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Research Organization of Information and Systems
National Institute of Informatics

Machine Learning for Graph Structured Data

Introduction to Big Data Science (ビッグデータ概論)

Mahito Sugiyama (杉山麿人)

Example of Learning from Data
(from mlss.tuebingen.mpg.de/2013/schoelkopf_whatisML_slides.pdf)

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  - What are succeeding numbers?

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1, 2, 4, 7, 11, 16, . . . $(a_n = a_{n-1} + n - 1)$

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$$1, 2, 4, 7, 12, 20, \ldots \quad (a_n = a_{n-1} + a_{n-2} + 1)$$

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$$1, 2, 4, 7, 13, 24, \ldots \quad (a_n = a_{n-1} + a_{n-2} + a_{n-3})$$

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1, 2, 4, 7, 14, 28	(divisors of 28)

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1, 2, 4, 7, 1, 1, 5, . . .	(decimals of $\pi = 3.1415\ldots$, $e = 2.718\ldots$)

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- 1107 results (!) in the online encyclopedia (`https://oeis.org/`)

Analyze Learning as Scientific Problem

- Which is the correct answer (or generalization) for succeeding numbers of $1, 2, 4, 7, \ldots$?
  - Any answer is possible!

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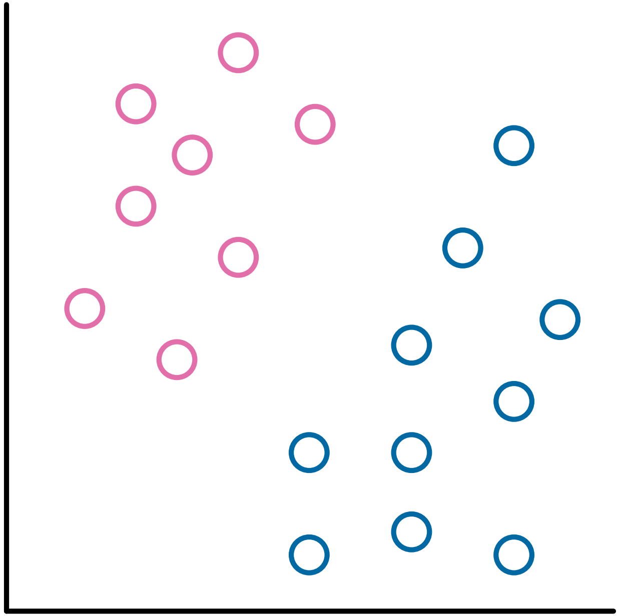
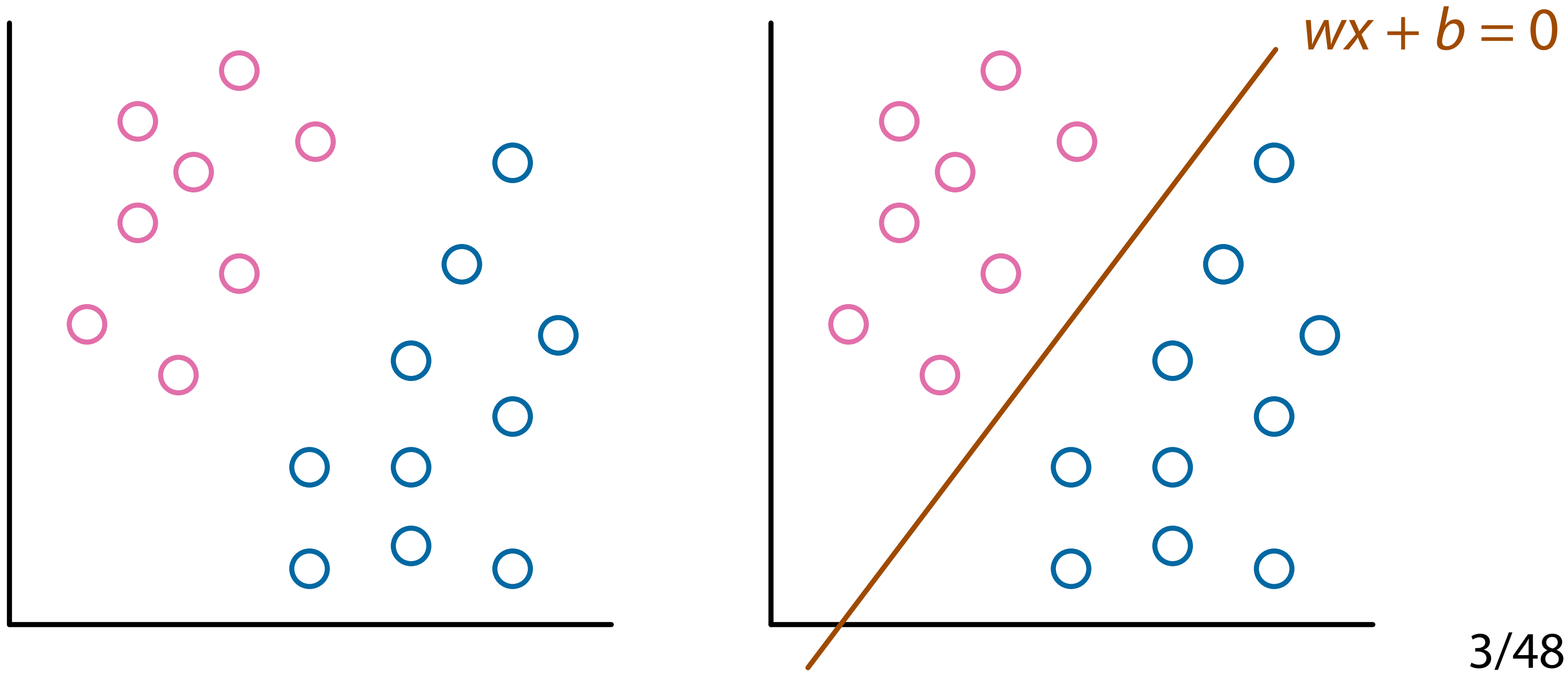
- We should take two points into consideration:
  (i) We need to formalize the problem of "learning"
    - There are two agents (teacher and learner) in learning, which are different from "computation"

  (ii) Learning is an infinite process
    - A learner usually never knows that the current hypothesis is perfectly correct

Learning of Binary Classifier



Learning of Binary Classifier



Example: Perceptron (by F. Rosenblatt, 1958)

- **Learning target**: two subsets $F, G \subseteq \mathbb{R}^d$ s.t. $F \cap G = \emptyset$
  - Assumption: F and G are linearly separable
    - There exists a function (classifier) $f_*(\boldsymbol{x}) = \langle \boldsymbol{w}_*, \boldsymbol{x} \rangle + b$ s.t. $f_*(\boldsymbol{x}) > 0 \quad \forall \boldsymbol{x} \in F, \qquad f_*(\boldsymbol{x}) < 0 \quad \forall \boldsymbol{x} \in G$

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      $f_*(\boldsymbol{x}) > 0 \quad \forall \boldsymbol{x} \in F, \qquad f_*(\boldsymbol{x}) < 0 \quad \forall \boldsymbol{x} \in G$
- **Hypotheses**: hyperplanes on $\mathbb{R}^d$
  - If we consider a linear equation $f(\boldsymbol{x}) = \langle \boldsymbol{w}, \boldsymbol{x} \rangle + b$, each line can be uniquely specified by a pair of two parameters $(\boldsymbol{w}, b)$ (hypothesis)

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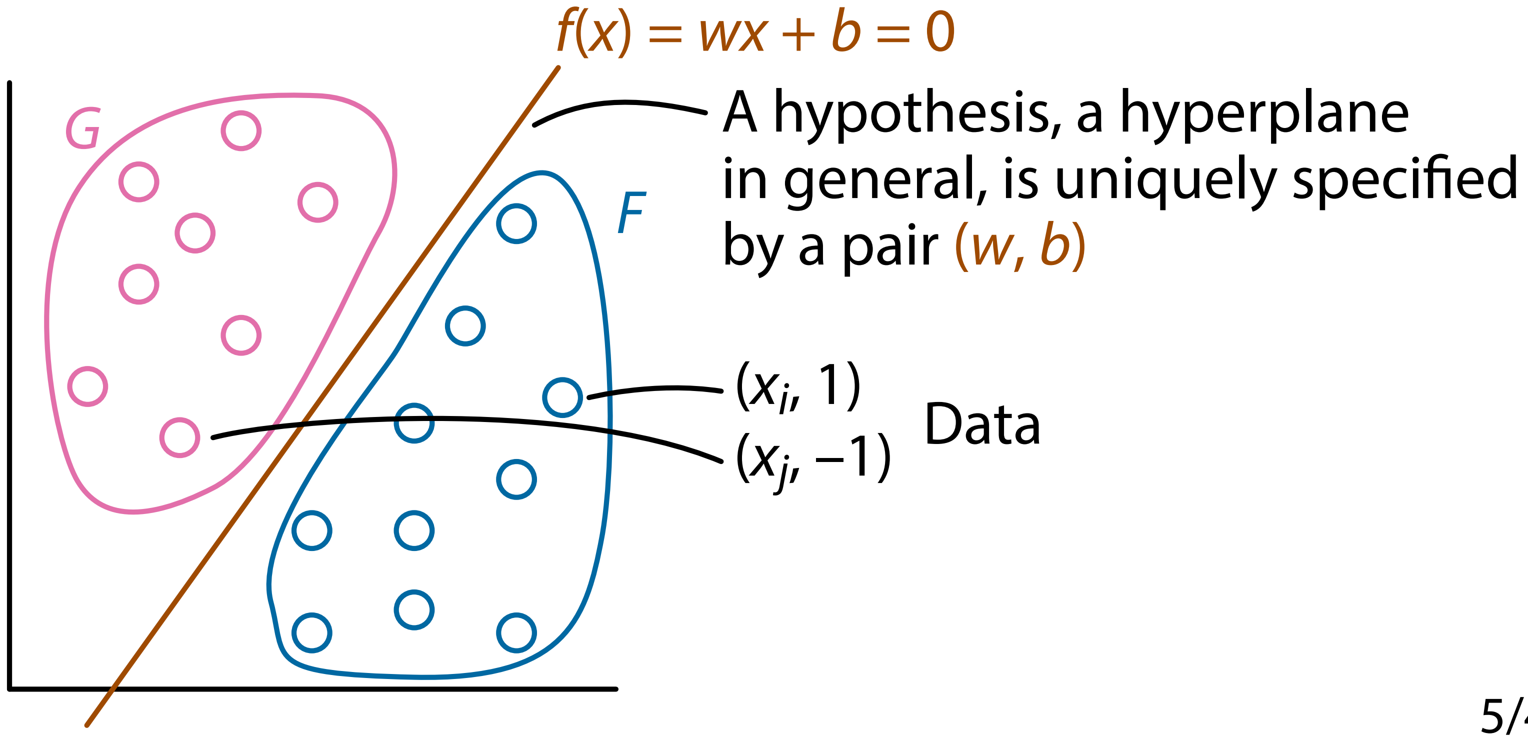
- **Data**: a sequence of pairs $(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \dots$
  - $(\boldsymbol{x}_i, y_i)$: (a real-valued vector in $\mathbb{R}^d$, a label)
  - $\boldsymbol{x}_i \in F \cup G$, $y_i \in \{1, -1\}$, and $y_i = 1$ ($y_i = -1$) if $\boldsymbol{x}_i \in F$ ($\boldsymbol{x}_i \in G$)

Learning Model for Perceptron



Learning Procedure of Perceptron

1. $\boldsymbol{w} \leftarrow 0, b \leftarrow 0$ (or a small random value) // initialization
2. **for** $i = 1, 2, 3, \ldots$ **do**
3. Receive i-th pair $(\boldsymbol{x}_i, y_i)$
4. Compute $a = \sum_{j=1}^{d} w^j x_i^j + b$
5. **if** $y_i \cdot a < 0$ **then** // $\boldsymbol{x}_i$ is misclassified
6. $\boldsymbol{w} \leftarrow \boldsymbol{w} + y_i \boldsymbol{x}_i$ // update the weight
7. $b \leftarrow b + y_i$ // update the bias
8. **end if**
9. **end for**

Correctness of Perceptron

- It is guaranteed that a perceptron always converges to a correct classifier
  - A correct classifier is a function f s.t.

    $$f(\boldsymbol{x}) > 0 \quad \forall \boldsymbol{x} \in F,$$
    $$f(\boldsymbol{x}) < 0 \quad \forall \boldsymbol{x} \in G$$

  - The convergence theorem

- Note: there are (infinitely) many functions that correctly classify F and G
  - A perceptron converges to one of them

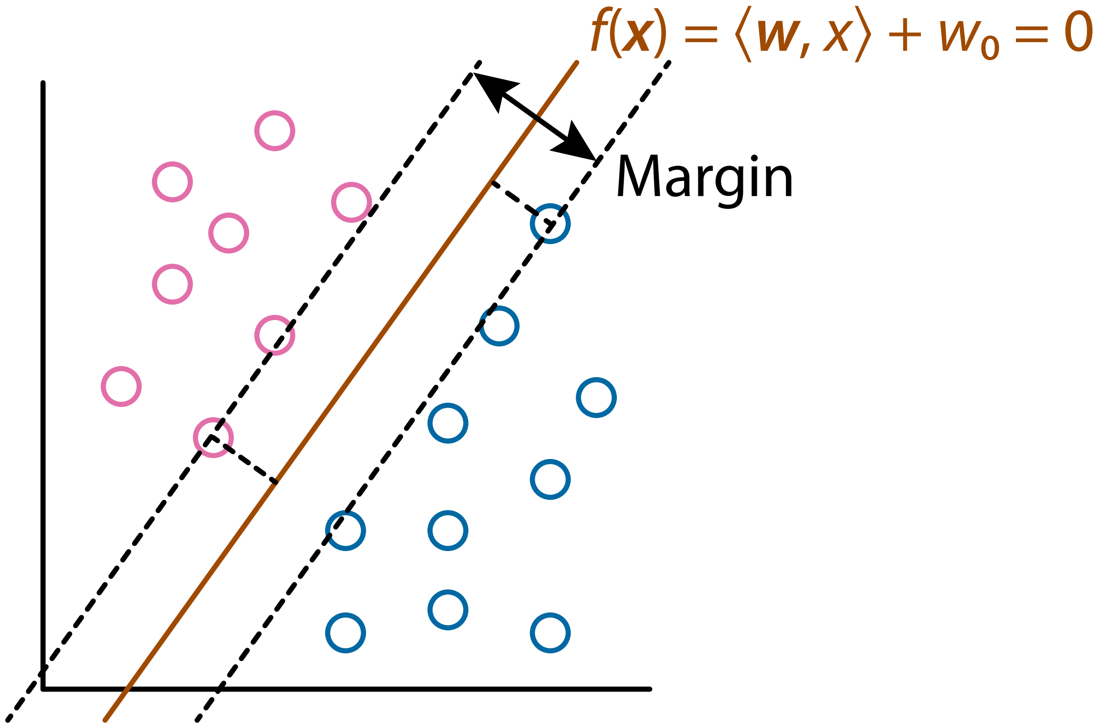
Summary: Perceptron

Target	Two disjoint subsets of $\mathbb{R}^d$
Representation	Two parameters $(\boldsymbol{w}, b)$ of linear equation $f(\boldsymbol{x}) = \langle \boldsymbol{w}, \boldsymbol{x} \rangle + b$
Data	Real vectors from target subsets
Algorithm	Perceptron
Correctness	Convergence theorem

Support Vector Machines (SVMs)

- A dataset D is separable by $f \iff y_i f(\boldsymbol{x}_i) > 0, \forall i \in \{1, 2, \ldots, n\}$
- The margin is the distance from the classification hyperplane to the closest data point
- Support vector machines (SVMs) tries to find a hyperplane that maximize the margin

Margin



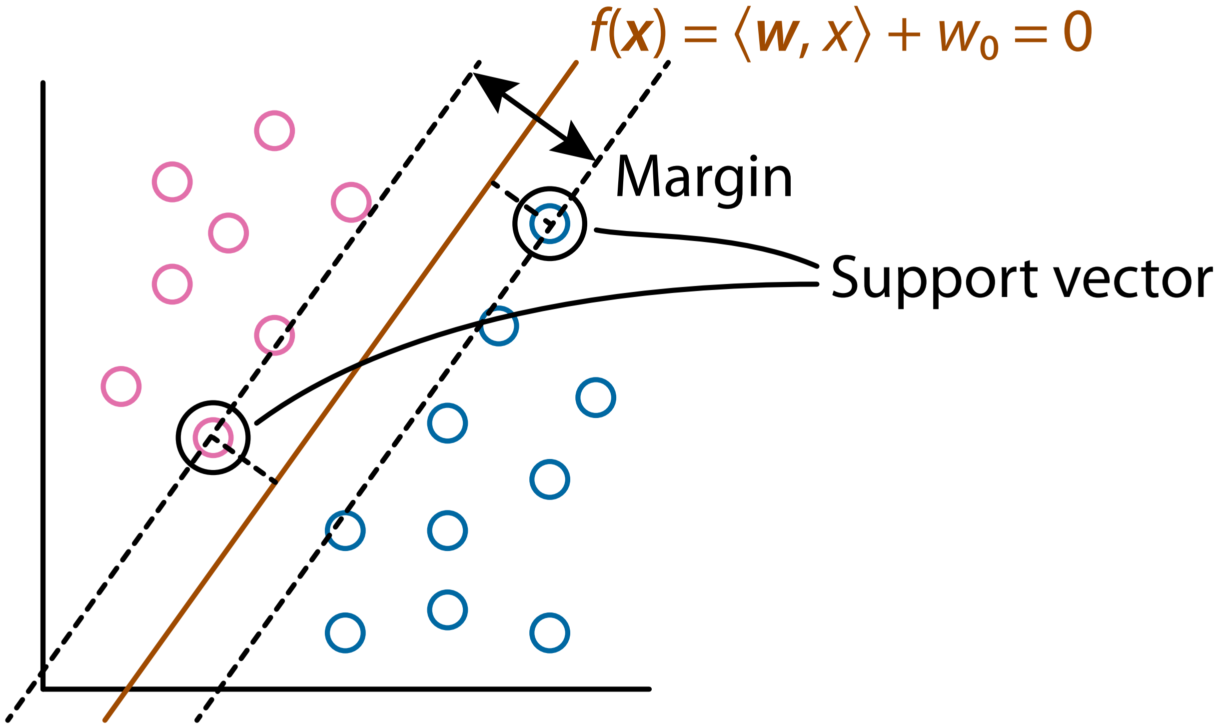
Formulation of SVMs

- The distance from a point $\boldsymbol{x}_i$ to a hyperplane $f(\boldsymbol{x}) = \langle \boldsymbol{w}, \boldsymbol{x} \rangle + w_0$ is
$$\frac{|f(\boldsymbol{x}_i)|}{||\boldsymbol{w}||} = \frac{|\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + w_0|}{||\boldsymbol{w}||}$$
- Since $y_i f(\boldsymbol{x}_i) > 0$ should be satisfied, assume that there exists $M > 0$ such that $y_i f(\boldsymbol{x}_i) \geq M$ for all $i \in \{1, 2, \dots, n\}$
- The margin maximization problem can be written as
$$\max_{\boldsymbol{w}, w_0, M} \frac{M}{||\boldsymbol{w}||} \quad \text{subject to } y_i f(\boldsymbol{x}_i) \geq M, i \in \{1, 2, \dots, n\}$$
  - $M = \min_{i \in \{1,2,\dots,n\}} |\langle \boldsymbol{w}, x_i \rangle + w_0|$

Hard Margin SVMs

- We can eliminate M and obtain
$$\max_{\boldsymbol{w}, w_0} \frac{1}{||\boldsymbol{w}||} \quad \text{subject to } y_i f(\boldsymbol{x}_i) \geq 1, i \in \{1, 2, \ldots, n\}$$
- This is equivalent to
$$\min_{\boldsymbol{w}, w_0} ||\boldsymbol{w}||^2 \quad \text{subject to } y_i f(\boldsymbol{x}_i) \geq 1, i \in \{1, 2, \ldots, n\}$$
  - The standard formulation of hard margin SVMs
  - There are data points x_i satisfying $y_i f(\boldsymbol{x}_i) = 1$, called support vectors
  - The solution does not change even data points that are not support vectors are removed

Margin

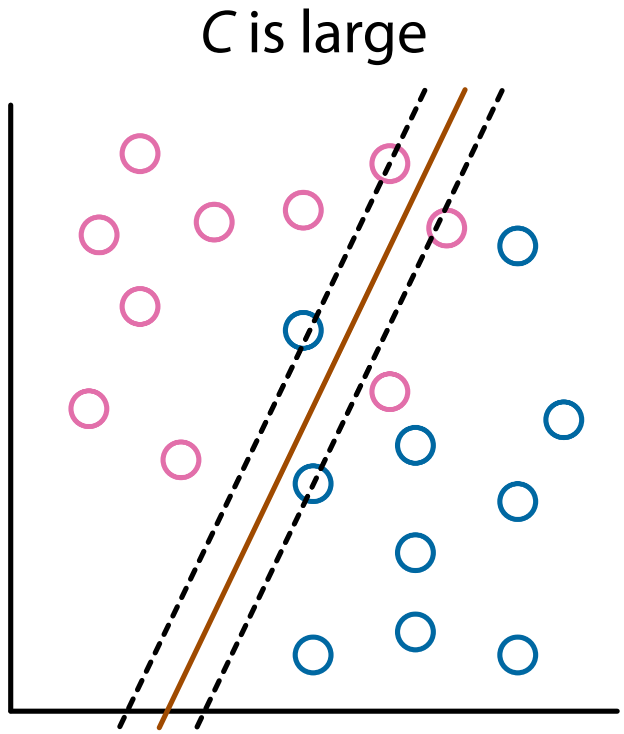


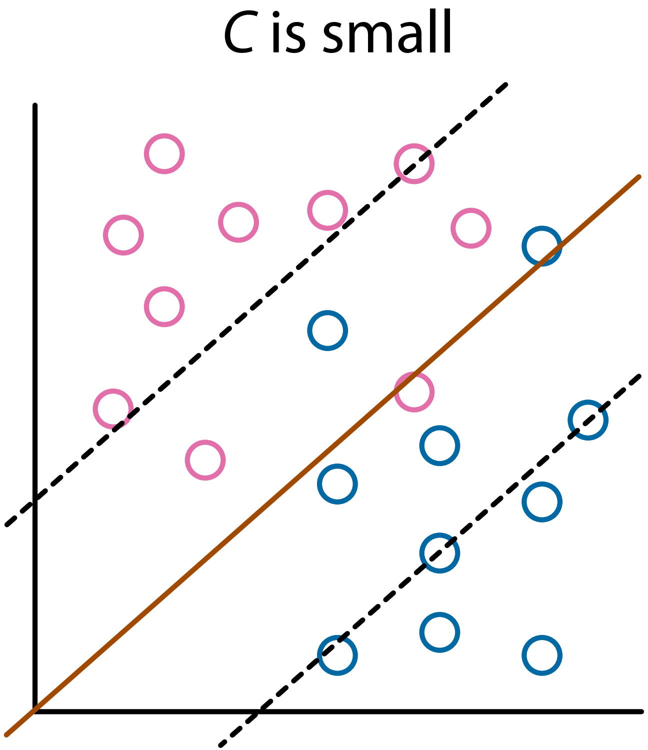
$f(\boldsymbol{x}) = \langle \boldsymbol{w}, x \rangle + w_0 = 0$
Margin
Support vector

Soft Margin

- Datasets are not often separable
- Extend SV classification to soft margin by relaxing $\langle \boldsymbol{w}, \boldsymbol{x} \rangle + w_0 \geq 1$
- Change the constraint $y_i f(\boldsymbol{x}_i) \geq 1$ using the slack variable ξ_i to
  $$y_i f(\boldsymbol{x}_i) = y_i (\langle \boldsymbol{w}, \boldsymbol{x} \rangle + w_0) \geq 1 - \xi_i, \quad i \in \{1, 2, \ldots, n\}$$
- The formulation of soft margin SVM (C-SVM) is
  $$\min_{\boldsymbol{w}, w_0, \boldsymbol{\xi}} \frac{1}{2} ||\boldsymbol{w}||^2 + C \sum_{i \in \{1,2,\ldots,n\}} \xi_i \quad \text{s.t. } y_i f(\boldsymbol{x}_i) \geq 1 - \xi_i, \xi_i \geq 0, i \in \{1, 2, \ldots, n\}$$
  - C is called the regularization parameter

Soft Margin





Data Point Location

- $y_i f(\boldsymbol{x}_i) > 1$: $\boldsymbol{x}_i$ is outside margin
  - These points do not affect to the classification hyperplane
- $y_i f(\boldsymbol{x}_i) = 1$: $\boldsymbol{x}_i$ is on margin
- $y_i f(\boldsymbol{x}_i) < 1$: $\boldsymbol{x}_i$ is inside margin
  - These points do not exist in hard margin
- Points on margin and inside margin are support vectors

Dual Problem (1/4)

- The formulation of C-SVM

$$\min_{\boldsymbol{w}, w_0, \boldsymbol{\xi}} \frac{1}{2}||\boldsymbol{w}||^2 + C \sum_{i \in \{1,2,\ldots,n\}} \xi_i \quad \text{s.t. } y_i f(\boldsymbol{x}_i) \geq 1 - \xi_i, \xi_i \geq 0, i \in \{1, 2, \ldots, n\}$$

  is called the primal problem

- This is usually solved via the dual problem

- Make the Lagrange function using $\boldsymbol{a} = (a_1, \ldots, a_n), \boldsymbol{\mu} = (\mu_1, \ldots, \mu_n)$:

$$L(\boldsymbol{w}, w_0, \boldsymbol{\xi}, \boldsymbol{a}, \boldsymbol{\mu}) = \frac{1}{2}||\boldsymbol{w}||^2 + C \sum_{i \in [n]} \xi_i - \sum_{i \in [n]} a_i\big(y_i f(\boldsymbol{x}_i) - 1 + \xi_i\big) - \sum_{i \in [n]} \mu_i \xi_i$$

  - $[n] = \{1, 2, \ldots, n\}$

Dual Problem (2/4)

- Let us consider

$$D(\boldsymbol{\alpha}, \boldsymbol{\mu}) = \min_{\boldsymbol{w}, w_0, \boldsymbol{\xi}} L(\boldsymbol{w}, w_0, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\mu})$$

and its maximization

$$\max_{\boldsymbol{\alpha} \geq 0, \boldsymbol{\mu} \geq 0} D(\boldsymbol{\alpha}, \boldsymbol{\mu}) = \max_{\boldsymbol{\alpha} \geq 0, \boldsymbol{\mu} \geq 0} \min_{\boldsymbol{w}, w_0, \boldsymbol{\xi}} L(\boldsymbol{w}, w_0, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\mu})$$

- The inside minimization is achieved when

$$\frac{\partial L}{\partial \boldsymbol{w}} = \boldsymbol{w} - \sum_{i \in [n]} \alpha_i y_i \boldsymbol{x}_i = 0, \quad \frac{\partial L}{\partial w_0} = -\sum_{i \in [n]} \alpha_i y_i = 0, \quad \frac{\partial L}{\partial \xi_i} = C - \alpha_i - \mu_i = 0$$

Dual Problem (3/4)

- Putting the three conditions to the Lagrange function to remove $\boldsymbol{w}$, w_o, and $\boldsymbol{\xi}$, yielding

$$L = \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i\in[n]}\xi_i - \sum_{i\in[n]}\alpha_i\big(y_i f(\boldsymbol{x}_i) - 1 + \xi_i\big) - \sum_{i\in[n]}\mu_i\xi_i$$

$$= \frac{1}{2}\|\boldsymbol{w}\|^2 - \sum_{i\in[n]}\alpha_i y_i\langle\boldsymbol{w},\boldsymbol{x}_i\rangle - w_o\sum_{i\in[n]}\alpha_i y_i + \sum_{i\in[n]}\alpha_i + \sum_{i\in[n]}(C - \alpha_i - \mu_i)\xi_i$$

$$= -\frac{1}{2}\sum_{i,j\in[n]}\alpha_i\alpha_j y_i y_j\langle\boldsymbol{x}_i,\boldsymbol{x}_j\rangle + \sum_{i\in[n]}\alpha_i$$

Dual Problem (4/4)

- It can be proved that $\max_{\boldsymbol{\alpha}\geq 0, \boldsymbol{\mu}\geq 0} \min_{\boldsymbol{w}, w_0, \boldsymbol{\xi}} L(\boldsymbol{w}, w_0, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\mu})$, that is, the dual problem

$$\max_{\boldsymbol{\alpha}} -\frac{1}{2}\sum_{i,j\in[n]} \alpha_i \alpha_j y_i y_j \langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle + \sum_{i\in[n]} \alpha_i \quad \text{s.t.} \sum_{i\in[n]} \alpha_i y_i = 0,\ 0 \leq \alpha_i \leq C, i \in [n]$$

is equivalent to the primal problem

$$\min_{\boldsymbol{w}, w_0, \boldsymbol{\xi}} \frac{1}{2}||\boldsymbol{w}||^2 + C \sum_{i\in\{1,2,\ldots,n\}} \xi_i \quad \text{s.t. } y_i f(\boldsymbol{x}_i) \geq 1 - \xi_i, \xi_i \geq 0, i \in [n]$$

KKT (Karush-Kuhn-Tucker) condition

- The necessary conditions for a solution to be optimal:

$$\frac{\partial L}{\partial \boldsymbol{w}} = \boldsymbol{w} - \sum_{i \in [n]} \alpha_i y_i \boldsymbol{x}_i = 0, \ \frac{\partial L}{\partial w_0} = -\sum_{i \in [n]} \alpha_i y_i = 0, \ \frac{\partial L}{\partial \xi_i} = C - \alpha_i - \mu_i = 0$$

$$-(y_i f(\boldsymbol{x}_i) - 1 + \xi_i) \le 0, \ -\xi_i \le 0,$$

$$\alpha_i \ge 0, \ \mu_i \ge 0,$$

$$\alpha_i(y_i f(\boldsymbol{x}_i) - 1 - \xi_i) = 0, \ \mu_i \xi_i = 0,$$

$$i \in [n]$$

Recovering Primal Variables

- Using these conditions, from the optimal $\boldsymbol{\alpha}$, we have

$$f(\boldsymbol{x}) = \sum_{i \in [n]} \alpha_i y_i \langle \boldsymbol{x}_i, \boldsymbol{x} \rangle + w_0,$$

$$w_0 = y_i - \sum_{j \in [n]} \alpha_j y_j \langle \boldsymbol{x}_j, \boldsymbol{x}_i \rangle, \quad \forall i \in \{i \in [n] \mid 0 < \alpha_i < C\}$$

  - Since the second condition holds for all $i \in \{i \in [n] \mid 0 < \alpha_i < C\}$, one can take the average to avoid numerical errors

Data Point Location

- $y_i f(\boldsymbol{x}_i) > 1 \iff \alpha_i = 0$: $\boldsymbol{x}_i$ is outside margin
  - These points do not affect to the classification hyperplane
- $y_i f(\boldsymbol{x}_i) = 1 \iff 0 < \alpha_i < C$: $\boldsymbol{x}_i$ is on margin
- $y_i f(\boldsymbol{x}_i) < 1 \iff \alpha_i = C$: $\boldsymbol{x}_i$ is inside margin
  - These points do not exist in hard margin
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How to Solve?

- The (dual) problem:

  $$\max_{\boldsymbol{a}} -\frac{1}{2}\boldsymbol{a}^T Q\boldsymbol{a} + \mathbf{1}^T\boldsymbol{a} \quad \text{s.t. } \boldsymbol{y}^T\boldsymbol{a} = 0,\ 0 \le \boldsymbol{a} \le C\mathbf{1}$$

  – $Q \in \mathbb{R}^{n\times n}$ is the matrix such that $q_{ij} = y_i y_j \langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle$

- Since analytical solution is not available, iterative approach for continuous optimization with constraints is needed

- One of standard methods is the active set method

Active Set Method

- Divide the set $[n]$ of indices into three sets:

$$O = \{i \in [n] \mid a_i = 0\}$$
$$M = \{i \in [n] \mid 0 < a_i < C\}$$
$$I = \{i \in [n] \mid a_i = C\}$$

  – O and I are called active sets

- The problem can be solved w.r.t. $i \in M$, yielding

$$\begin{bmatrix} Q_M & \mathbf{y}_M \\ \mathbf{y}_M^T & 0 \end{bmatrix} \begin{bmatrix} a_M \\ v \end{bmatrix} = -C \begin{bmatrix} Q_{M,I} & \mathbf{1} \\ \mathbf{1}^T & \mathbf{y}_I \end{bmatrix} + \begin{bmatrix} \mathbf{1} \\ 0 \end{bmatrix}$$

  – This can be directly solved if Q_M is positive definite

Algorithm 1: Active Set Method

activeSetMethod(D)

  Initialize M, I, O

  while *there exists i s.t.* $y_i f(\boldsymbol{x}_i) < 1, i \in O$ *or* $y_i f(\boldsymbol{x}_i) > 1, i \in I$ **do**

    Update M, I, O

    repeat

      $\boldsymbol{\alpha}_M^{\text{new}} \leftarrow$ the solution of the above equation

      $\boldsymbol{d} \leftarrow \boldsymbol{\alpha}_M^{\text{new}} - \boldsymbol{\alpha}_M$

      $\boldsymbol{\alpha}_M \leftarrow \boldsymbol{\alpha}_M + \eta \boldsymbol{d}$; // the maximum η satisfying $\boldsymbol{\alpha}_M \in [0, C]^{|M|}$

      Move $i \in M$ from M to I or O if $\alpha_i = C$ or $\alpha_i = 0$

    until $\boldsymbol{\alpha}_M = \boldsymbol{\alpha}_M^{new}$;

Extension to Nonlinear Classification

- To achieve nonlinear classification, convert each data point $\boldsymbol{x}$ to some point $\varphi(\boldsymbol{x})$, and $f(\boldsymbol{x})$ becomes

  $f(\boldsymbol{x}) = \langle \boldsymbol{w}, \varphi(\boldsymbol{x}) \rangle + w_0$

- The dual problem becomes

  $$\max_{\boldsymbol{\alpha}} -\frac{1}{2} \sum_{i,j \in [n]} \alpha_i \alpha_j y_i y_j \langle \varphi(\boldsymbol{x}_i), \varphi(\boldsymbol{x}_j) \rangle + \sum_{i \in [n]} \alpha_i \ \text{ s.t. } \sum_{i \in [n]} \alpha_i y_i = 0,\ 0 \le \alpha_i \le C, i \in [n]$$

  - Only the dot product $\langle \varphi(\boldsymbol{x}_i), \varphi(\boldsymbol{x}_j) \rangle$ is used!
  - We do not even need to know $\varphi(\boldsymbol{x}_i)$ and $\varphi(\boldsymbol{x}_j)$

- Kernel function: $K(\boldsymbol{x}_i, \boldsymbol{x}_j) = \langle \varphi(\boldsymbol{x}_i), \varphi(\boldsymbol{x}_j) \rangle$

C-SVM with Kernel Trick

- Using the kernel function K, we have

$$\max_{\boldsymbol{\alpha}} -\frac{1}{2}\sum_{i,j\in[n]} \alpha_i \alpha_j y_i y_j K(\boldsymbol{x}_i, \boldsymbol{x}_j) + \sum_{i\in[n]} \alpha_i \ \text{ s.t. } \sum_{i\in[n]} \alpha_i y_i = 0,\ 0 \le \alpha_i \le C, i \in [n]$$

  - The technique of using K is called kernel trick

Positive Definite Kernel

- A kernel $K : \Omega \times \Omega \to \mathbb{R}$ is a positive definite kernel if
  (i) $K(x, y) = K(y, x)$
  (ii) For $x_1, x_2, \dots, x_n$, the $n \times n$ matrix

$$(K_{ij}) = \begin{bmatrix} K(x_1, x_1) & K(x_2, x_1) & \dots & K(x_n, x_1) \\ K(x_1, x_2) & K(x_2, x_2) & \dots & K(x_n, x_2) \\ \dots & \dots & \dots & \dots \\ K(x_1, x_n) & K(x_2, x_n) & \dots & K(x_n, x_n) \end{bmatrix}$$

  is positive (semi-)definite, that is, $\sum_{i,j=1}^{n} c_i c_j K(x_i, x_j) \geq 0$ for any $c_1, c_2, \dots, c_n \in \mathbb{R}$
  - $(K_{ij}) \in \mathbb{R}^{n \times n}$ is called the Gram matrix

Popular Positive Definite Kernels

- Linear Kernel

$$K(\boldsymbol{x}, \boldsymbol{y}) = \langle \boldsymbol{x}, \boldsymbol{y} \rangle$$

- Gaussian (RBF) kernel

$$K(\boldsymbol{x}, \boldsymbol{y}) = \exp\left(-\frac{1}{\sigma^2} \|\boldsymbol{x} - \boldsymbol{y}\|^2\right)$$

- Polynomial Kernel

$$K(\boldsymbol{x}, \boldsymbol{y}) = (\langle \boldsymbol{x}, \boldsymbol{y} \rangle + c)^c \qquad c, d \in \mathbb{R}$$

Simple Kernels

- The all-ones kernel

$$K(\boldsymbol{x}, \boldsymbol{y}) = 1$$

- The delta (Dirac) kernel

$$K(\boldsymbol{x}, \boldsymbol{y}) = \begin{cases} 1 & \text{if } \boldsymbol{x} = \boldsymbol{y}, \\ 0 & \text{otherwise} \end{cases}$$

Closure Properties of Kernels

- For two kernels K_1 and K_2, $K_1 + K_2$ is a kernel
- For two kernels K_1 and K_2, the product $K_1 \cdot K_2$ is a kernel
- For a kernel K and a positive scalar $\lambda \in \mathbb{R}^+$, λK is a kernel
- For a kernel K on a set D, its zero-extension:

  $$K_0(\boldsymbol{x}, \boldsymbol{y}) = \begin{cases} K(\boldsymbol{x}, \boldsymbol{y}) & \text{if } \boldsymbol{x}, \boldsymbol{y} \in D, \\ 0 & \text{otherwise} \end{cases}$$

  is a kernel

Kernels on Structured Data

- Given objects X and Y, decompose them into substructures S and T
- The R-convolution kernel K_R by Haussler (1999) is given as

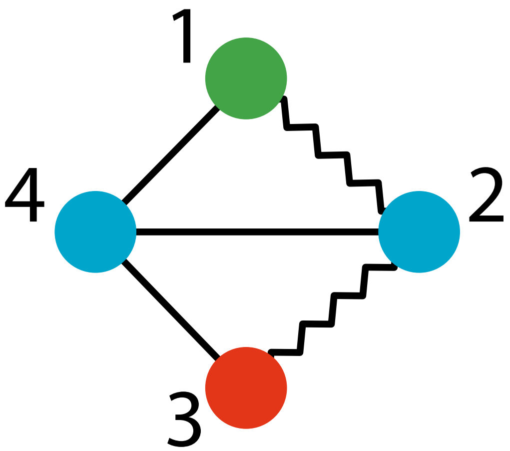
$$K_R(X, Y) = \sum_{s \in S, t \in T} K_{\text{base}}(s, t)$$

  - K_{base} is an arbitrary base kernel, often the delta kernel
- For example, X is a graph and S is the set of all subgraphs

What Is Graph?

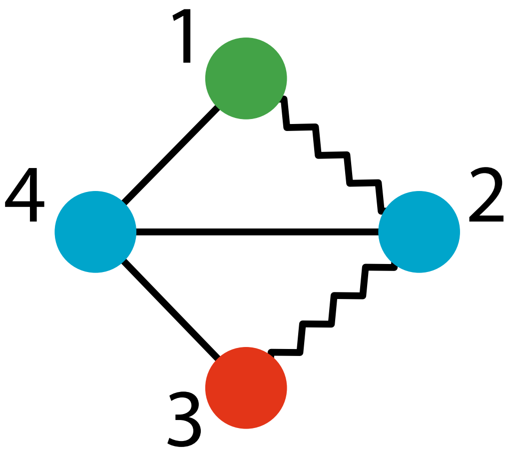
- An object consisting of vertices (nodes) connected with edges
- A graph is directed if the edges are directed, otherwise it is undirected
- A graph is written as $G = (V, E)$, where V is a vertex set and E is an edge set
- Labels can be associated with vertices and/or edges
  - If a function φ gives labels, the label of a vertex $v \in V$ is $\varphi(v)$ and that of an edge $e \in E$ is $\varphi(e)$

Example of Graph



- A graph $G = (V, E, \varphi)$
  - $V = \{1, 2, 3, 4\}$
  - $E = \{\{1, 2\}, \{1, 4\}, \{2, 3\}, \{2, 4\}, \{3, 4\}\}$
  - $\varphi(1)$ = green, $\varphi(2)$ = blue, $\varphi(3)$ = red, $\varphi(4)$ = blue
  - $\varphi(\{\{1, 2\})$ = zigzag, $\varphi(\{1, 4\})$ = straight, $\varphi(\{2, 3\})$ = zigzag, $\varphi(\{2, 4\})$ = straight, $\varphi(\{3, 4\}\})$ = straight

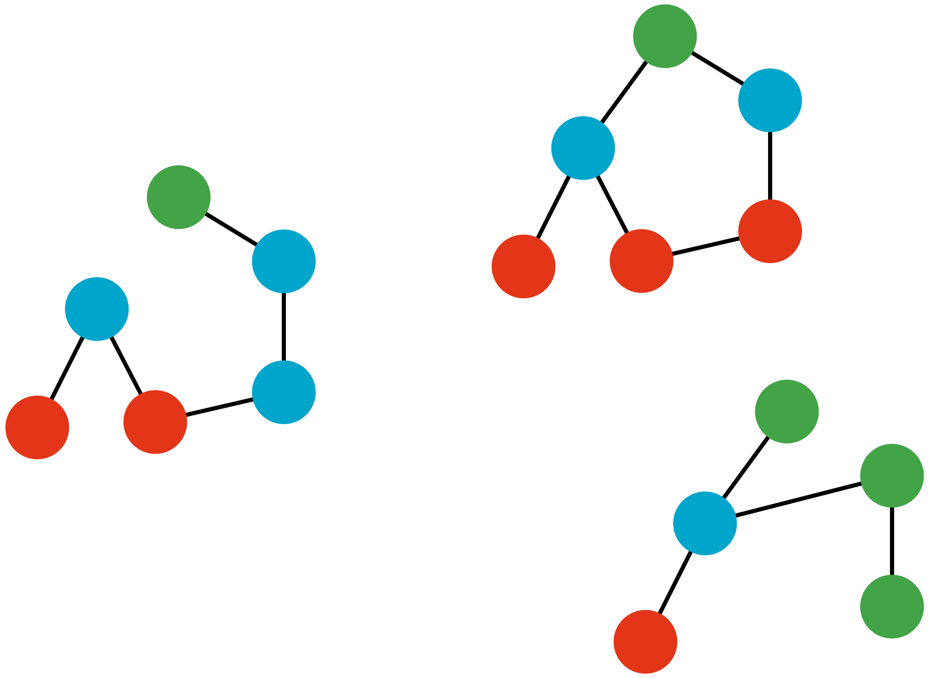
Example of Graph



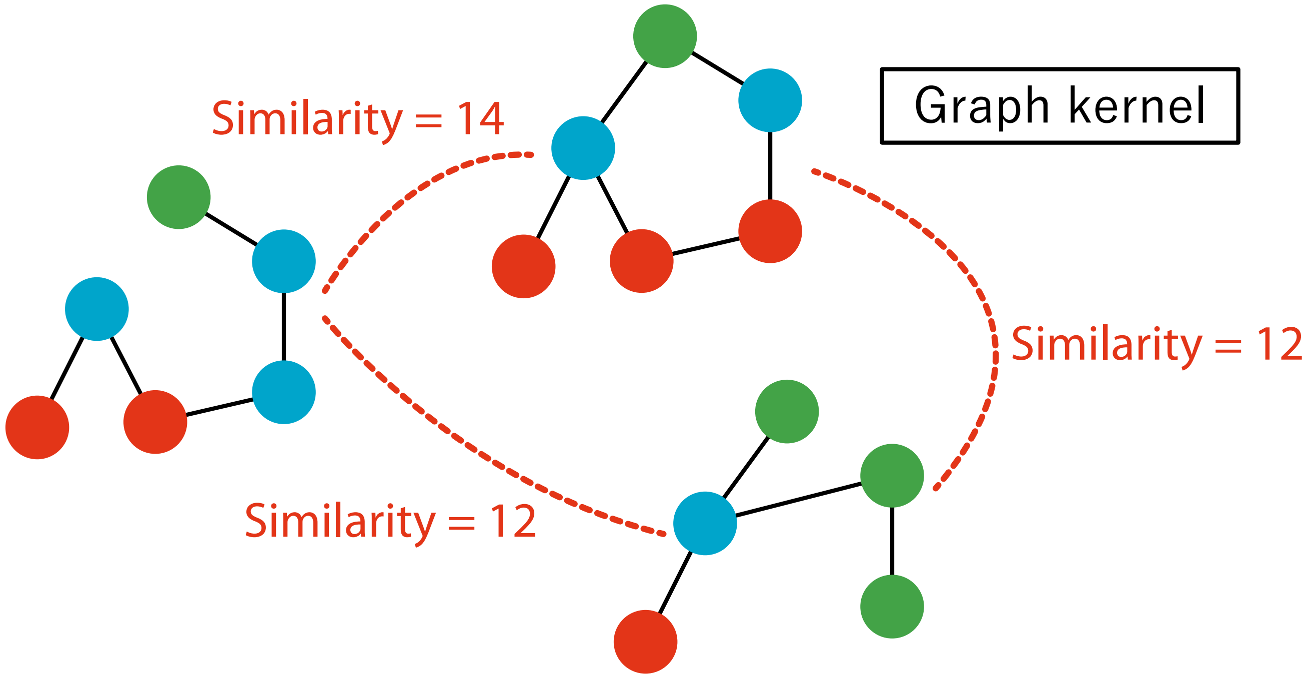
- The adjacency matrix

$$A = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$

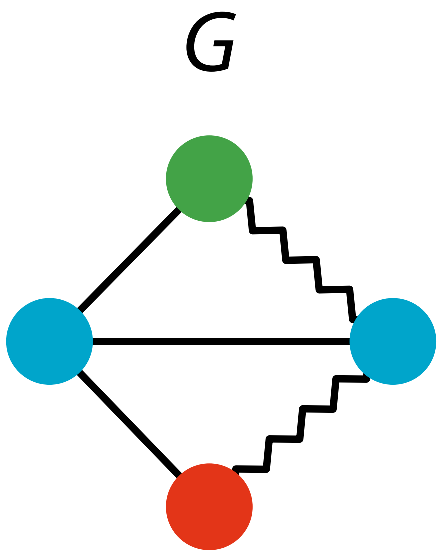
Similarity between Graphs

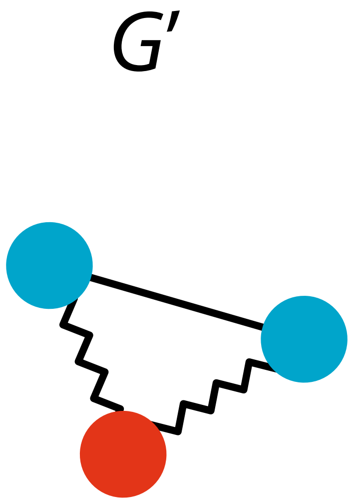


Similarity between Graphs



Example





Vertex Label Histogram Kernel

G	2	1	1
G'	2	0	1

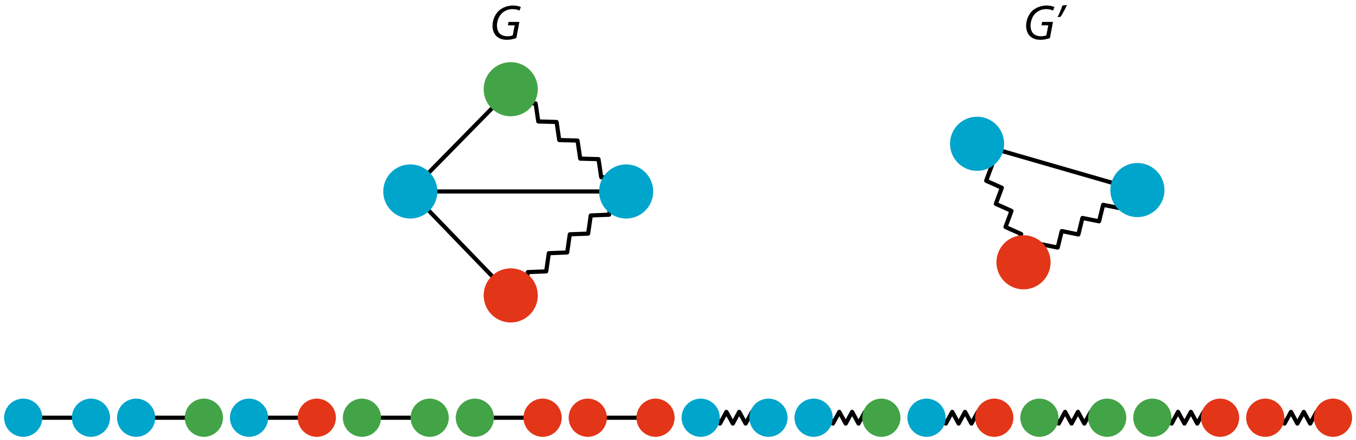
$$K_{\mathrm{VH}}(G, G') = 2 \cdot 2 + 1 \cdot 0 + 1 \cdot 1 = 5$$

Edge Label Histogram Kernel

G	3	2
G'	1	2

$$K_{EH}(G, G') = 3\cdot1 + 2\cdot2 = 7$$

Vertex-Edge Label Histogram Kernel



G	1	1	1	0	0	0	0	1	1	0	0	0
G'	1	0	0	0	0	0	0	0	2	0	0	0

$K_{\text{VEH}}(G, G') = 3$

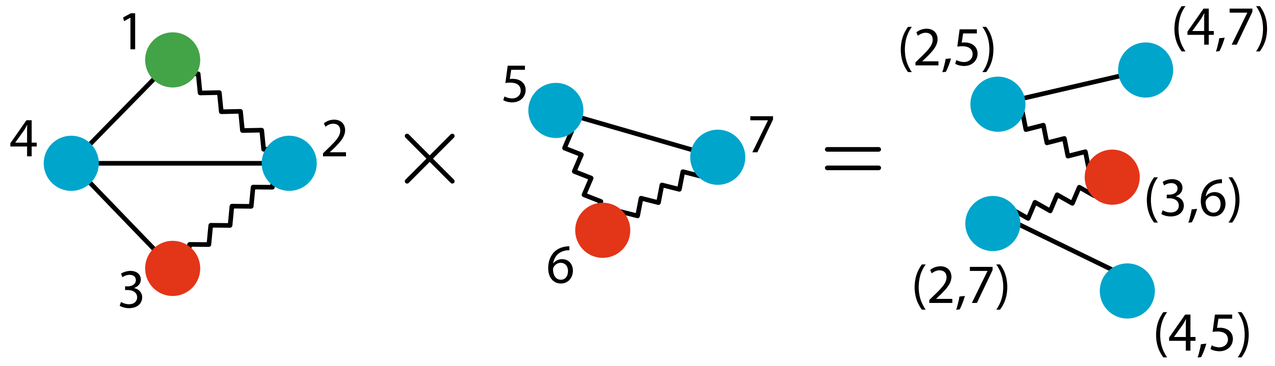
Product Graph

- The direct product $G_\times = (V_\times, E_\times, \varphi_\times)$ of $G = (V, E, \varphi)$, $G' = (V', E', \varphi')$:

$$V_\times = \{ (v, v') \in V \times V' \mid \varphi(v) = \varphi'(v') \},$$

$$E_\times = \left\{ ((u, u'), (v, v')) \in V_\times \times V_\times \;\middle|\; \begin{array}{l} (u, v) \in E,\ (u', v') \in E', \\ \varphi(u, v) = \varphi'(u', v') \end{array} \right\}$$

  - All labels are inherited



k-Step Random Walk Kernal

- The k-step (fixed-length-k) random walk kernel between G and G':

$$K_\times^k(G, G') = \sum_{i,j=1}^{|V_\times|} \left[\lambda_0 A_\times^0 + \lambda_1 A_\times^1 + \lambda_2 A_\times^2 + \cdots + \lambda_k A_\times^k\right]_{ij} \quad (\lambda_l > 0)$$

  - $A_\times$: The adjacency matrix of the product graph
  - The ij entry of $A_\times^n$ shows the number of paths from i to j

Geometric Random Walk Kernel

- $K_\times^\infty$ can be directly computed if $\lambda_\ell = \lambda^\ell$ for each $\ell \in \{0, \ldots, k\}$ (geometric series), resulting in the geometric random walk kernel:

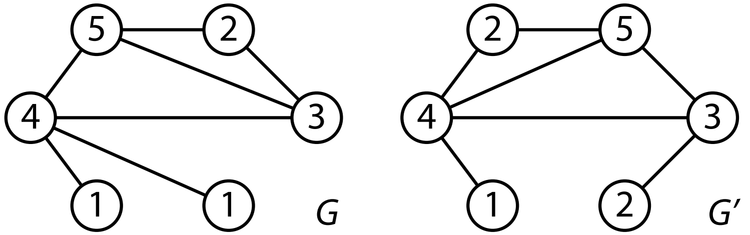
$$K_{\mathrm{GR}}(G, G') = \sum_{i,j=1}^{|V_\times|} \left[\lambda^0 A_\times^0 + \lambda^1 A_\times^1 + \lambda^2 A_\times^2 + \lambda^3 A_\times^3 + \cdots\right]_{ij} = \sum_{i,j=1}^{|V_\times|} \left[\sum_{\ell=0}^{\infty} \lambda^\ell A_\times^\ell\right]_{ij}$$

$$= \sum_{i,j=1}^{|V_\times|} \left[(\mathbf{I} - \lambda A_\times)^{-1}\right]_{ij}$$

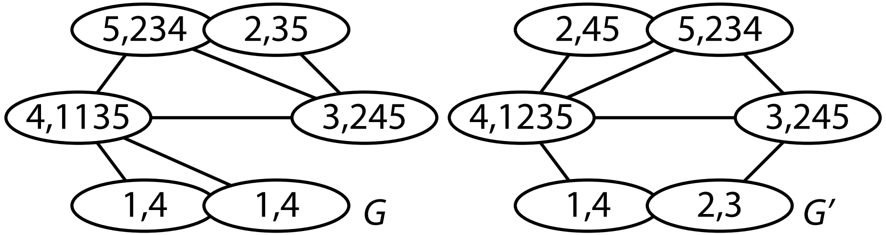
  - Well-defined only if $\lambda < 1/\mu_{\times,\max}$ ($\mu_{\times,\max}$ is the max. eigenvalue of $A_\times$)
  - $\delta_\times$ (min. degree) $\leq \bar{d}_\times$ (average degree) $\leq \mu_{\times,\max} \leq \Delta_\times$ (max. degree)

Weisfeiler–Lehman Kernel

Given graphs



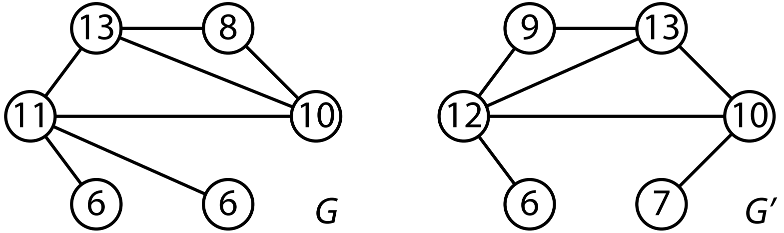
1st iteration



Re-labeling after 1st iteration

1,4	→ 6	3,245	→ 10
2,3	→ 7	4,1135	→ 11
2,35	→ 8	4,1235	→ 12
2,45	→ 9	5,234	→ 13

After 1st iteration



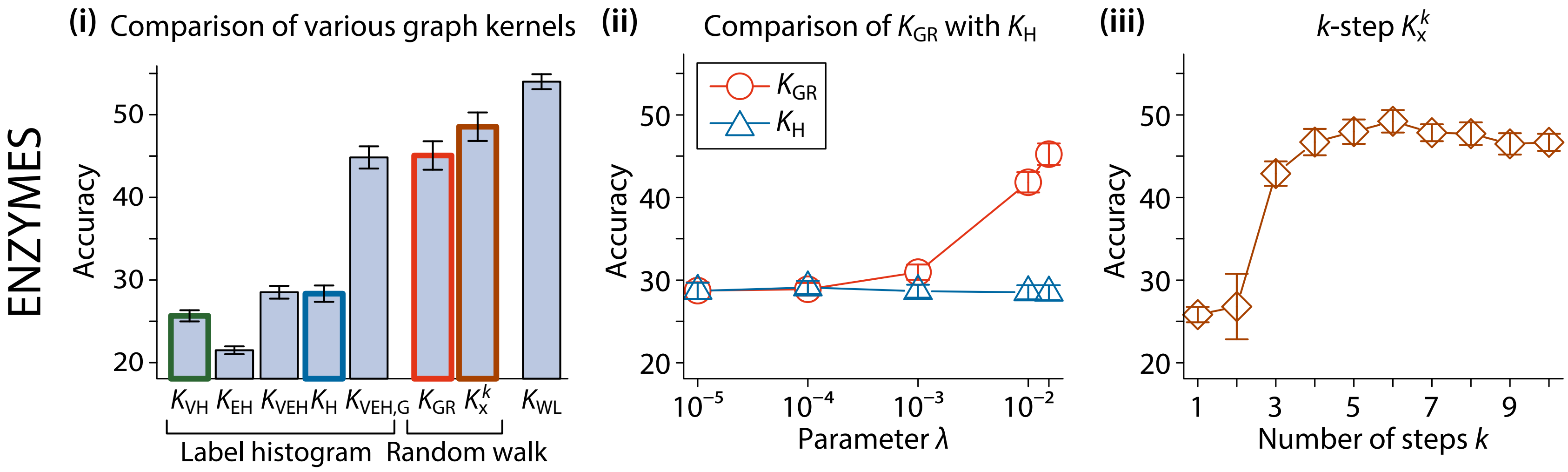
Weisfeiler–Lehman Kernel

- The kernel value becomes:

$$\begin{bmatrix} \text{label} \\ \varphi(G)^{(1)} \\ \varphi(G')^{(1)} \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 \\ 2 & 1 & 1 & 1 & 1 & 2 & 0 & 1 & 0 & 1 & 1 & 0 & 1 \\ 1 & 2 & 1 & 1 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 1 \end{bmatrix},$$

$$K^1_{\mathrm{WL}}(G, G') = 11$$

Performance Comparison



graphkernels Package

- A package for graph kernels available in R and Python
- R:
  `https://CRAN.R-project.org/package=graphkernels`
- Python:
  `https://pypi.org/project/graphkernels/`
- Paper:
  `https://doi.org/10.1093/bioinformatics/btx602`