Some problems and trends in data mining
データマイニングの課題とトレンド

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The talk aims to ...

➔ Introduce to basic concepts and techniques of data mining (DM).
データマイニング（ＤＭ）の基本概念と技法を紹介する.

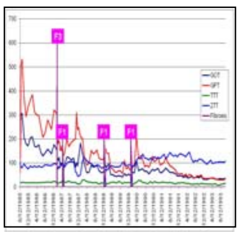
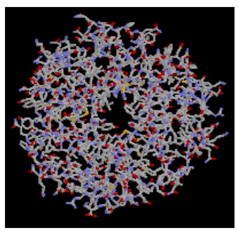
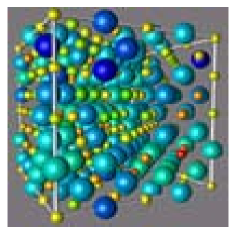
➔ Present some challenging data mining problems, and kernel methods as an emerging trend in this field.
データマイニングのチャレンジ課題およびこの分野で興隆しつつあるカーネル手法について説明する.

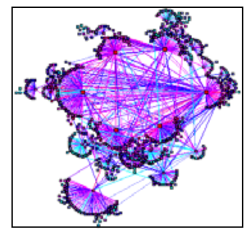
What motivated data mining?
データマイニングの必要性？

We are living in the most exciting of times: Computer and computer networks　もっともエキサイティングな時代：コンピュータとコンピュータ・ネットワーク

- Much more data around us then before. They are collected and stored in huge databases (millions of records, thousands of fields).
  前代未聞に膨大なデータに囲まれる生活．何百万件もの多岐に渡るデータデータは巨大データベースに格納されている．

- Many kinds of complexly structured data (non-vectorial).
  多種多様な複雑に構造化されたデータ（非ベクトル型）．

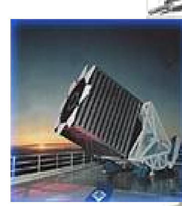


Astronomical data　天文学的データ

Astronomy is facing a major data avalanche:
天文学ではデータ崩壊の危機に瀕している

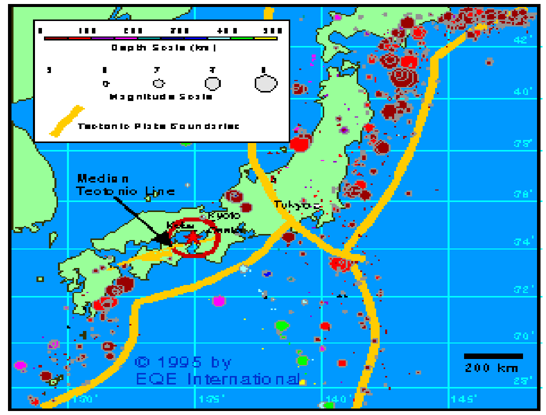
Multi-terabyte sky surveys and archives (soon: multi-petabyte), billions of detected sources, hundreds of measured attributes per source …
何テラバイトもの天空観測データ，何十億もの観測源，観測源ごとに何百もある属性

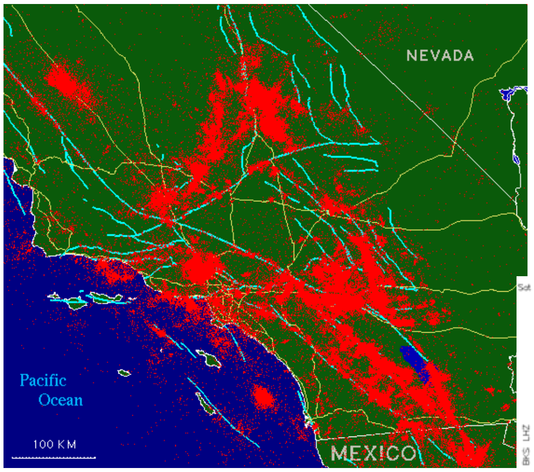




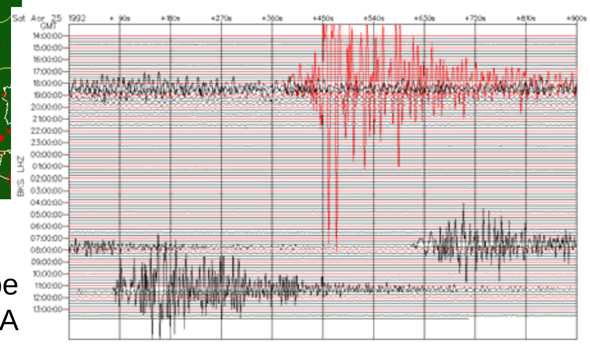

Earthquake data　地震データ

Japanese earthquakes
日本の地震1961-1994



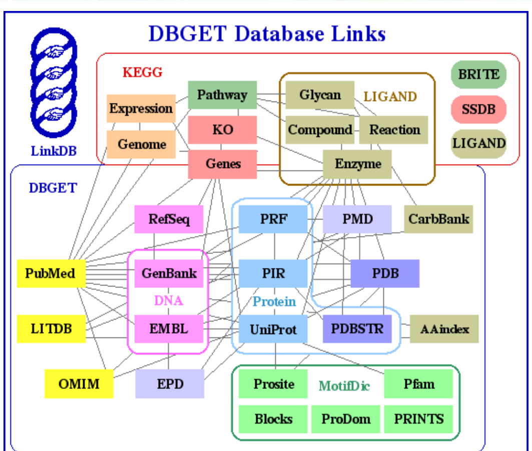


1932-1996

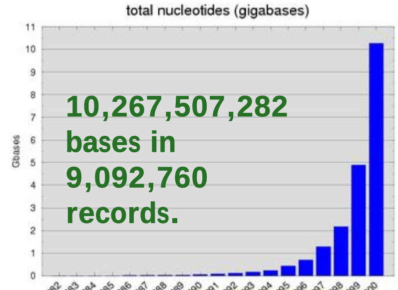


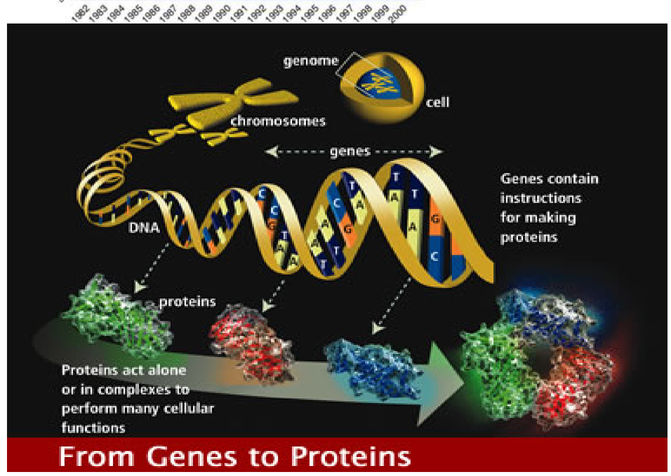
04/25/92 Cape
Mendocino, CA

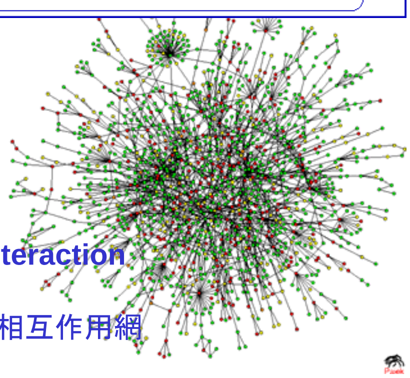
Explosion of biological data
爆発的な生物学データ



EMBL Database Growth
total nucleotides (gigabases)





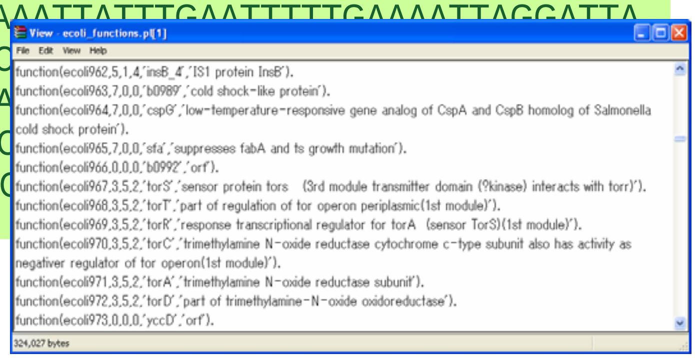


Protein interaction network
タンパク質相互作用網

How biological data look like?
生物学データの形式など

A portion of the DNA sequence, consisting of 1.6 million characters, is given as follows (about 350 characters, 4570 times smaller):
1600万文字からなるDNA配列の一部（4570分の一）

...TACATTAGTTATTACATTGAGAAACTTTATAATTAAAAAAGATTCATGTAAATT
TCTTATTTGTTTATTTAGAGGTTTTAAATTTAATTTCTAAGGGTTTGCTGGTTTC
ATTGTTAGAATATTTAACTTAATCAAATTATTTGAATTTTTTGAAAATTAGGATTA
ATTAGGTAAGTAAATAAAATTTCTC
GAGATAAAAATACTACTCTGTTTTA
GTTTATATATATGAAGTAGTTACCC
ATTAAGAGTGATGAAGTATATTATC



Many other kinds of biological data

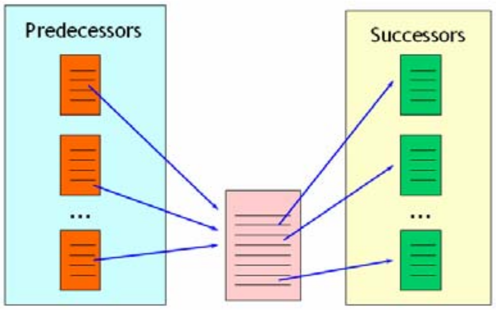
Text: huge sources of knowledge
テキスト：知識の大きな源

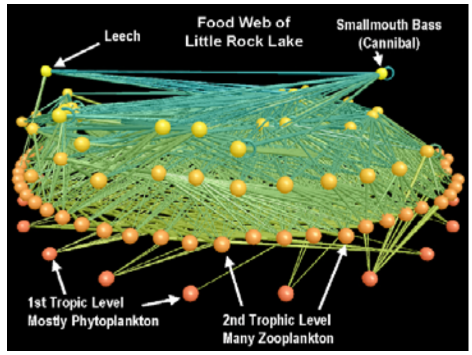
- Approximately **80%** of the world's data is held in unstructured formats (source: Oracle Corporation)
  世界中のデータの約80%が非構造化データ（オラクルによる）
- Example: MEDLINE is a source of life sciences and biomedical information, with nearly eleven million records
  例：生命科学・生物医学の情報源であるMEDLINEには約1100万件の論文情報がある
  - ➔ About 60,000 abstracts on hepatitis (そのうち6万件が肝炎)

36003: Biomed Pharmacother. 1999 Jun;53(5-6):255-63.
Pathogenesis of autoimmune hepatitis.
Institute of Liver Studies, King's College Hospital, London, United Kingdom.

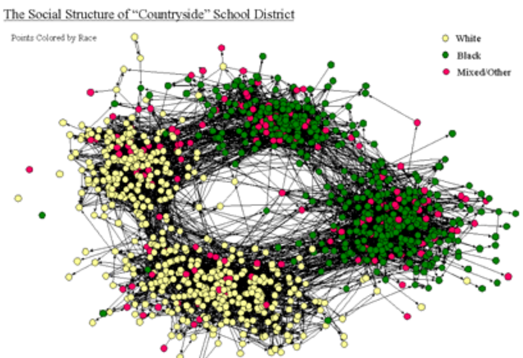
Autoimmune **hepatitis** (AIH) is an idiopathic disorder affecting the hepatic parenchyma. There are no morphological features that are pathognomonic of the condition but the characteristic histological picture is that of an interface hepatitis without other changes that are more typical of other liver diseases. It is associated with hypergammaglobulinaemia, high titres of a wide range of circulating auto-antibodies, often a family history of other disorders that are thought to have an autoimmune basis, and a striking response to immunosuppressive therapy. The pathogenetic mechanisms are not yet fully understood but there is now considerable circumstantial evidence suggesting that: (a) there is an underlying genetic predisposition to the disease; (b) this may relate to several defects in immunological control of autoreactivity, with consequent loss of self-tolerance to liver auto-antigens; (c) it is likely that an initiating factor, such as a hepatotropic viral infection or an idiosyncratic reaction to a drug or other hepatotoxin, is required to induce the disease in susceptible individuals, …

Web link data　　ウェブのリンクデータ



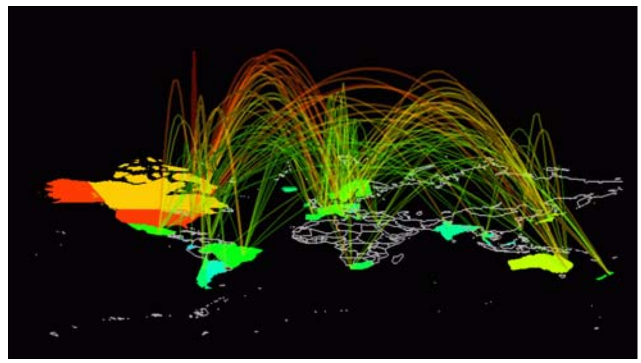


Food Web
[Martinez '91]



Friendship Network
[Moody '01]

Over 3 billion
documents



What is data mining?
データマイニングとは何か？

"Data-driven discovery of models and patterns from massive observational data sets"

大規模な観測データからのモデルおよびパターンのデータ駆動型発見

Statistics, Inference
統計学，推論

Languages, Representations
言語，表現

Engineering, Data Management
工学，データ管理

Applications 応用

Example: mining associations in market data
マーケット・バスケット分析（IBM）

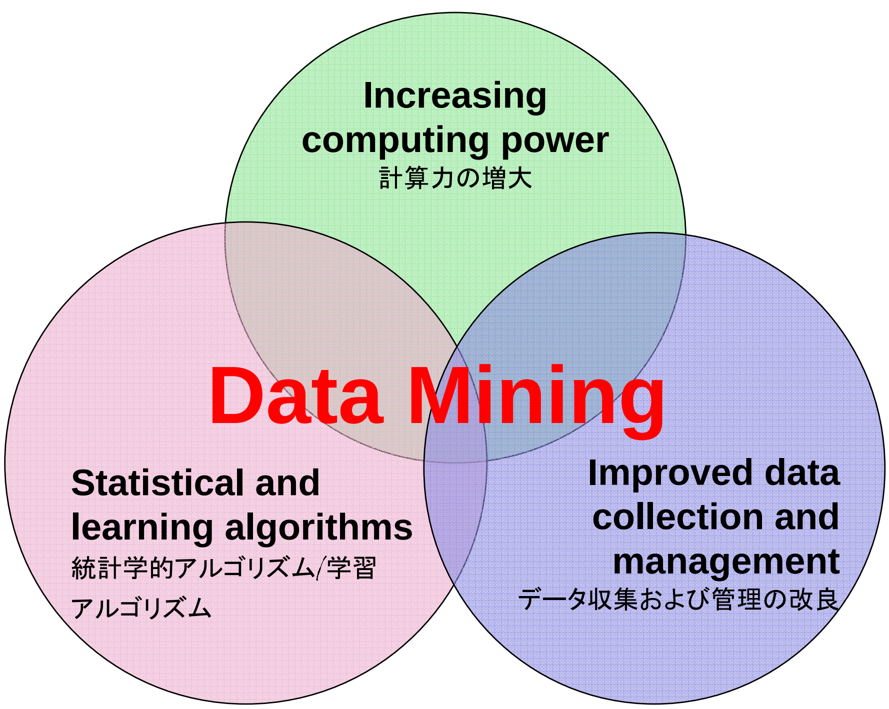
Super market data

"Young men buy diaper and beer together"
「紙おむつを買う男性は缶ビールを一緒に買うことが多い」

売上データ　データマイニング　20-30歳の男性　紙おむつ　ビール

（解釈：顧客像）紙おむつを買うように頼まれた男性がついでに自分用の缶ビールを購入していた　→ 今後の陳列に活かすことのできる知識.

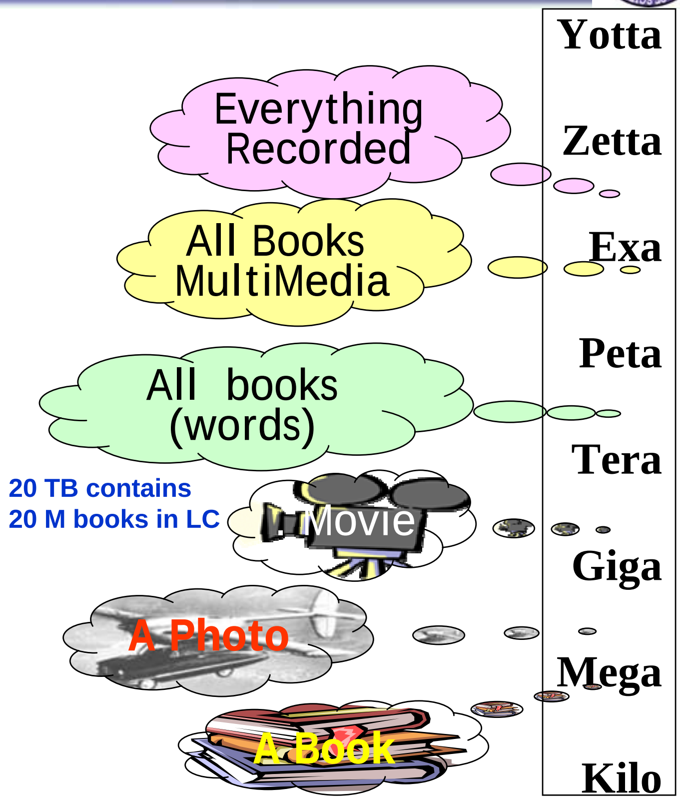
Convergence of thee technologies
3つのテクノロジーの集合



Improved data collection and management
データ収集および管理の改善

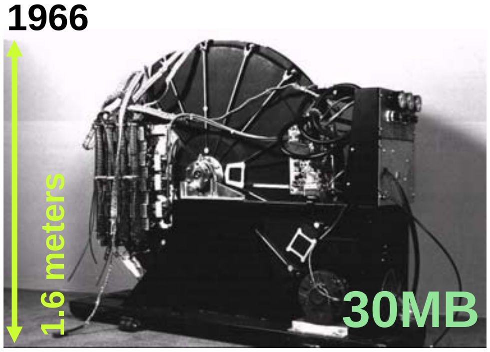
- Soon everything can be recorded and indexed
  すべてが記録され索引付けられる
- Most bytes will never be seen by humans
  ほとんどは人間が確認することはない
- What will be key technologies to deal with huge volumes of information sources?
  莫大な情報を取り扱うための主要技法は何か？

[“How much information is there?” Adapted from the invited talk of Jim Gray (Microsoft) at KDD’2003]

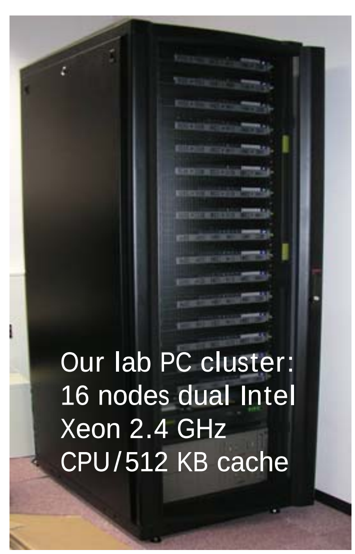


Increasing computing power
計算力の増大

1966

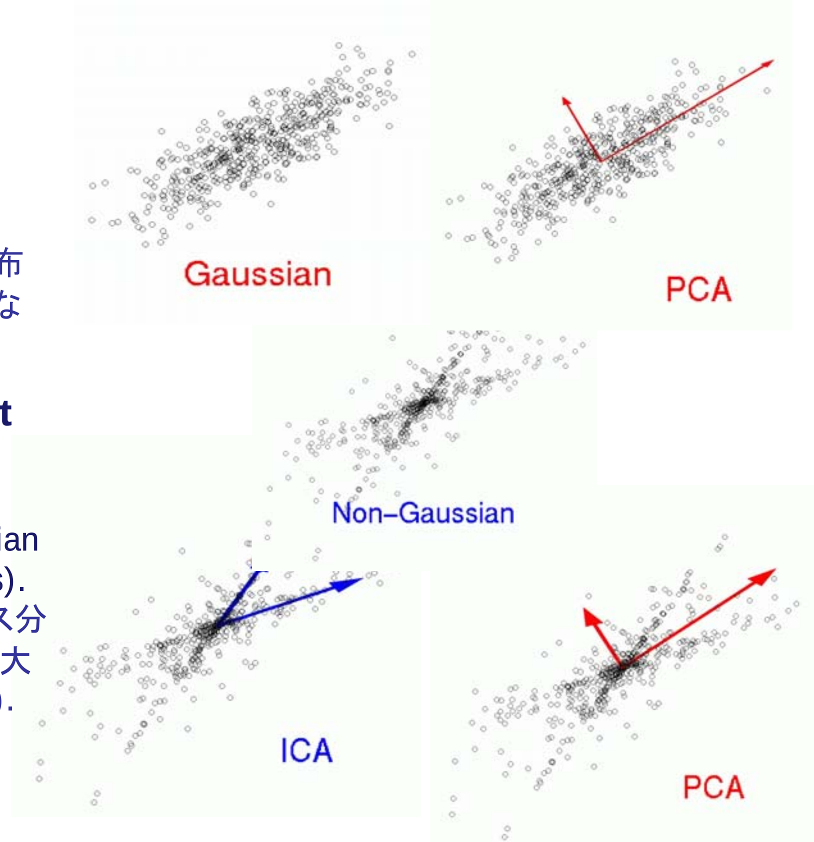


JAIST’s CRAY XT3
計算ノード:
CPU: AMD Opteron150
2.4GHz ×4×90
メモリ: 32GB ×90 ＝
2.88TB CPU間接続: 3Dトーラス結合帯域幅: CPU-CPU間 7.68GB/s(双方向)



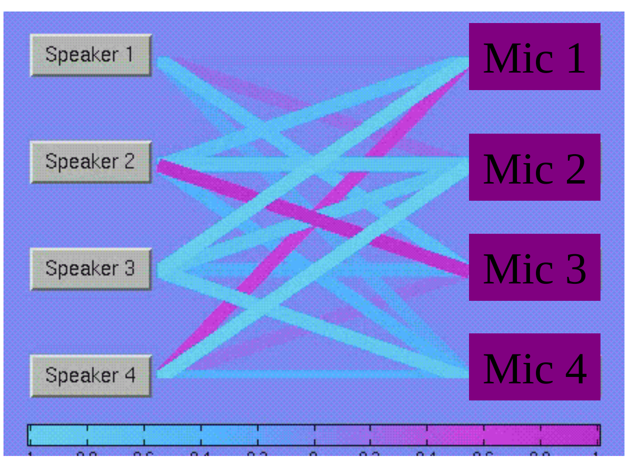
Statistical and learning algorithms
独立成分分析(ICA) vs. 主成分分析(PCA)

- **Principal Component Analysis (PCA)**
  finds directions of maximal variance in Gaussian data (second-order statistics).
  主成分分析(PCA): ガウス分布データにおいて分散が最大となる方向の発見(一次統計).
- **Independent Component Analysis (ICA)**
  finds directions of maximal independence in non-Gaussian data (higher-order statistics).
  独立成分分析 (ICA):非ガウス分布データにおいて独立性が最大となる方向の発見 (高次統計).

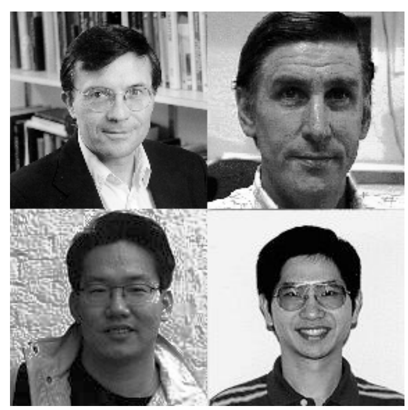


Statistical and learning algorithms
ICA: 複数センサで取得した信号データの分離

Perform ICA



Play Mixtures



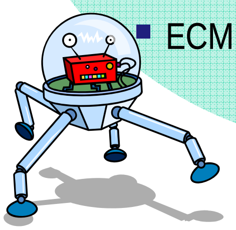
Terry Scott

Te-Won Tzyy-Ping

Play Components

Machine learning and data mining
研究領域とデータマイニング

- **Machine learning 機械学習**
  To build computer systems that learn as well as human does (science of learning from data).
  人間のように学習するコンピュータシステムを構築する（データからの学習の科学）
- ICML since 1982 (23th ICML in 2006), ECML since 1989.
- ECML/PKDD since 2001.



- **Data mining データマイニング**
  To find new and useful knowledge from large datasets (data engineering).
  大きなデータベースから新しく有用な知識を見つける（データ工学）
- ACM SIGKDD since 1995, PKDD and PAKDD since 1997 IEEE ICDM and SIAM DM since 2000, etc.

Knowledge discovery in databases (KDD) process
知識発見とデータマイニングのプロセス

a step in the KDD process consisting of methods that produce useful patterns or models from the data
データから有用なパターンやモデルを生成する手法からなるステップ

Maybe 70-90% of effort and cost in KDD 全体の70-90%の労力を要するステップ

1. Understand the domain and define problems
   領域を理解し問題を定義する
2. Collect and preprocess data
   データを収集し前処理する
3. Data mining
   Extract Patterns/Models
   パターン･モデルを抽出する
4. Interpret and evaluate discovered knowledge
   発見した知識を解釈し評価する
5. Putting the results in practical use
   結果を実践に用いる

KDD is inherently interactive and iterative
知識発見の本質は繰り返しとインタラクション

(In many cases, viewed KDD as data mining)

Data schemas vs. mining methods
データ·スキーマ vs. 学習手法

Types of data

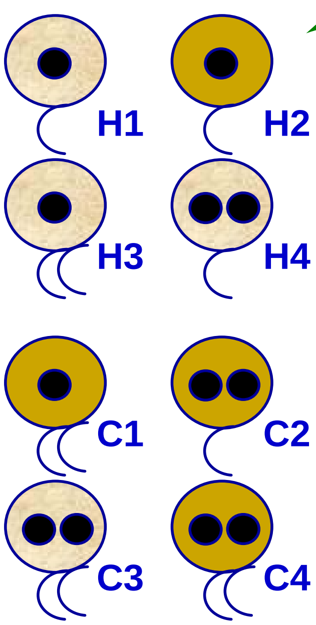
- Flat data tables 表形式データ
- Relational databases 関係DB
- Temporal & spatial data 時空間データ
- Transactional databases 取引データ
- Multimedia data マルチメディアデータ
- Genome databases ゲノムデータ
- Materials science data 材料データ
- Textual data テキストデータ
- Web data ウェブデータ
- etc.

Different data schemas

Mining tasks and methods
マイニングの課題と手法

- **Classification/Prediction 分類/予測**
  - ➔ Decision trees 決定木
  - ➔ Neural networks 神経回路網
  - ➔ Rule induction ルール帰納法
  - ➔ Support vector machines SVM
  - ➔ Hidden Markov Model 隠れマルコフ
  - ➔ etc.
- **Description 記述**
  - ➔ Association analysis 相関分析
  - ➔ Clustering クラスタリング
  - ➔ Summarization 要約
  - ➔ etc.

Dataset: cancerous and healthy cells
データ例：がん細胞と健康な細胞



Unsupervised data **Supervised data**

	color	#nuclei	#tails
H1	light	1	1
H2	dark	1	1
H3	light	1	2
H4	light	2	1
C1	dark	1	2
C2	dark	2	1
C3	light	2	2
C4	dark	2	2

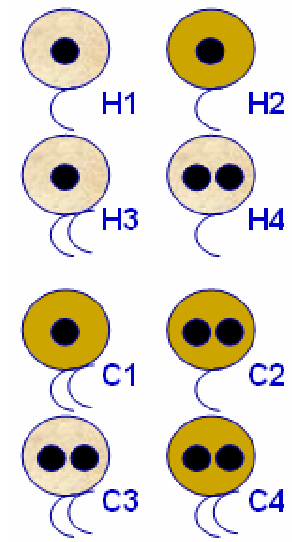
Primary tasks of data mining
データマイニングの第一の課題

- Predictive mining tasks perform inference on the current data in order to make prediction or classification.
（予測的マイニングの課題は，未知のデータの予測を目的として，現在のデータに関する推論を行うことである）

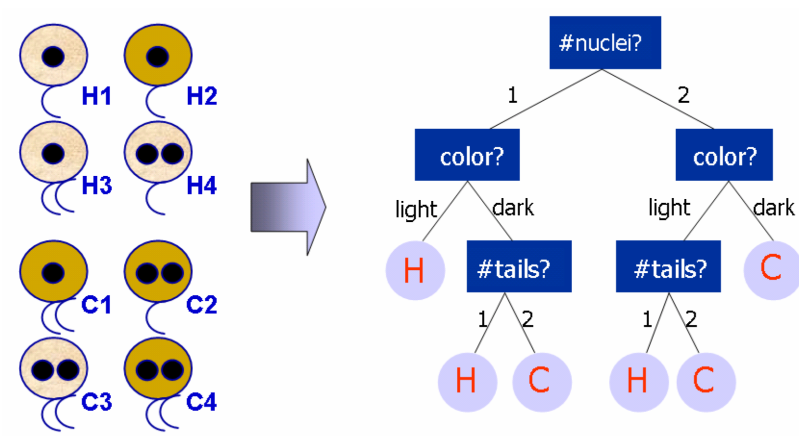
  Ex. IF “color = dark” and “#nuclei =2”
  THEN cancerous

- Descriptive mining tasks characterize the properties of the data in the database.
（記述的マイニングの課題は，データベース中のデータの全般的特性を特徴付ける記述を与えることである）

  Ex. “Healthy cells usually have one nuclei while cancerous ones have two”



Mining with decision trees
決定木によるマイニング



- Generalize classification models in form of trees.
木構造の一般的な分類モデル
- Well known methods and systems:
著名な手法とシステム:

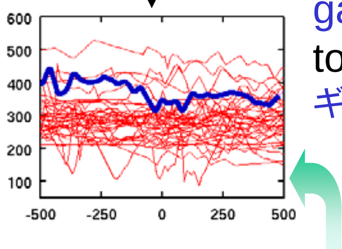
  CART (Breiman et al.), C4.5, See5 (Quinlan)

Some problems: 問題点

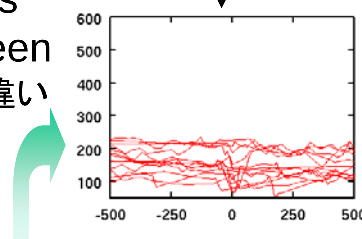
- Learning decision trees from huge datasets (data access)
大規模データからの学習
- Learning decision trees from complexly structured data
複雑に構造化されたデータからの学習の場合は？
- Decision tree ensembles: random forests (Breiman, 2001)
組合わせによる決定木：ランダム· フォレストなど

Decision trees with complex split tests
複合分割テストによる決定木

Study of liver cirrhosis (LC) in active data mining
アクティブマイニングでの肝硬変の研究



gap: difference of dissimilarities to the standard example between
ギャップ:標準事例との差異に関する違い

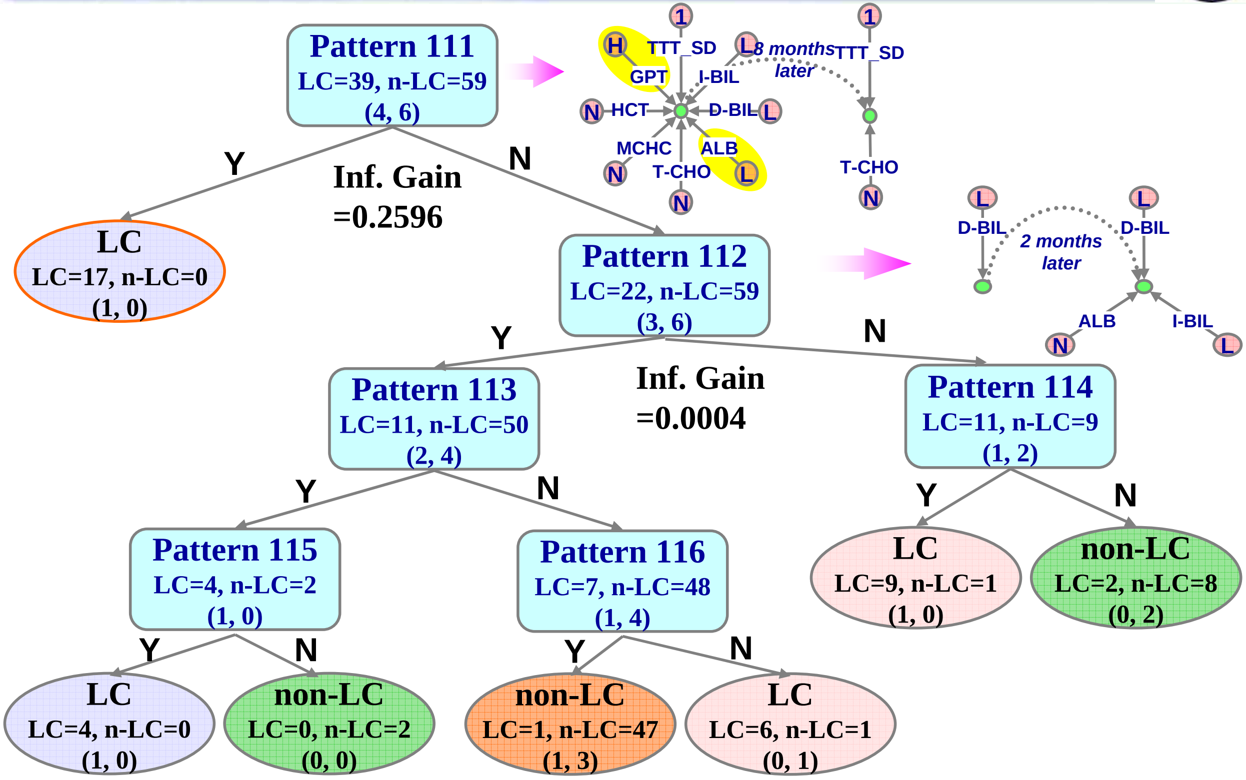


the most dissimilar red curve to the blue curve
青い線ともっとも違う赤い線

the most similar red curve to the blue curve
青い線に最も近い赤い線

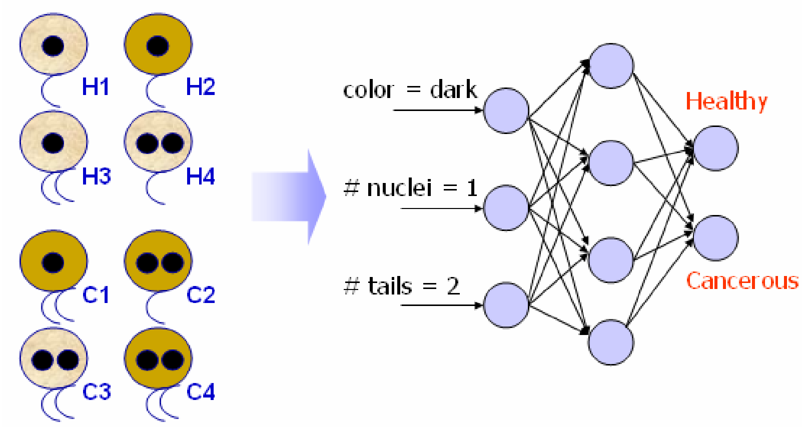
(Suzuki group, Yokohama Nat. Univ. Accuracy 88.2%)

Decision trees with complex split tests
複合分割テストによる決定木



Motoda's group, Osaka Univ., Prediction accuracy: 87.5% by 10-CV

Mining with neural networks
神経回路網によるマイニング

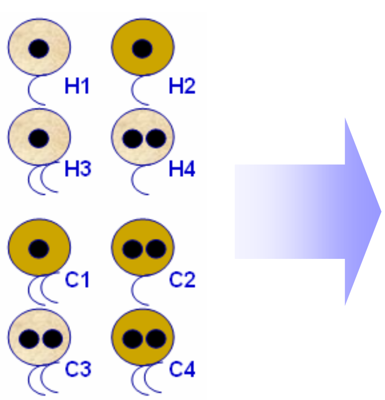


- Multi layer neural networks
  多層神経回路網
- Well known methods: 著名手法 backpropagation, SOM, etc.

Some problems: 課題

- Difficult to understand the learned function (weights)
  学習結果の関数(重み)を理解することが困難
- Not easy to incorporate domain knowledge
  背景知識との組合わせは容易ではない

Mining associations
相関ルールによるマイニング



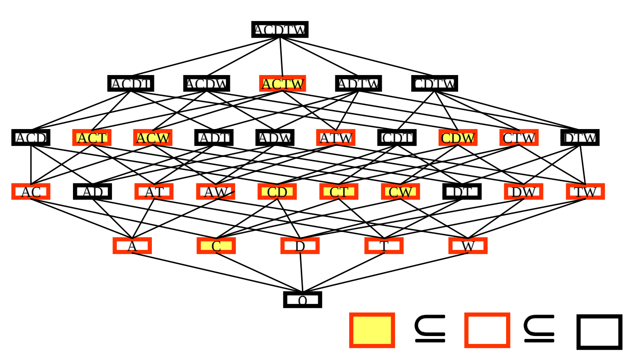
Number of nuclei = 1
→
Healthy cells

(support = 37.5%, confidence = 75%)

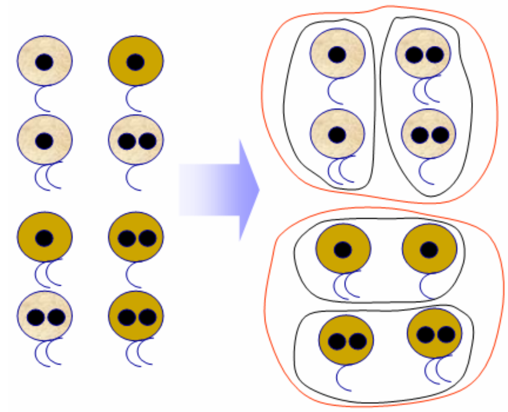
- Associations among itemsets
  アイテム集合間の相関
- Apriori algorithm (Agrawal, 1983). Variants: PF-growth, closed-frequent itemsets, multi level association rules, etc.

Some problems: 課題

- Database scan reduction: partitioning, hashing, sampling, find non-redundant rules
  データベース走査の低減：分割、ハッシュ、サンプリング、非冗長ルール
- New measures of association (Interestingness and exceptional rules)
  相関に関する新指標



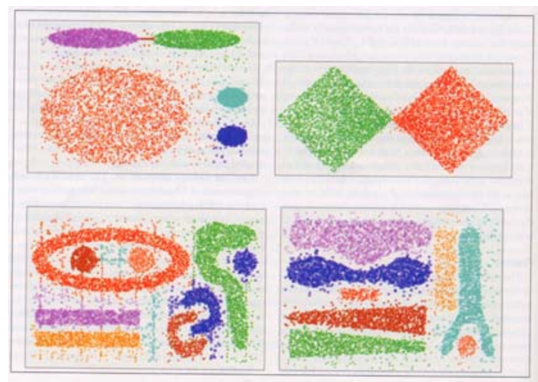
Mining clusters
クラスタリングによるマイニング



- Partitioning clustering　非階層型
- Hierarchical clustering　階層型
- Model-based clustering　モデルベース
- Density-based clustering　密度ベース
- Grid-based clustering　グリッドベース

Some problems: 課題

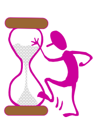
- Find clusters with arbitrary shapes
  任意の形のクラスタを見つける
- Finding clusters from complex and huge datasets (e.g., Web communities)
  複雑で巨大なデータからクラスタを見つける



Challenges in data mining
データマイニングにおけるチャレンジ

Large data sets (10^6-10^{12} bytes) and high dimensionality (10^2-10^3 attributes)　規模と次元数
[Problems: efficiency, scalability?]　効率、スケーラビリティ

Different types of data in different forms (mixed numeric, symbolic, text, image, voice,...)
データの形式やタイプ
[Problems: quality, effectiveness?]　質、効果



Data and knowledge are changing
変化し続けるデータや知識

Human-computer interaction and visualization
人間ーコンピュータのインタラクションと視覚化

Numerical vs. symbolic data
数値データと絞るデータ

Combinatorial search in hypothesis spaces (machine learning)
仮説空間における組合わせ探索

Attribute	Numerical	Symbolic	
No structure ＝ ≠		Places, Color	Nominal (categorical)
Ordinal structure ＝≠≧	Age, Temperature, Taste,	Rank, Resemblance	Ordinal
Ring structure ＝≠≧＋×	Income, Length		Measurable

Often matrix-based computation (multivariate data analysis)
通常は行列ベースの計算（多変量データ解析）

Text mining　　テキストマイニング

Text Mining = Data Mining (applied to textual data)
+ Language Engineering

テキストマイニング ＝ データマイニング (テキストへの応用) ＋ 言語工学

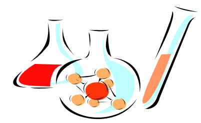
Areas related to text mining: 関連分野

- Computational linguistics (NLP) 計算言語学
- Information extraction 情報抽出
- Information retrieval 情報検索
- Web mining ウェブマイニング
- Regular data mining 通常のデータマイニング

A typical example of text mining
テキストマイニングの典型例

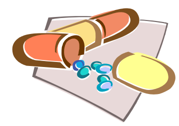
生物医学文献タイトルからの科学的根拠の抽出
(Swanson & Smalheiser, 1997)

- ✓ “stress is associated with migraines” “ストレスは片頭痛を伴う”
- ✓ “stress can lead to loss of magnesium”
  “ストレスはマグネシウム損失の原因となる”
- ✓ “calcium channel blockers prevent some migraines”
  “カルシウム拮抗薬は片頭痛を予防することがある”
- ✓ “magnesium is a natural calcium channel blocker”
  “マグネシウムは天然のカルシウム拮抗薬である”



抜粋した文の断片を人間の医学専門知識を使って組合せ，文献にない新しい仮説を導き出す

- ✓ Magnesium deficiency may play a role in some kinds of migraine headache
  マグネシウムはある種の片頭痛に関与するらしい

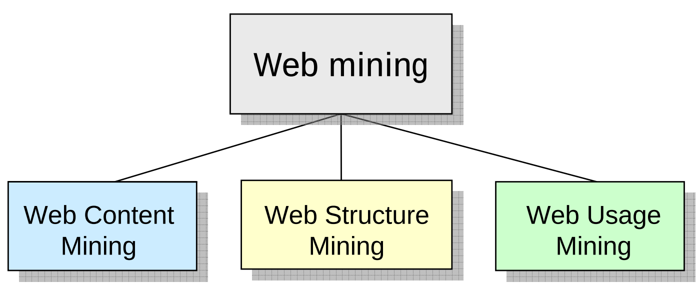


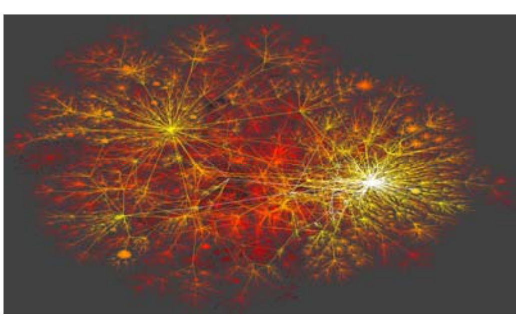
Web mining　　ウェブマイニング

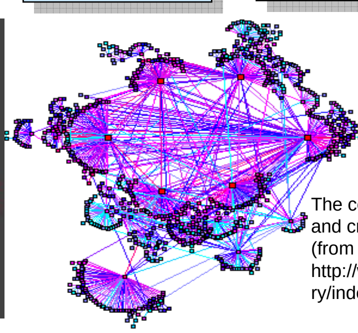
Web Mining = Data Mining (applied to Web documents and services) + Web technology

ウェブマイニング ＝ データマイニング(ウェブ文書やサービスへの応用) ＋ ウェブ工学

Areas related to Web mining:
- Information extraction
- Information retrieval
- Text mining
- Regular data mining







The contemporary robots travel on the Web and create maps like this.
(from http://www.caida.org/projects/internetatlas/gallery/index.xml)

Bioinformatics　バイオインフォマティクス

Bioinformatics = Data Mining + Machine Learning + Biological Databases

バイオインフォマティクス ＝ データマイニング ＋ 機械学習 ＋ 生物学データ

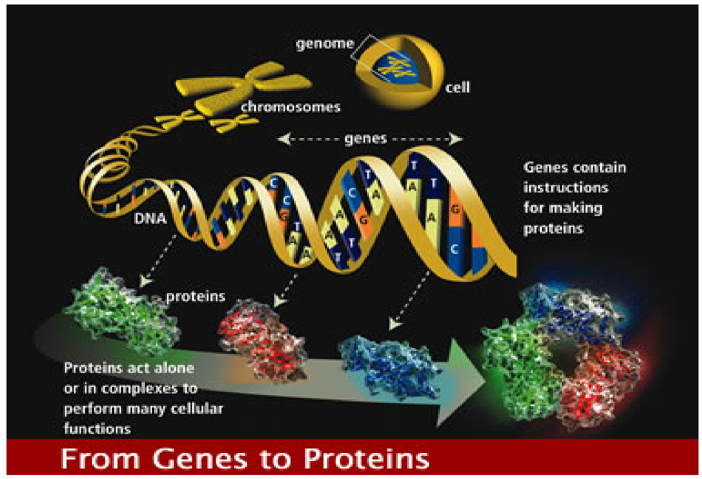
Sequence analysis
- Sequence alignment
- DNA sequence analysis
- Statistical sequence matching

Genomics
- Gene finding & prediction
- Functional genomics
- Structural genomics

Proteomics
- Functional proteomics
- Structural proteomics
- Structure, function relationship

Other problems
- Gene expression analysis
- Pathway analysis
- Protein-protein interaction

DNA → RNA → protein
Sequence → Structure → Function
Interaction → Network → Function



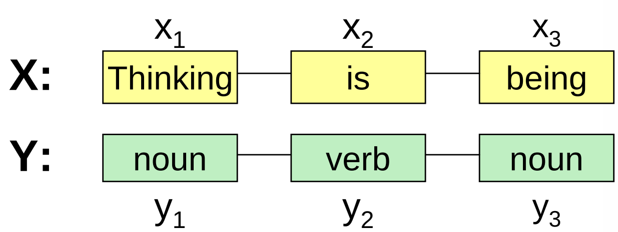
The talk aims to ...

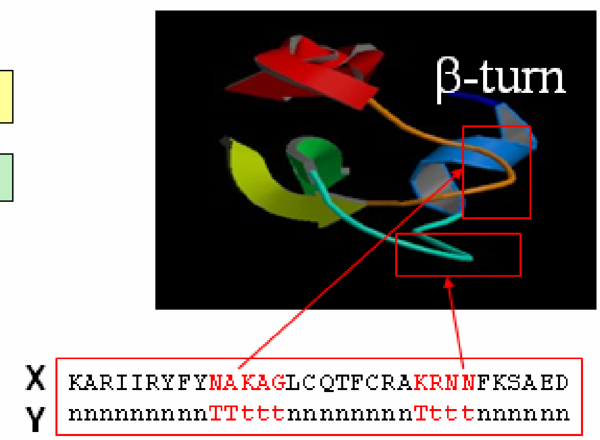
➔ Introduce to basic concepts and techniques of data mining (DM).
データマイニング（ＤＭ）の基本概念と技法を紹介する.

➔ Present some challenging data mining problems, and kernel methods as an emerging trend in this field.
データマイニングのチャレンジ課題およびこの分野で興隆しつつあるカーネル手法について説明する.

A typical problem: Labeling sequence data
配列データのラベル付け

- **X** is a random variable over data sequences　Xはデータ系列の確率変数
- **Y** is a random variable over label sequences whose labels are assumed to range over a finite label alphabet A
  Yはラベル系列の確率変数で有限のラベルアルファベット群Aにあると仮定
- *Problem*: Learn how to give labels from a closed set **Y** to a data sequence **X**　課題：閉集合Yからデータ系列Xへのラベル付け学習

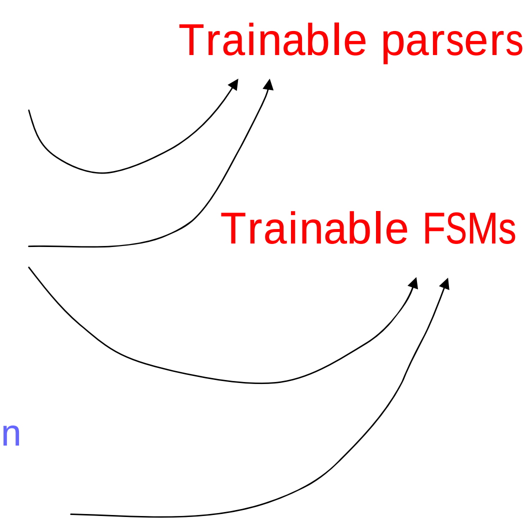




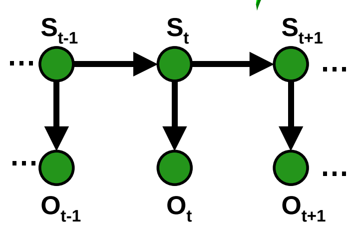
- POS tagging, phrase types, etc. (NLP),
- Named entity recognition (IE)
- Modeling protein sequences (CB)
- Image segmentation, object recognition (PR)
- etc.

Archeology of natural language processing (NLP)
自然言語処理の考古学

- 1990s–2000s: Statistical learning
  統計的学習
  - → algorithms, evaluation, corpora
- 1980s: Standard resources and tasks
  標準リソースとタスク
  - → Penn Treebank, WordNet, MUC
- 1970s: Kernel (vector) spaces
  カーネル（ベクトル）空間
  - → clustering, information retrieval (IR)
- 1960s: Representation transformation
  表現形式の変換
  - → Finite state machines (FSM)
    and Augmented transition networks (ATNs)
- 1960s: Representation—beyond the word level
  一語単位を超える表現へ
  - → lexical features, tree structures, networks



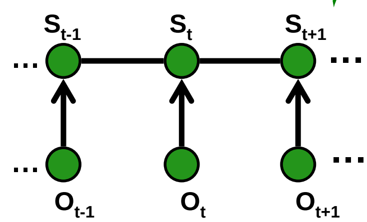
Trainable finite state machines



Hidden Markov Models (HMMs)

[Baum et al., 1970]

- Generative
- Need independence assumption
- Local optimum
- Local normalization

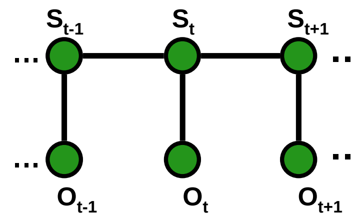


Maximum Entropy Markov Models (MEMMs)

[McCallum et al., 2000]

- Discriminative
- No independence assumption
- Global optimum
- Local normalization

More accurate then HMMs



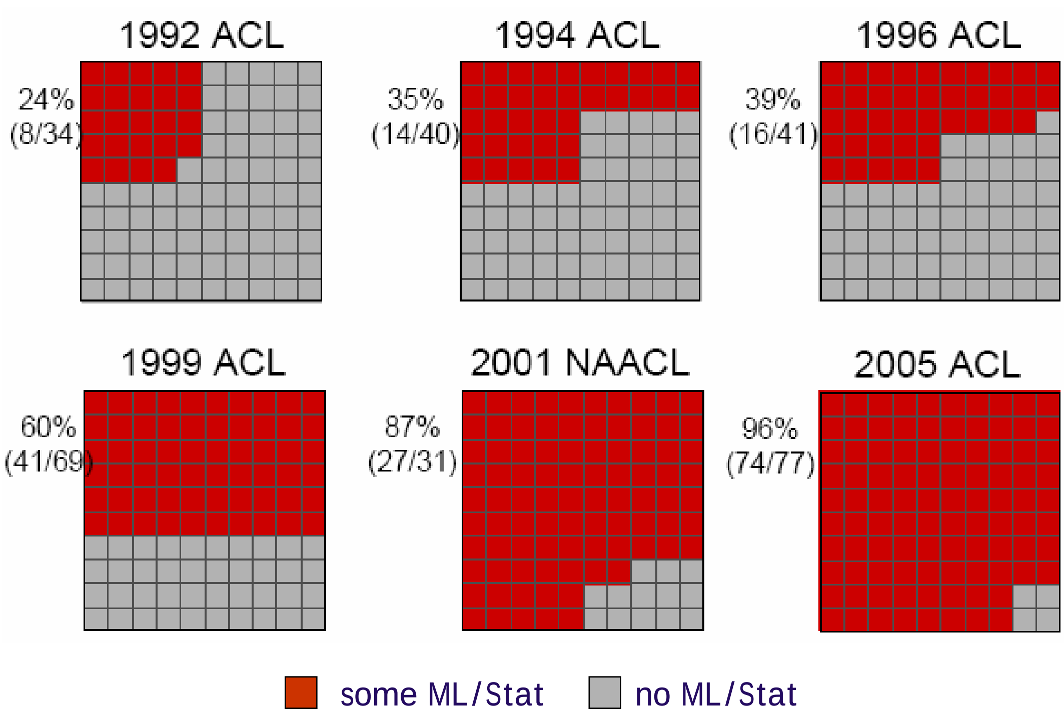
Conditional Random Fields (CRFs)

[Lafferty et al., 2001]

- Discriminative
- No independence assumption
- Global optimum
- Global normalization

More accurate then MEMMs

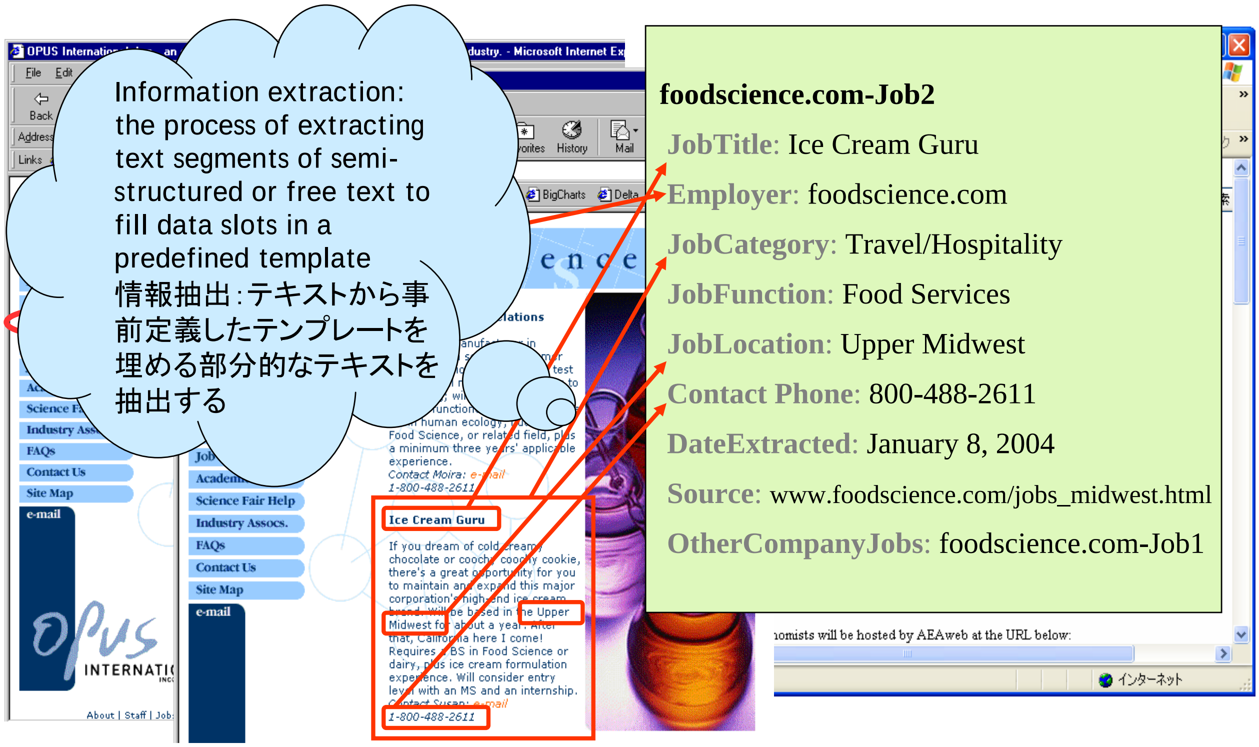
Machine learning and statistics in NLP
NLPにおける機械学習と統計学



(Marie Claire, ECML/PKDD 2005)

Finding “things” but not “pages”

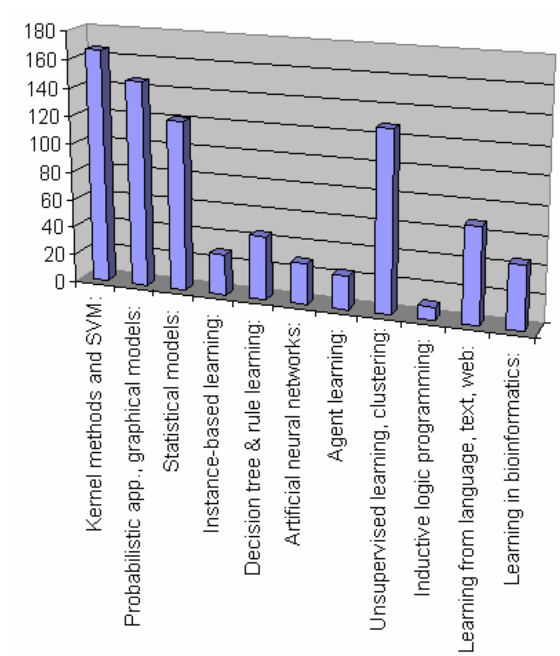
情報抽出(Information Extraction) vs. 情報検索(Information Retrieval)



Kernel methods and support vector machines

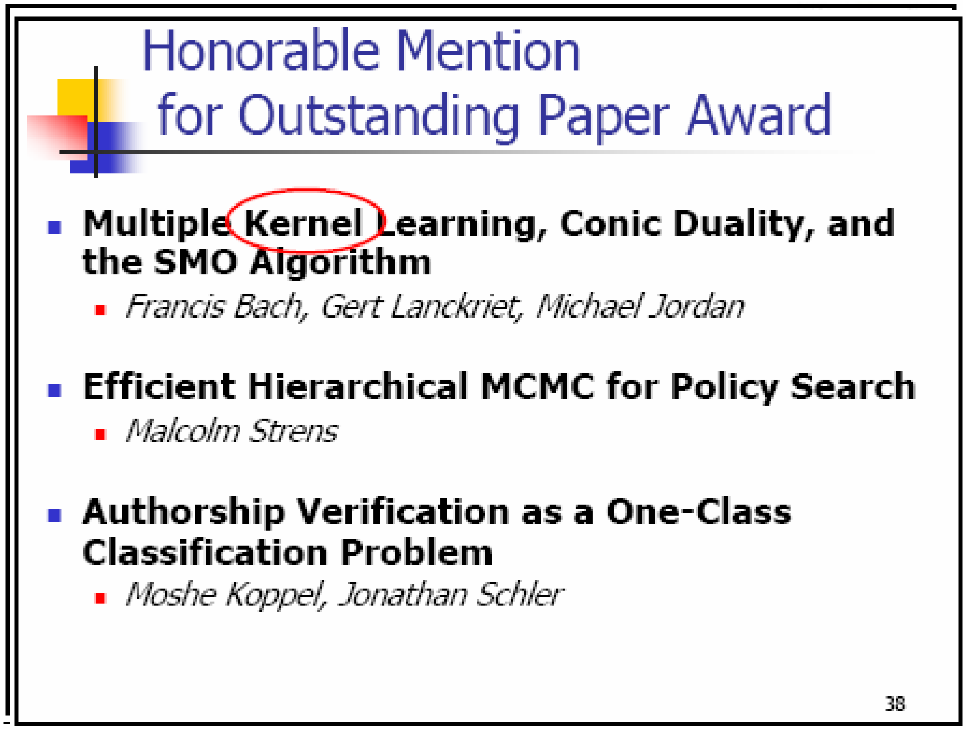
カーネル手法とサポートベクトルマシン

Kernel methods & SVM	**166**
Probabilistic, graphical models	146
Unsupervised learning, clustering	128
Statistical models	121
Language, Text & web	68
Learning in bioinformatics	45
ANN	29
ILP	9
CRF	13



ICML 2006 (720 abstracts)

Observed from ICML 2004

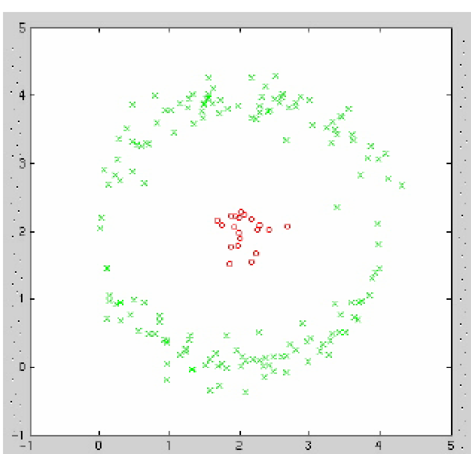


(Russ Greiner, ICML'04 PC co-chair)

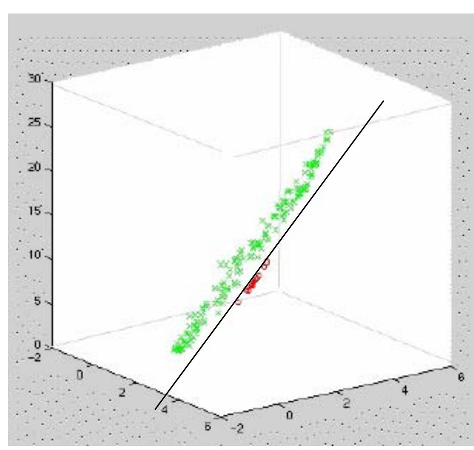
Kernel methods: the basic idea
カーネル手法：基本的な考え方

Converting data into another high dimensional space can make data become linear separable

データを高次元空間に変換することで、線形分離を可能にする



$\phi : \mathcal{X} = \Re^2 \rightarrow \mathcal{H} = \Re^3$

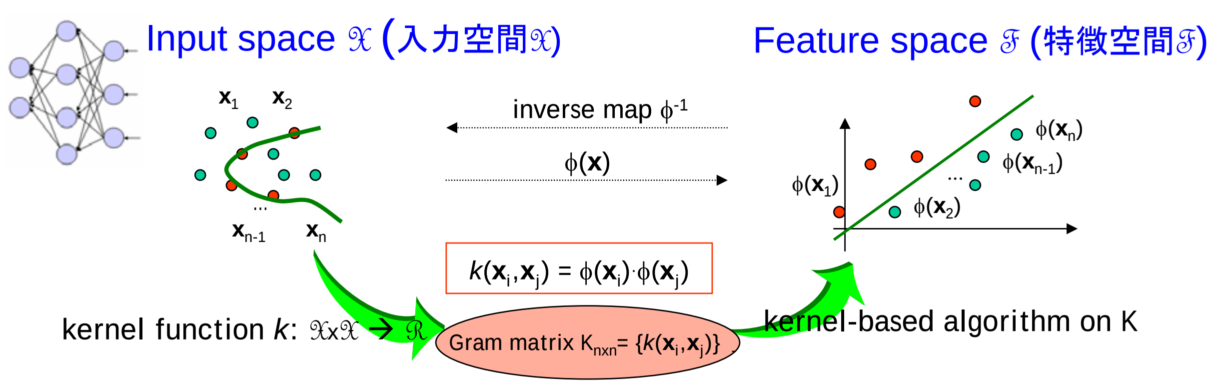


$(x_1, x_2) \mapsto (x_1, x_2, x_1^2 + x_2^2)$

Kernel methods: a bit of history
カーネル手法：歴史を少し

- Linear learning machines (perceptrons, 1956) has one big problem of insufficient capacity. Minsky and Pappert (1969) highlighted the weakness of perceptrons.
  線形機械学習(パーセプトロン)にはミンスキー等に指摘される弱点があった
- Neural networks (since 1980s) overcame the problem by glueing together many thresholded linear units (multi-layer neural networds: solved problem of capacity but ran into training problems of speed and multiple local minima).
  神経回路網(1980年代以降)は閾値を持つ多くの線形ユニットの組合 せ(多層神経回路網)で弱点を克服したが実行速度と局所解が課題
- The kernel methods approach (since 2000s) is to stick with linear functions but work in a *high dimensional feature space.*
  カーネル手法によるアプローチ(2000年以降）は線形関数を維持しつつ高次元の特徴空間に対応

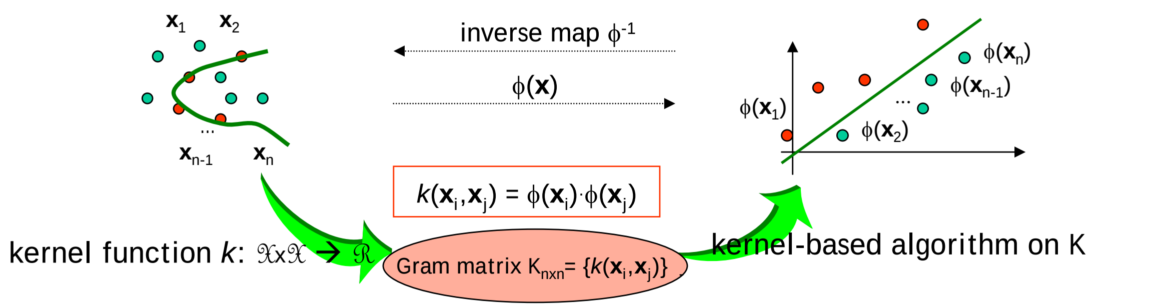
Kernel methods: the scheme
カーネル手法：スキーマ



- Map the data from 𝔛 into a (high-dimensional) vector space, the feature space 𝔉, by applying the feature map ϕ on the data points **x**.
- Find a linear (or other easy) pattern in 𝔉 using a well-known algorithm (that works on the Gram matrix).
- By applying the inverse map, the linear pattern in 𝔉 can be found to correspond to a complex pattern in 𝔛.
- This implicitly by only making use of inner products in 𝔉 (kernel trick)

Kernel methods: math background

Input space $\mathcal{X}$ (入力空間$\mathcal{X}$)　　Feature space $\mathcal{F}$ (特徴空間$\mathcal{F}$)



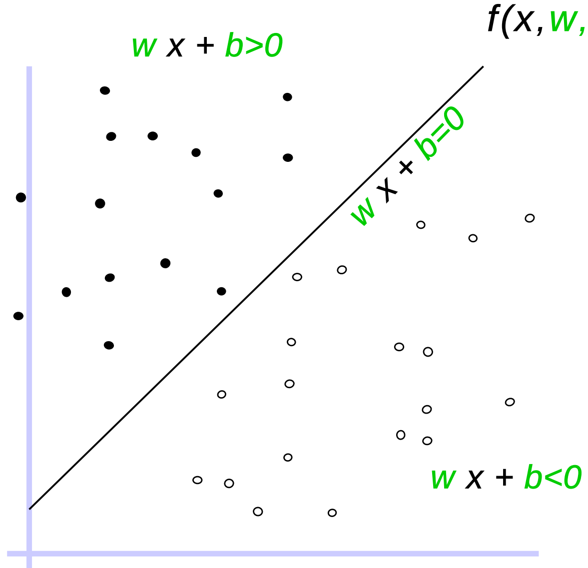
Linear algebra, probability/statistics, functional analysis, optimization

- **Mercer theorem**: Any positive definite function can be written as an inner product in some feature space.
- **Kernel trick**: Using kernel matrix instead of inner product in the feature space.
- **Representer theorem**: Every minimizer of $\min_{f\in\mathcal{H}}\{C(f,\{x_i,y_i\})+\Omega(\|f\|_H)\}$ admits a representation of the form $f(.)=\sum_{i=1}^{m}\alpha_i K(.,x_i)$

Support vector machines: key ideas

- • denotes +1
- ◦ denotes -1

$f(x,w,b) = sign(w\ x + b)$



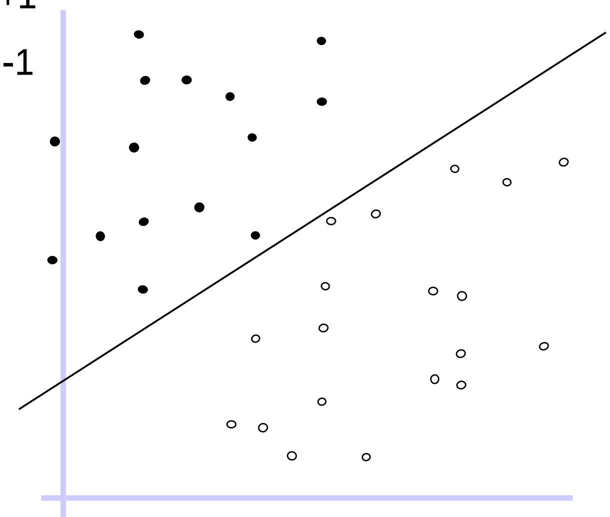
How would you classify this data?

(Pages 46-52 from Andrew Moore's SVM tutorial)

Support vector machines: key ideas

$f(x,w,b) = sign(w\ x + b)$

- denotes +1
- ◦ denotes -1



How would you classify this data?

Support vector machines: key ideas

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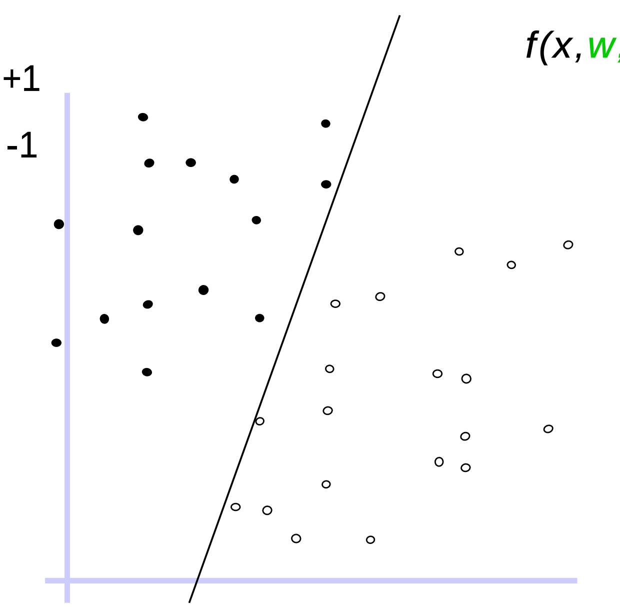
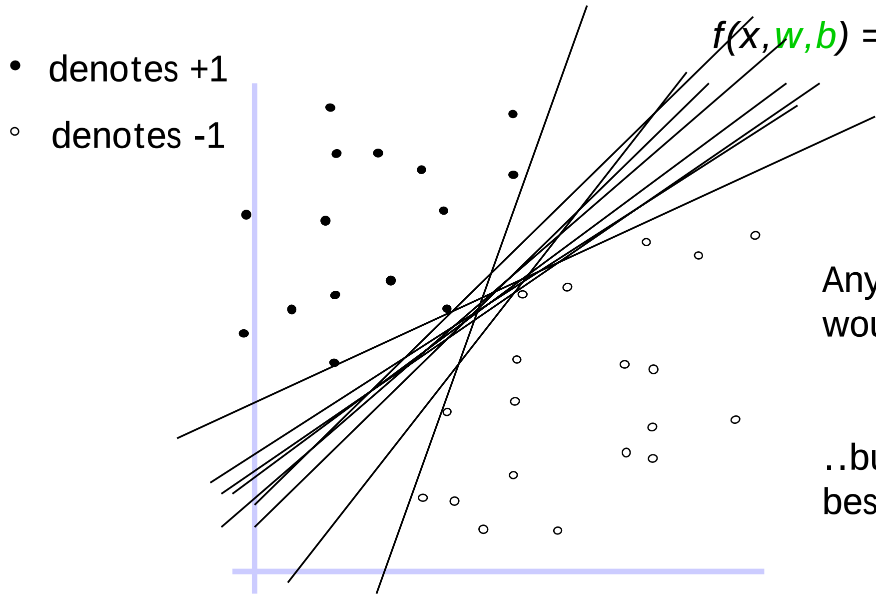


How would you classify this data?

Support vector machines: key ideas

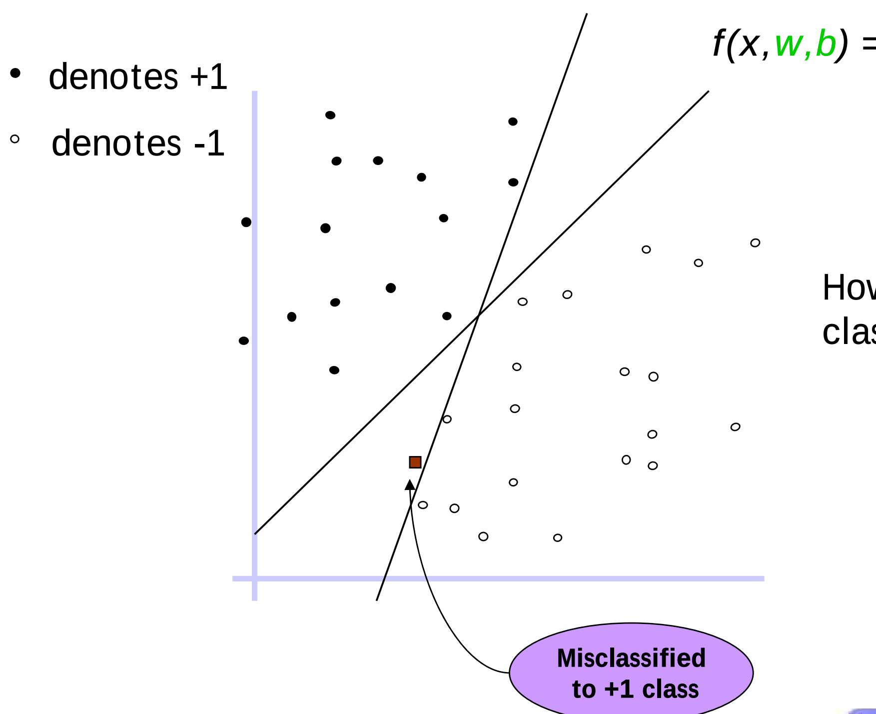


$f(x,w,b) = sign(w\ x + b)$

Any of these would be fine..

..but which is best?

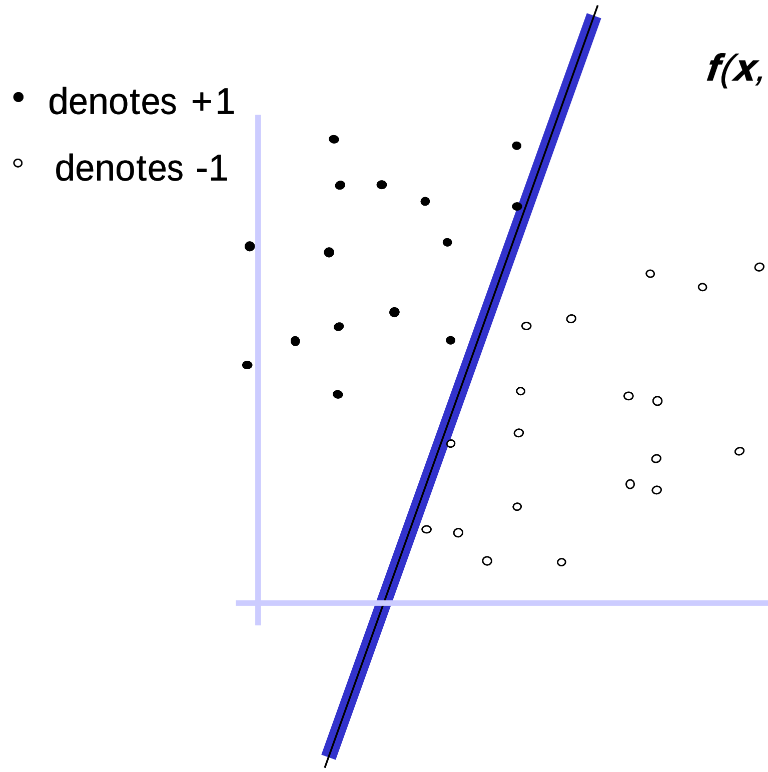
Support vector machines: key ideas



$f(x,w,b) = sign(w\ x + b)$

How would you classify this data?

Classifier margin

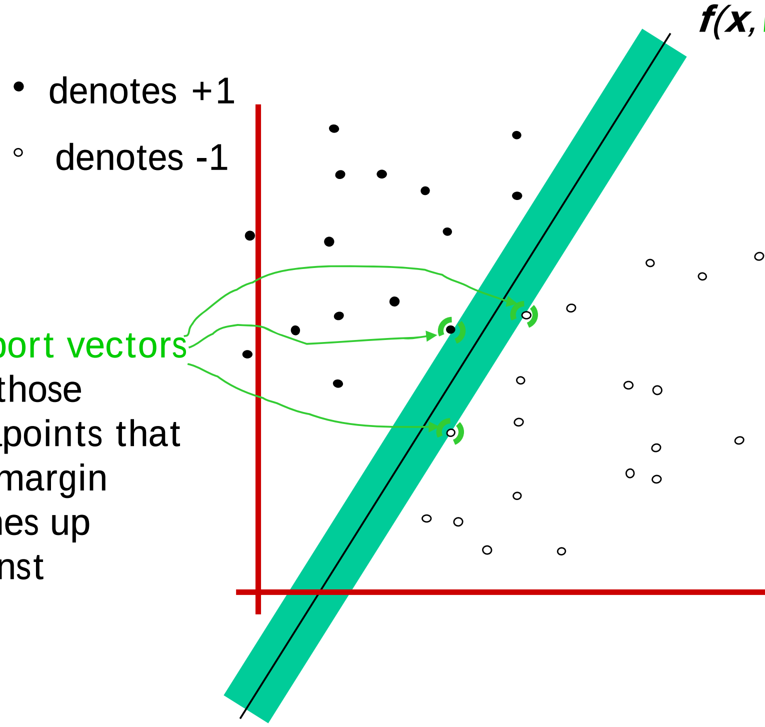


f(x,w,b) = sign(w x + b)

Define the margin of a linear classifier as the width that the boundary could be increased by before hitting a datapoint.

Maximum margin

f(x,w,b) = sign(w x + b)



Support vectors are those datapoints that the margin pushes up against

The maximum margin linear classifier is the linear classifier with the maximum margin

(maximum margin is equivalent to minimum $1/\|\mathbf{w}\|$)

Support vector machines

Soft margin problem

$$\min_{\mathbf{w},b,\xi_1,\ldots,\xi_n} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{n}\xi_i$$

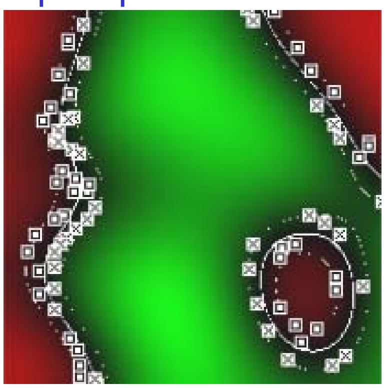
$$\forall i, \begin{cases} \xi_i \geq 0 \\ \xi_i - 1 + y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 0 \end{cases}$$

Equivalent to dual problem

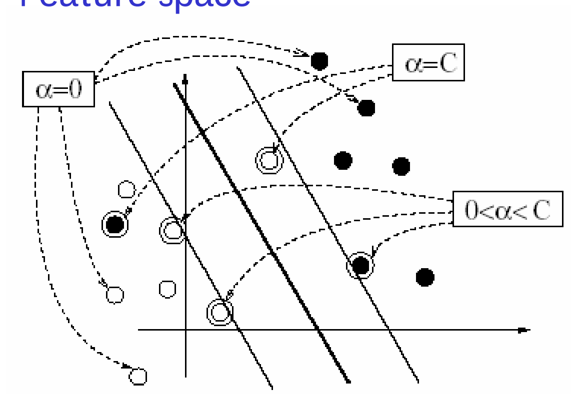
$$W(\boldsymbol{\alpha}) = -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j \mathbf{x}_i^T \mathbf{x}_j + \sum_{i=1}^{n}\alpha_i$$

$$\begin{cases} \sum_{i=1}^{n} y_i \alpha_i = 0 \\ 0 \leq \alpha_i \leq C \quad \text{for } i = 1,\ldots,n \end{cases}$$

Input space



Feature space



Some of our recent results

- Improving prediction performance of CRFs (KDD'05, ACM Trans. ALIP'06)
- High-performance training of CRFs for large-scale applications (HPCS'06)
- Sentence reduction (in text summarization) by SVM (COLING'04)
- Model for emerging trend detection (PAKDD'06, KSSJ)
- Prediction and analysis of β-turns in protein structures (GIW'03, JBCB'05) and histone modifications by SVM (GIW'05) and CRFs (ICMLB'06)
- Simplifying support vector machines (ICML'05, IEEE Trans. Neural Network)
- Manifolds in imbalanced data learning (IEEE ICDM'06)
- Kernel matrix evaluation measure (IJCAI'07, sumitted)

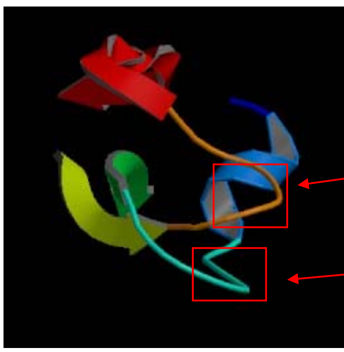
Prediction of β-turns and γ-turns by SVM
(GIW'03, JBCB'05)

Protein sequence

RPDFCLEPPYTGPCKARIIRYFYNAKAGL
CQTFVYGGCRAKRNNFKSAEDCMRTCGGA

Predict by SVM

β-turns

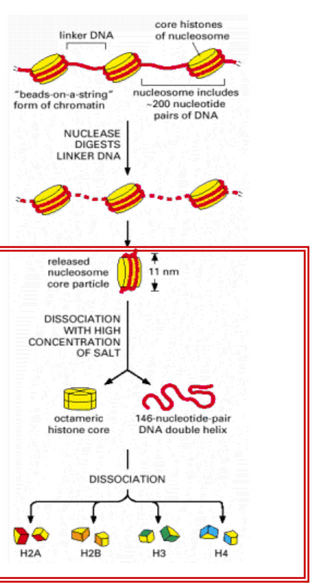


RPDFCLEPPYTGPCKARIIRYFYNAKAGL
nnnnnnnnnnnnnnnnnnnnnnnTTtttn

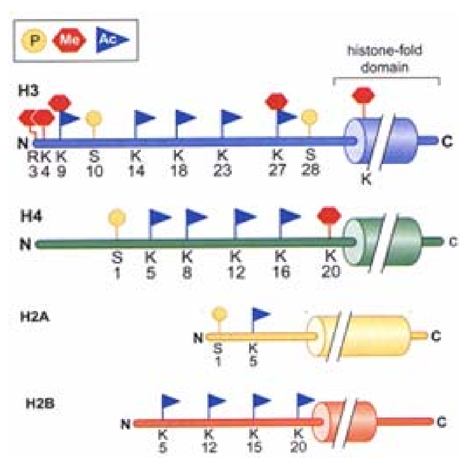
CQTFVYGGCRAKRNNFKSAEDCMRTCGGA
nnnnnnnnnnnTtttnnnnnnnnnnnnnn

Prediction of histone modifications in DNA
(GIW'05, BioMed Central 2006)

Histone modifications: Some amino acids of histone proteins (H3, H4, H2A, H2B) in nucleosomes are modified by added methyl group (methylation), acetyl group (acetylation), or other chemical groups.



146 pairs of DNA in nucleosomes are wrapped around a core of histone proteins.



Prediction of histone modifications in DNA
(GIW'05, BioMed Central 2006)

From DNA sequences

CACTACGGGCCTGTGTACATTCTGCGCGACATTCACCCAGTGTGCAGTGTGAGAGGTACAGGTGGCGCATGTGGTGTGCGCCACACACGTTGGCACC

To **computationally** predict:
- H3, H4 occupancy
- Acetylation state
- Methylation state

To find characteristics of areas at which H3, H4 occupancy, histone acetylation and methylation are at high and low levels.

The accuracy and correlation coefficient of qualitative prediction are consistent with experimental approach.

SVMs simplification
(ICML'05, IEEE Trans. Neural Networks 2006)

To replace original machine

$$y = sign\left(\sum_{i=1}^{Ns} \alpha_i K(x_i, x) + b\right)$$

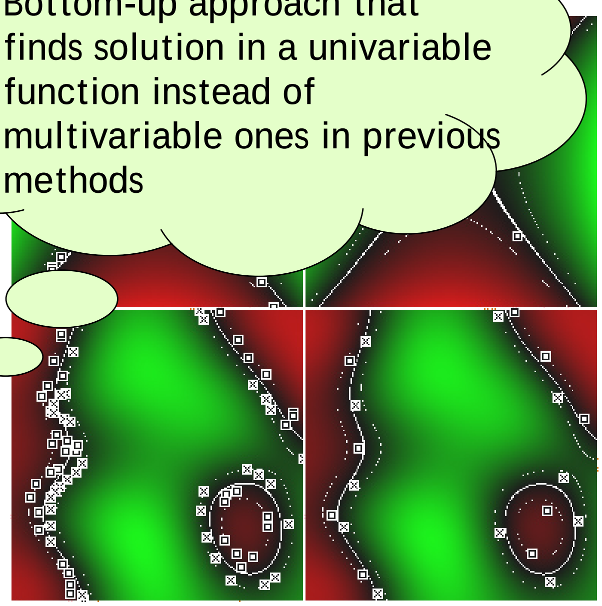
by a simplified machine

$$y' = sign\left(\sum_{j=1}^{Nz} \beta_j K(z_j, x) + b\right) \quad (2)$$

with $N_Z < N_S$
(1) and (2) are similar

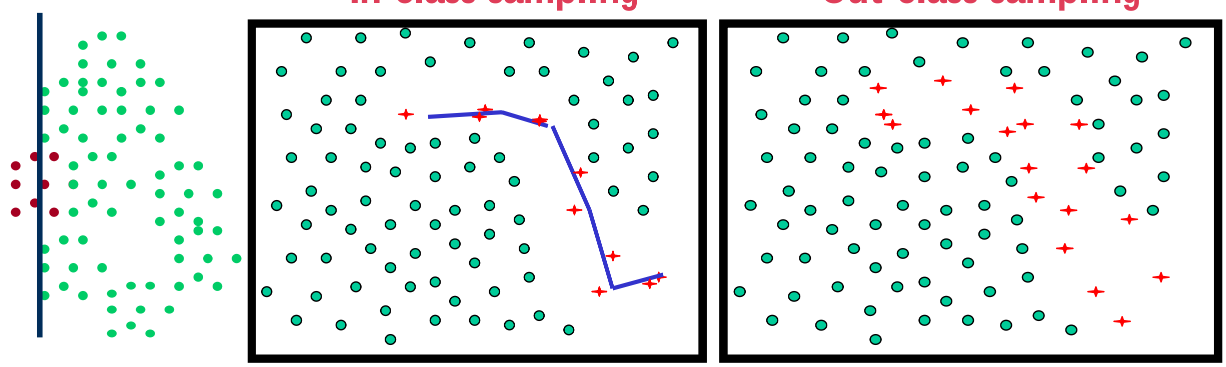
$\{(z_i, \beta_j)\}_{j=1,\ldots,Nz}$ – reduced vectors

Bottom-up approach that finds solution in a univariable function instead of multivariable ones in previous methods



Manifold for imbalanced data learning
(IEEE ICDM'06)

- Flexible assumption: Data having manifold structures.
- Up sampling data to make it exhibit manifold structures → give rise to patterns of interest.
- Our algorithms outperform SVMs and SMOTE (Chawla et al, JAIR'02).



Kernel matrix evaluation
(IJCAI 2007)

- Popular efficient measure of kernel matrix KTA (Kernel Target Alignment, Cristianini 2002) has fundamental limitations
- A sufficient but not necessary condition.
- Proposed the new measure FSM (Feature Space-based Kernel Matrix Evaluation Measure) using the data distribution in the feature space that is efficient, having desirable properties.
- Implication of FSM is vast.

Comparing directly matrices in the input spaces (入力空間$\mathcal{X}$)

$$KTA(K,y) = \frac{\langle K, y.y^T \rangle_F}{\sqrt{\langle K,K \rangle_F \langle y.y^T, y.y^T \rangle_F}}$$

Comparing data images distributions in the feature space (特徴空間$\mathfrak{F}$)

$$FSM(K,y) = \frac{var_+ + var_-}{\|\phi_- - \phi_+\|}$$

Summary

- Data mining is a emerging interdisciplinary area with great interests from both research and industry.
  データマイニングは急激に発展している学際領域であり，研究としても産業としても大きな関心を集めている.

- Many challenges in data mining, especially in mining complexly structured data.
  マイニング，特に複雑に構造化されたデータのマイニングにおけるチャレンジ課題は多い.

- Kernel methods are a new emerging trend with mathematical foundations and high performance in solving hard problems of pattern analysis.
  カーネル手法は数学的基盤をもち，難しいパターン認識の問題を性能よく解決できる新しく進展しつつあるトレンドである.

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