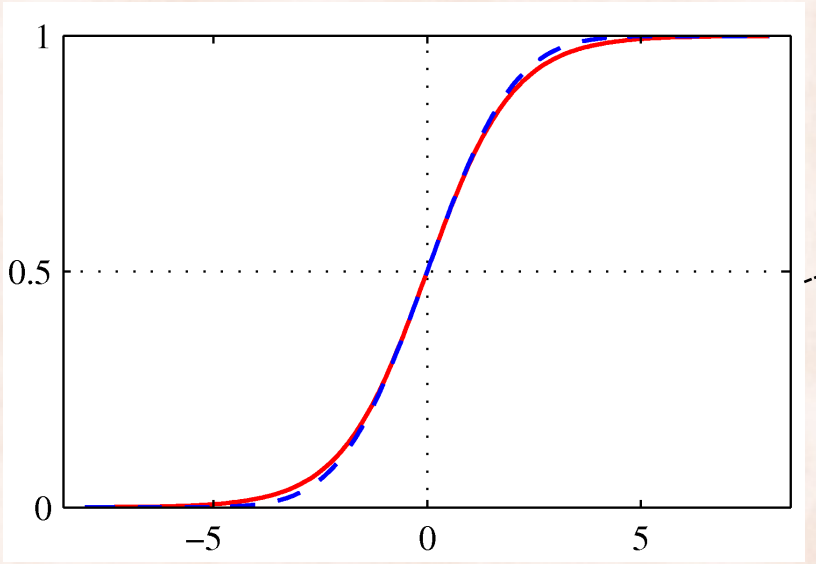
log odds

$$a(\mathbf{x}) = \ln \frac{p(\mathbf{x}\,|\,C_1)p(C_1)}{p(\mathbf{x}\,|\,C_2)p(C_2)} = \ln \frac{p(C_1\,|\,\mathbf{x})}{p(C_2\,|\,\mathbf{x})}$$

Probabilistic Generative Models: Binary Classification (K = 2)

- If $a(\mathbf{x})$ is a linear function of x $\Rightarrow$ $p(C_1 \mid \mathbf{x})$ is a *generalized linear model*:

$$p(C_1 \mid \mathbf{x}) = \frac{1}{1+\exp(-a(\mathbf{x}))} = \sigma(a(\mathbf{x})) = \sigma(\boldsymbol{\lambda}^T \mathbf{x})$$



$\sigma(a)$ is a *squashing function*

The Naïve Bayes Model

- Assume binary features $x_i \in \{0,1\}$:

$$\Rightarrow p(\mathbf{x} \mid C_k) = \prod_{i=1}^{M} p(x_i \mid C_k)$$

$$= \prod_{i=1}^{M} \mu_{ki}^{x_i} (1-\mu_{ki})^{1-x_i} \quad \text{, where} \quad \mu_{ki} = p(x_i = 1 \mid C_k)$$

$$\Rightarrow p(C_k \mid \mathbf{x}) = \frac{\exp(a_k(\mathbf{x}))}{\sum_j \exp(a_j(\mathbf{x}))}$$

$$\text{, where } a_k(\mathbf{x}) = \sum_{i=1}^{M} \{x_i \ln \mu_{ki} + (1-x_i)\ln(1-\mu_{ki})\} + \ln p(C_k)$$

$$= \boldsymbol{\lambda}_k^T \mathbf{x} \quad \Rightarrow \text{NB is a } \textit{generalized linear model.}$$

Probabilistic Generative Models: Multiple Classes (K ≥ 2)

- Model class-conditional $p(\mathbf{x}\,|C_k)$ as well as the priors $p(C_k)$, then use Bayes's theorem to find $p(C_k \mid \mathbf{x})$:

$$p(C_k \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid C_k)p(C_k)}{\sum_j p(\mathbf{x} \mid C_j)p(C_j)}$$

$$= \frac{\exp(a_k(\mathbf{x}))}{\sum_j \exp(a_j(\mathbf{x}))}$$

normalized exponential i.e. softmax function

where $a_k(\mathbf{x}) = \ln p(\mathbf{x} \mid C_k)p(C_k)$

- If $a_k(\mathbf{x}) = \boldsymbol{\lambda}_k^T \mathbf{x} \Rightarrow p(C_k \mid \mathbf{x})$ is a *generalized linear model.*