Machine Learning in BioMedical Informatics

: Support Vector Machines & Semi-Supervised Learning

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Abstract: Machine Learning in BioMedical Informatics

The emergence of the fields of **bio-** and **medical- informatics** has alleviated the burden of solving the related biological or medical domain problems, saving the **time and cost** required for **wet-lab experiments** or **patient treatments**, and it also has provided **predictions** that guide the next experiments or treatments.

In **biomedical informatics**, **machine learning** has played a central role in dealing with the flood of data. The **goal of this talk** is to raise **awareness** and **comprehension** of **machine learning** so that the domain specialists can properly match the task at hand to the corresponding analytical approach.

Abstract: Machine Learning in BioMedical Informatics

We start by **categorizing** the types of the tasks with given data and introduce the **general machine learning schemes** that fit best to each of the categories. We then explore **representative models** from traditional statistical models to the most recent ones such as **support vector machines (SVM)** and **semi-supervised learning (SSL)**

To exemplify how biological or medical questions can benefit from **machine learning**, we present several **up-to-date research projects**: **protein functional class** prediction based on genome and proteome data, **breast cancer** survivability prediction based on clinical data of patients, and clinical outcome prediction of **brain- and ovarian cancer** based on genome to phenome data.

Outline

Preliminaries	Data & Tasks
Machine Learning	Machine Learning Fields of Machine Learning Machine Learning Models
Support Vector Machines (SVM)	Kernel Method Basic Idea of SVM
Semi-Supervised Learning (SSL)	Fundamentals Problem Setting Family of Algorithm Graph-based SSL
Case Examples (SVM vs. SSL)	[Intra-Relation] Single Data Source [Integration] Multiple Data Sources
Closing Remarks	Future Work

Data & Tasks

- **Prediction**
  - Classification
  - Regression
- **Description**
  - Clustering
  - Feature Description
  - Outlier Detection
- **Dimensionality Reduction**
  - Feature Selection
  - Feature Extraction
- **Data Reduction (Sample Selection)**
- **Data Integration**

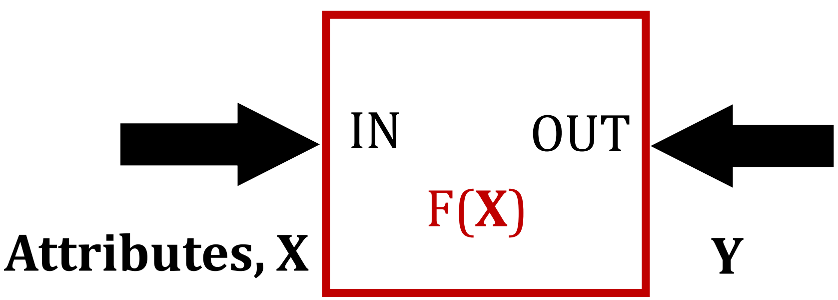
Machine Learning

Machine Learning : Algorithms or Techniques that allow computers to "learn" using "data"

1

"TRAINING"

Develop Model
With **Known Data**

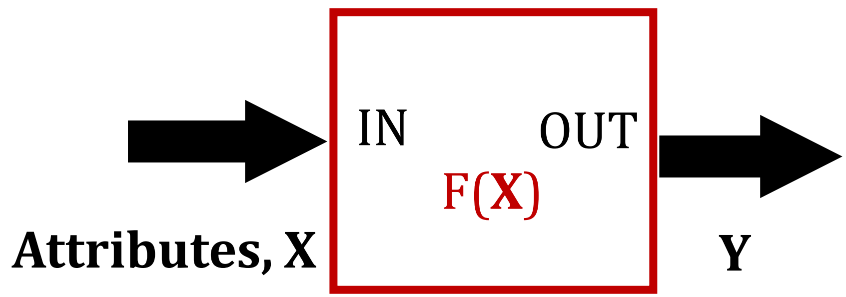


Determine F(X)

2

"TEST/EVALUATION"

Use Model
For **New Data**



Y = F(X)

The Fields of Machine Learning

The **field of machine learning** has traditionally been divided into **three sub-fields**:

Supervised Learning

Unsupervised Learning

Reinforcement Learning

The Fields of Machine Learning: Supervised Learning

The **field of machine learning** has traditionally been divided into **three sub-fields**:

Supervised Learning

The learning system observes a **labeled training set** consisting of **(attribute, label) pairs**, denoted by $\{(x_1, y_1), \ldots, (x_n, y_n)\}$.

The ***goal*** is to predict the **label y** for any new input with feature x.

A supervised learning task is called ***regression*** **when y ∈ R**, and ***classification*** when **y** takes a set of **discrete values**.

Unsupervised Learning

Reinforcement Learning

The Fields of Machine Learning: Unsupervised Learning

The **field of machine learning** has traditionally been divided into **three sub-fields**:

Supervised Learning

Unsupervised Learning

The learning system observes an **unlabeled set of items**, represented by their attributes $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$.

The ***goal*** is to **organize the items:** Typical unsupervised learning tasks includes ***clustering*** that groups items into clusters**;** ***outlier detection*** which determines if a new item **x** is significantly different from items seen so far; ***dimensionality reduction*** which maps **x** into a low dimensional space, while preserving certain properties of the dataset.

Reinforcement Learning

The Fields of Machine Learning: Reinforcement Learning

The **field of machine learning** has traditionally been divided into **three sub-fields**:

Supervised Learning

Unsupervised Learning

Reinforcement Learning

The learning system repeatedly **observes** the ***environment "x,"*** **performs** an ***action "a,"*** and **receives** a ***reward "r."***

The ***goal*** is to choose the actions that ***maximize the future rewards.***

SUPPORT VECTOR MACHINES (SVM)

SVM: Kernel Methods

Why KM?

- Kernel methods can operate on very **general types of data** and can detect very **general types of relations**

- Various tasks-- $\left\{\begin{array}{l}\textbf{PCA,}\\ \textbf{CCA,}\\ \textbf{FA,}\\ \textbf{DA,}\\ \textbf{Clustering}\end{array}\right\}$ can be performed on diverse data $\left\{\begin{array}{l}\textbf{vectors,}\\ \textbf{sequences,}\\ \textbf{text,}\\ \textbf{images,}\\ \textbf{graphs}\end{array}\right\}$

- **Integration of different types of data** is easy and natural

SVM: Wrap-up

$$\min_{0\le \alpha_i \le C} W(\alpha_i, b) = \frac{1}{2}\sum_{i,j=1}^{M} \alpha_i \alpha_j y_i y_j K(\vec{x}_i, \vec{x}_j) - \sum_{i=1}^{M} \alpha_i + b\sum_{i=1}^{M} y_i \alpha_i$$

KKT

$$\frac{\partial W(\alpha_i, b)}{\partial \alpha_i} = \sum_{j=1}^{M} y_i y_j K(\vec{x}_i, \vec{x}_j)\alpha_j + y_i b - 1 = y_i \bar{f}(x_j) - 1$$

$$\frac{\partial W(\alpha_i, b)}{\partial b} = \sum_{j=1}^{M} y_j \alpha_j = 0$$

where $\bar{f}(\vec{x}) = \sum_{\mathrm{i}=1}^{\mathrm{M}} y_{\mathrm{i}} \alpha_{\mathrm{i}} K(\vec{x}_{\mathrm{i}}, \vec{x}) + b$

Semi-Supervised Learning: Learning Schemes

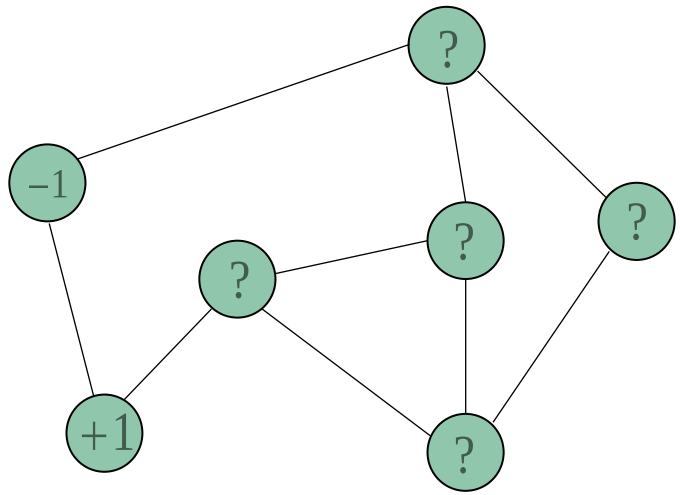
Supervised Learning

"Semi"-Supervised Learning

Unsupervised Learning

Reinforcement Learning

Graph-based SSL: WRAP-UP



Objective Function $$\min_{\boldsymbol{f}} \quad \mu\, \boldsymbol{f}^T L\, \boldsymbol{f} + (\boldsymbol{f}-\boldsymbol{y})^T(\boldsymbol{f}-\boldsymbol{y})$$

Solution $$\boldsymbol{f} = \{\, \boldsymbol{I} + \mu L \,\}^{-1} \boldsymbol{y}$$

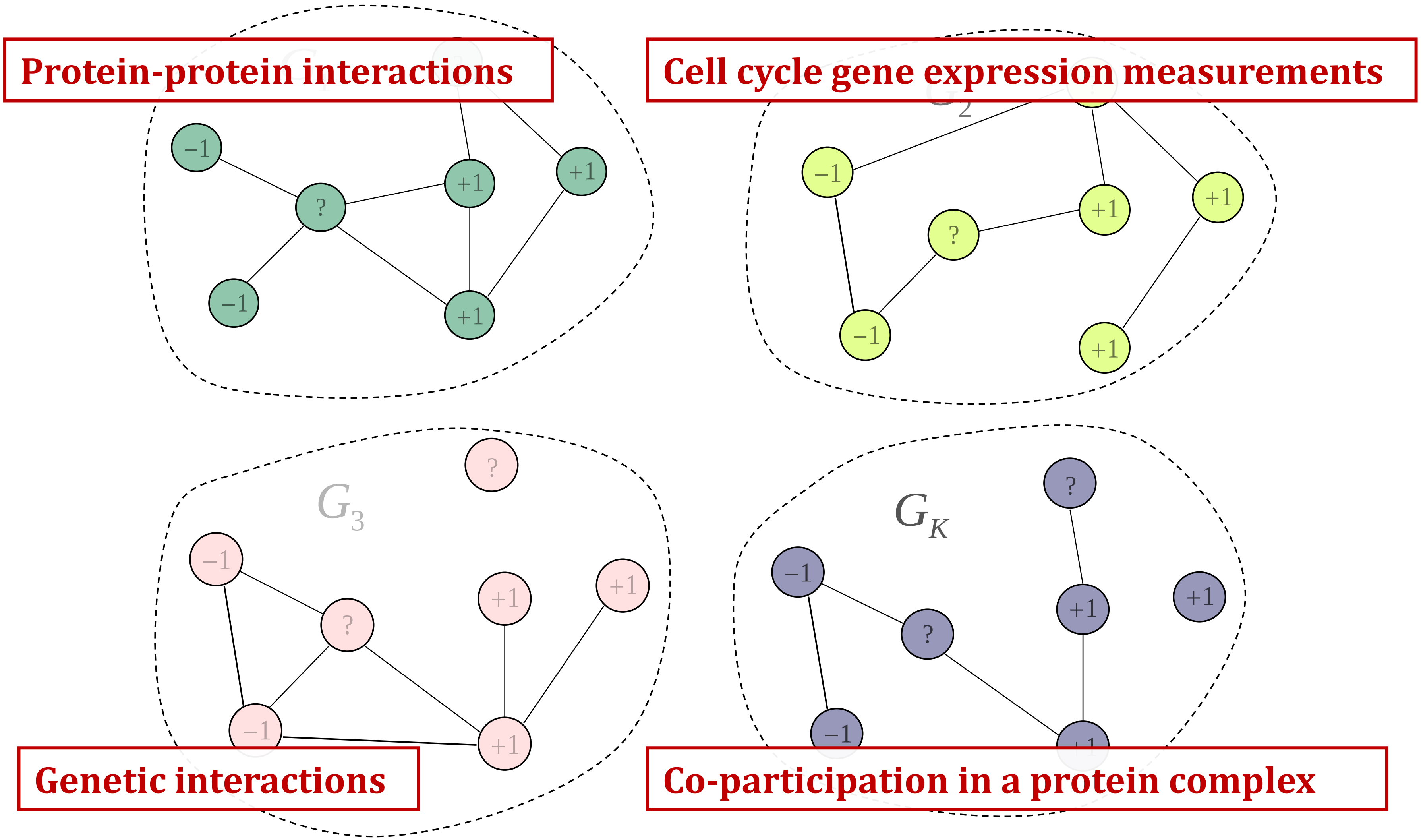
where $L = D - W,\ D = diag(d_i),\ \ d_i = \sum_j w_{ij}$

Abstract: Data Integration

Data Integration is concerned with the **integration of different or heterogeneous data sources** in order to **enhance the total information** about the problem at hand**.**

Each of data sources contains **partly independent** and **partly complementary** pieces of information about the problem**...**

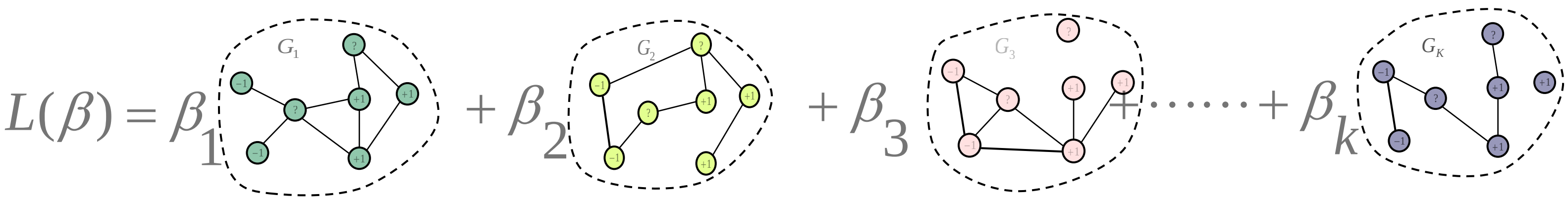
If Multiple Graphs are Given?



Graph Integration using SSL

Linear Combination of Laplacians

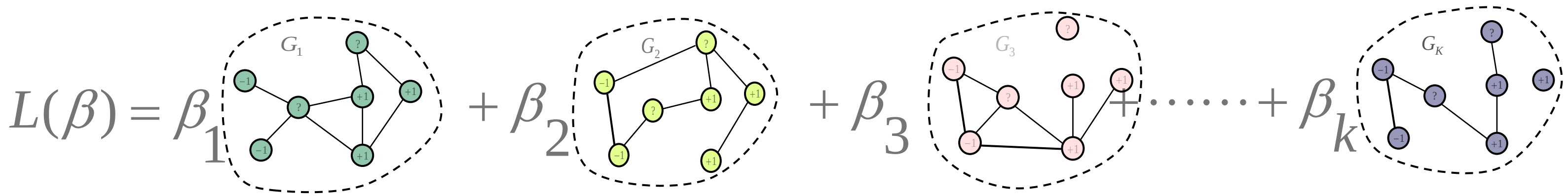
$$L(\beta) = \sum_{k=1}^{K} \beta_k L_k$$



How to Find Combining Weights ?

Graph Integration using SSL

Mutiple Graph (Data) Integration



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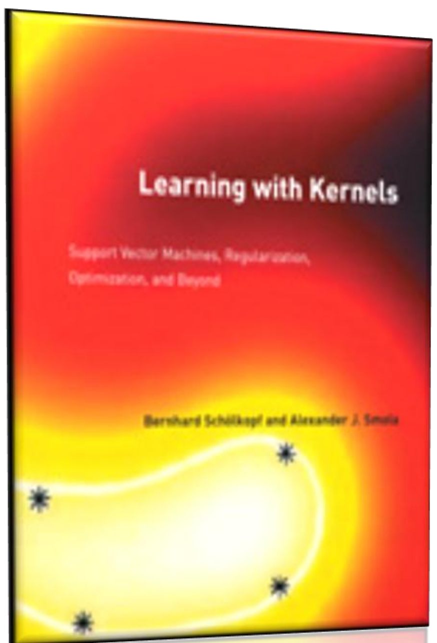

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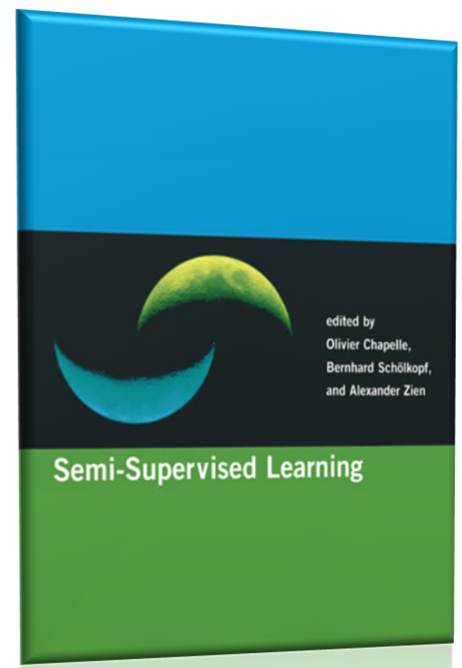

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