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Inter-University Research Institute Corporation /
Research Organization of Information and Systems
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SVM and Kernel Methods

Data Mining 10 (データマイニング)

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Today's Outline

- Today's topic is support vector machines (SVMs) and kernel methods
- SVM performs binary classification by maximizing the margin
  - It is a popular supervised classification method
- SVM can perform nonlinear classification for structured data using kernel trick
- Graph kernels for classification for graph structured data

Classification Problem Setting

- Given a supervised dataset $D = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \ldots, (\boldsymbol{x}_n, y_n)\}$, $\boldsymbol{x}_i \in \mathbb{R}^d$ (feature vector), $y_i \in C = \{-1, 1\}$ (label)
- Use a decision function (hyperplane) in the form of

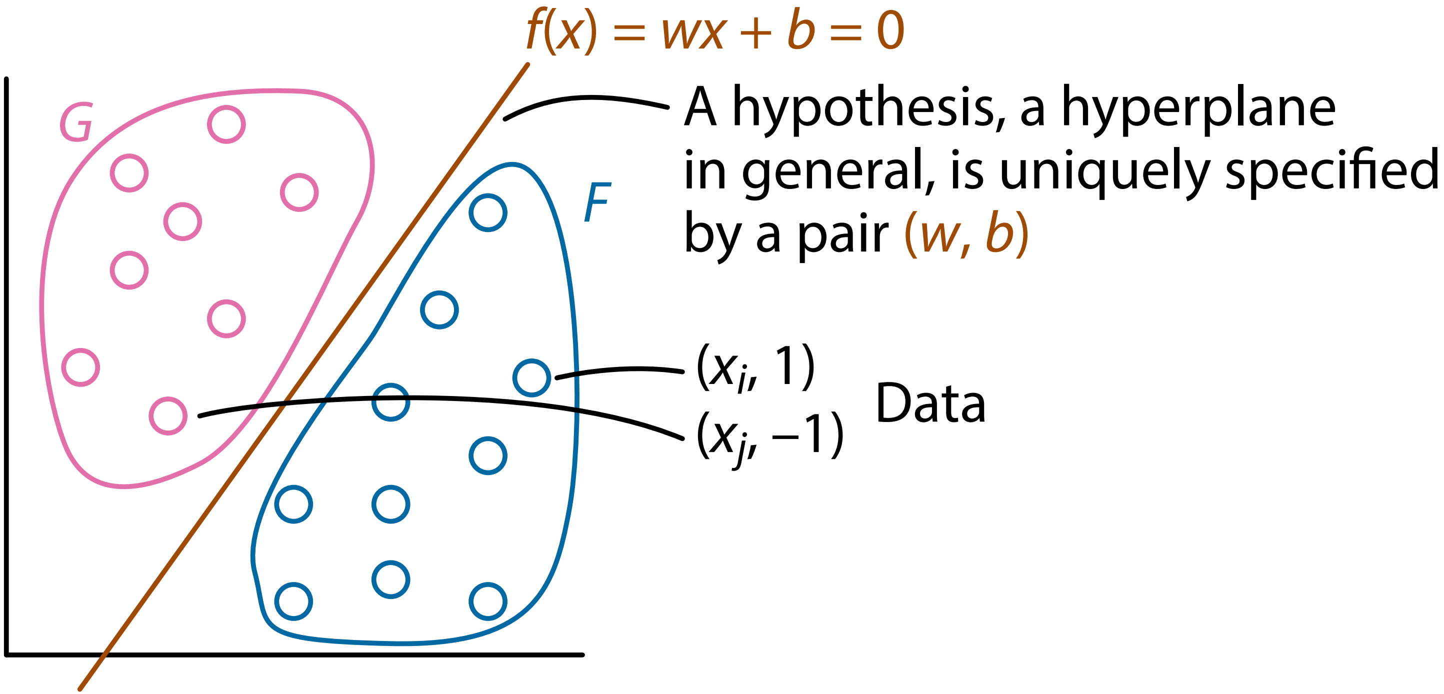
$$f(\boldsymbol{x}) = \langle \boldsymbol{w}, \boldsymbol{x} \rangle + w_0 = \sum_{j=1}^{d} w^j x^j + w_0$$

- A classifier $g(\boldsymbol{x})$ is given as

$$g(\boldsymbol{x}) = \begin{cases} 1 & \text{if } f(\boldsymbol{x}) > 0, \\ -1 & \text{if } f(\boldsymbol{x}) < 0 \end{cases}$$

- Goal: Find $(\boldsymbol{w}, w_0)$ that correctly classifies the dataset

Classification by Hyperplane



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

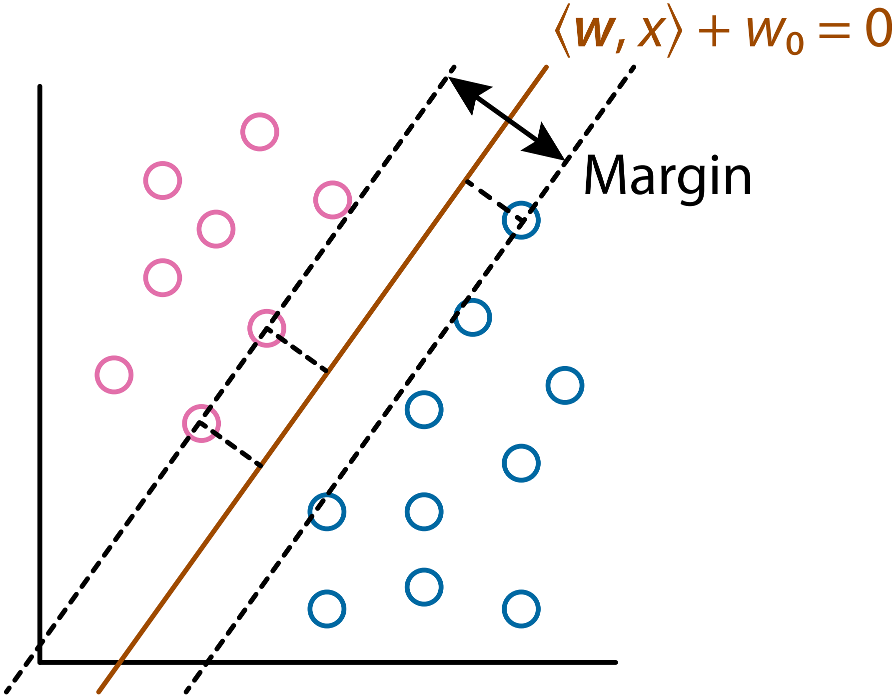
Correctness of Perceptron

- It is guaranteed that a perceptron always converges to a correct classifier
  - A correct classifier is a function f s.t.
    $f(\boldsymbol{x}) > 0$ if $y = 1$,
    $f(\boldsymbol{x}) < 0$ if $y = -1$
  - The convergence theorem
- Note: there are (infinitely) many functions that correctly classify F and G
  - A perceptron converges to one of them

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 maximizes the margin

Margin



Formulation of SVMs

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

Hard Margin SVMs

- We can eliminate B and obtain

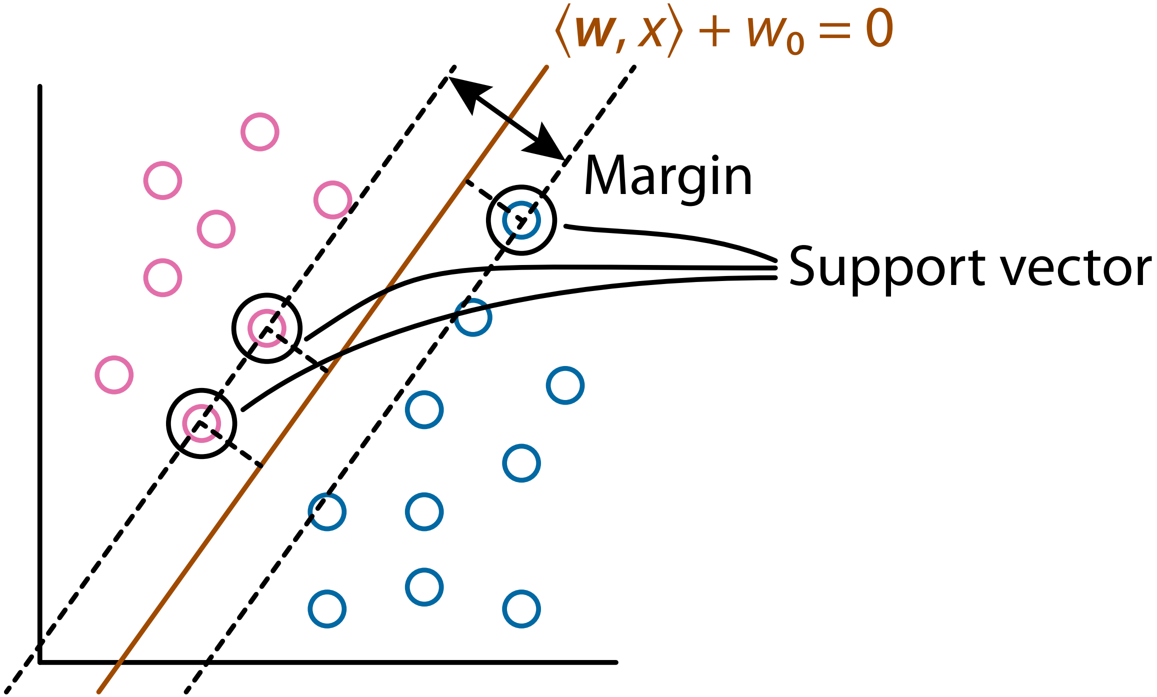
$$\max_{\boldsymbol{w}, w_0} \frac{1}{||\boldsymbol{w}||} \quad \text{subject to } y_i f(\boldsymbol{x}_i) \geq 1, i \in \{1, 2, \dots, n\}$$

- This is equivalent to

$$\min_{\boldsymbol{w}, w_0} ||\boldsymbol{w}||^2 \quad \text{subject to } y_i f(\boldsymbol{x}_i) \geq 1, i \in \{1, 2, \dots, n\}$$

  - The standard formulation of hard margin SVMs
  - There are data points $\boldsymbol{x}_i$ 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



Soft Margin

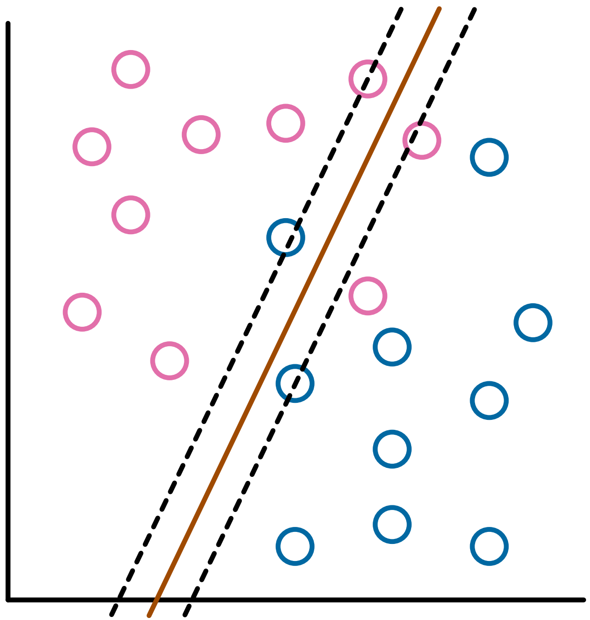
- Datasets are not often separable
- Extend SV classification to soft margin by relaxing $\langle \boldsymbol{w}, \boldsymbol{x} \rangle + w_0 \geq 1$
- Change the constraint $y_i f(\boldsymbol{x}_i) \geq 1$ using the slack variable ξ_i to

  $$y_i f(\boldsymbol{x}_i) = y_i (\langle \boldsymbol{w}, \boldsymbol{x} \rangle + w_0) \geq 1 - \xi_i, \quad i \in \{1, 2, \dots, n\}$$
- The formulation of soft margin SVM (C-SVM) is

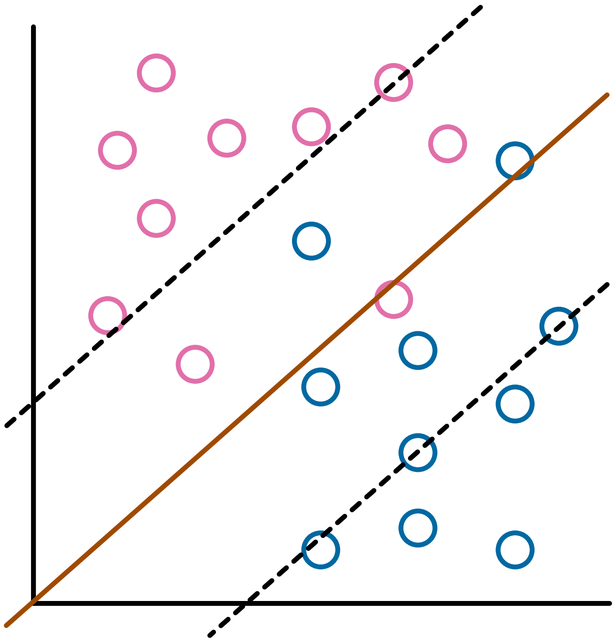
  $$\min_{\boldsymbol{w}, w_0, \xi} \frac{1}{2} \|\boldsymbol{w}\|^2 + C \sum_{i \in \{1,2,\dots,n\}} \xi_i \quad \text{s.t. } y_i f(\boldsymbol{x}_i) \geq 1 - \xi_i, \xi_i \geq 0, i \in \{1, 2, \dots, n\}$$
  - C is called the regularization parameter

Soft Margin

C is large



C is small



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 $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n), \boldsymbol{\mu} = (\mu_1, \ldots, \mu_n)$:

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

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

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

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

Dual Problem (3/4)

- Putting the three conditions to the Lagrange function to remove $\boldsymbol{w}$, w_0, and $\boldsymbol{\xi}$, yielding

$$
\begin{aligned}
L &= \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i\in[n]}\xi_i - \sum_{i\in[n]}\alpha_i\big(y_i f(\boldsymbol{x}_i) - 1 + \xi_i\big) - \sum_{i\in[n]}\mu_i\xi_i \\
&= \frac{1}{2}\|\boldsymbol{w}\|^2 - \sum_{i\in[n]}\alpha_i y_i\langle\boldsymbol{w},\boldsymbol{x}_i\rangle - w_0\sum_{i\in[n]}\alpha_i y_i + \sum_{i\in[n]}\alpha_i + \sum_{i\in[n]}(C-\alpha_i-\mu_i)\xi_i \\
&= -\frac{1}{2}\sum_{i,j\in[n]}\alpha_i\alpha_j y_i y_j\langle\boldsymbol{x}_i,\boldsymbol{x}_j\rangle + \sum_{i\in[n]}\alpha_i
\end{aligned}
$$

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

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

$$\text{subject to } \sum_{i\in[n]} \alpha_i y_i = 0,\ 0 \leq \alpha_i \leq C,\ i \in [n]$$

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:

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

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

$$\alpha_i \geq 0,\ \mu_i \geq 0,$$

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

$$i \in [n]$$

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
- Points on margin and inside margin are support vectors

How to Solve?

- The (dual) problem:

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

  - $Q \in \mathbb{R}^{n \times n}$ 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:

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

  - O and I are called active sets

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

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

  - 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
      $\boldsymbol{d} \leftarrow \boldsymbol{\alpha}_M^{\text{new}} - \boldsymbol{\alpha}_M$
      $\boldsymbol{\alpha}_M \leftarrow \boldsymbol{\alpha}_M + \eta \boldsymbol{d}$; // max. 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 $\phi(\boldsymbol{x})$, and $f(\boldsymbol{x})$ becomes

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

- The dual problem becomes

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

  $$\text{subject to } \sum_{i \in [n]} \alpha_i y_i = 0,\ 0 \leq \alpha_i \leq C, i \in [n]$$

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

C-SVM with Kernel Trick

- Use a kernel function: $K(\boldsymbol{x}_i, \boldsymbol{x}_j) = \langle \phi(\boldsymbol{x}_i), \phi(\boldsymbol{x}_j) \rangle$
- We have

$$\max_{\boldsymbol{\alpha}} -\frac{1}{2} \sum_{i,j \in [n]} \alpha_i \alpha_j y_i y_j K(\boldsymbol{x}_i, \boldsymbol{x}_j) + \sum_{i \in [n]} \alpha_i$$

$$\text{subject to } \sum_{i \in [n]} \alpha_i y_i = 0, \ 0 \le \alpha_i \le C, i \in [n]$$

  - The technique of using K is called kernel trick

Kernel Regression

- From regression:

$$\min_{\boldsymbol{\beta}} \sum_{i=1}^{N} (y_i - \boldsymbol{x}_i^T \boldsymbol{\beta})^2$$

to kernel regression:

$$\min \sum_{i=1}^{N} (y_i - f(\boldsymbol{x}_i))^2 = \min_{\boldsymbol{\alpha} \in \mathbb{R}^n} \sum_{i=1}^{N} \left(y_i - \sum_{j=1}^{N} \alpha_j K(\boldsymbol{x}_j, \boldsymbol{x}_i) \right)^2$$

  - Solved as $\boldsymbol{\alpha} = K^{-1} \boldsymbol{y}$
  - For a new data point $\boldsymbol{x}'$, its prediction is given as $\sum_{i=1}^{N} \alpha_i K(\boldsymbol{x}_i, \boldsymbol{x}')$
  - (Kernel) ridge regression (by adding $\lambda ||\boldsymbol{\beta}||_2^2$) is often used

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 (called Gram 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 semidefinite. Equivalent conditions of PSD are
  - There exists B s.t. $(K_{ij}) = B^T B$
  - $\boldsymbol{c}^T (K_{ij}) \boldsymbol{c} \geq 0$ for any $\boldsymbol{c} \in \mathbb{R}^n$
  - All eigenvalues of (K_{ij}) are nonnegative

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

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

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

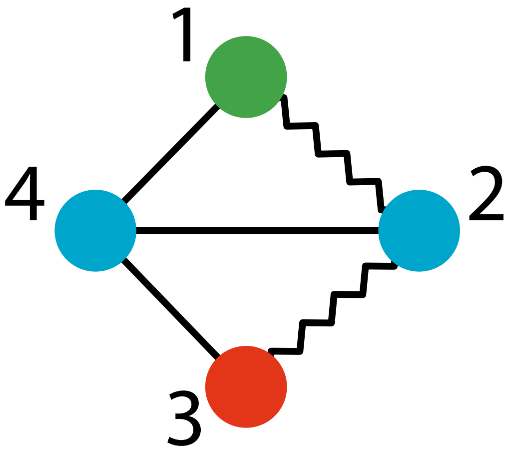
$$K_R(X, Y) = \sum_{s \in S, t \in T} K_{\text{base}}(s, t)$$

  - 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?

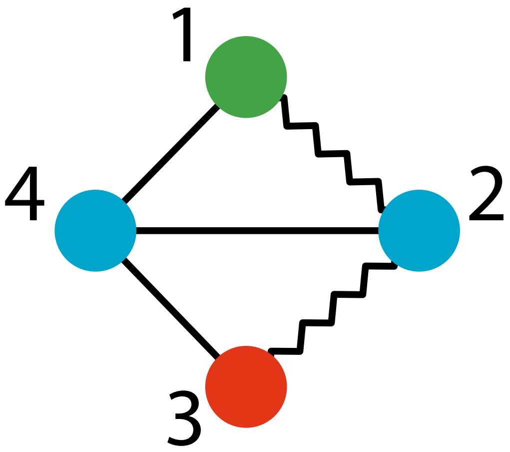
- An object consisting of vertices (nodes) connected with edges
- A graph is directed if the edges are directed,
  otherwise it is undirected
- A graph is written as $G = (V, E)$, where V is a vertex set and
  E is an edge set
- Labels can be associated with vertices and/or edges
  - If a function ϕ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

Example of Graph



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

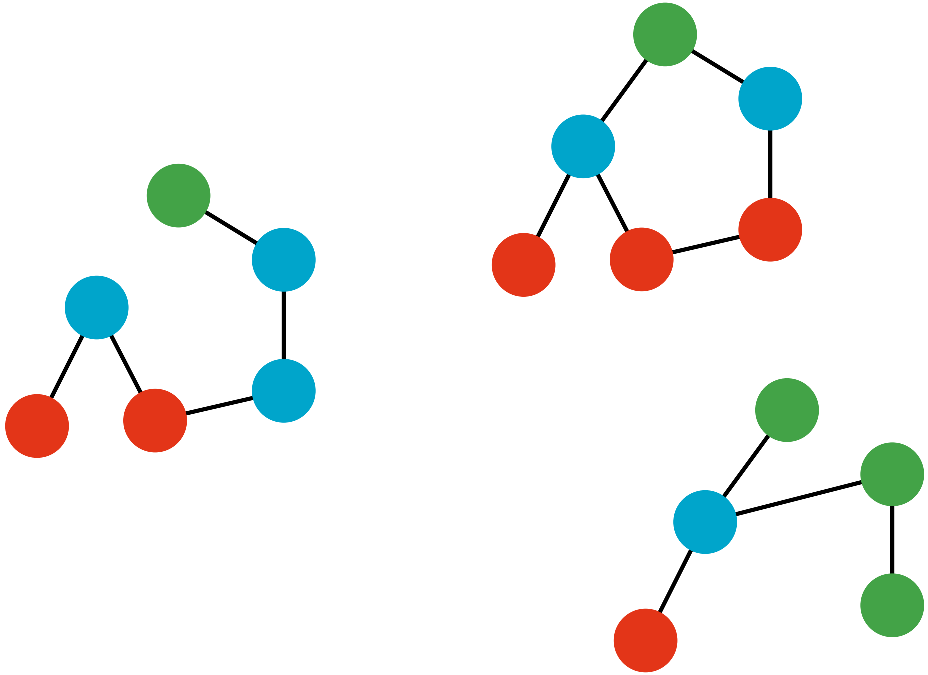
Example of Graph



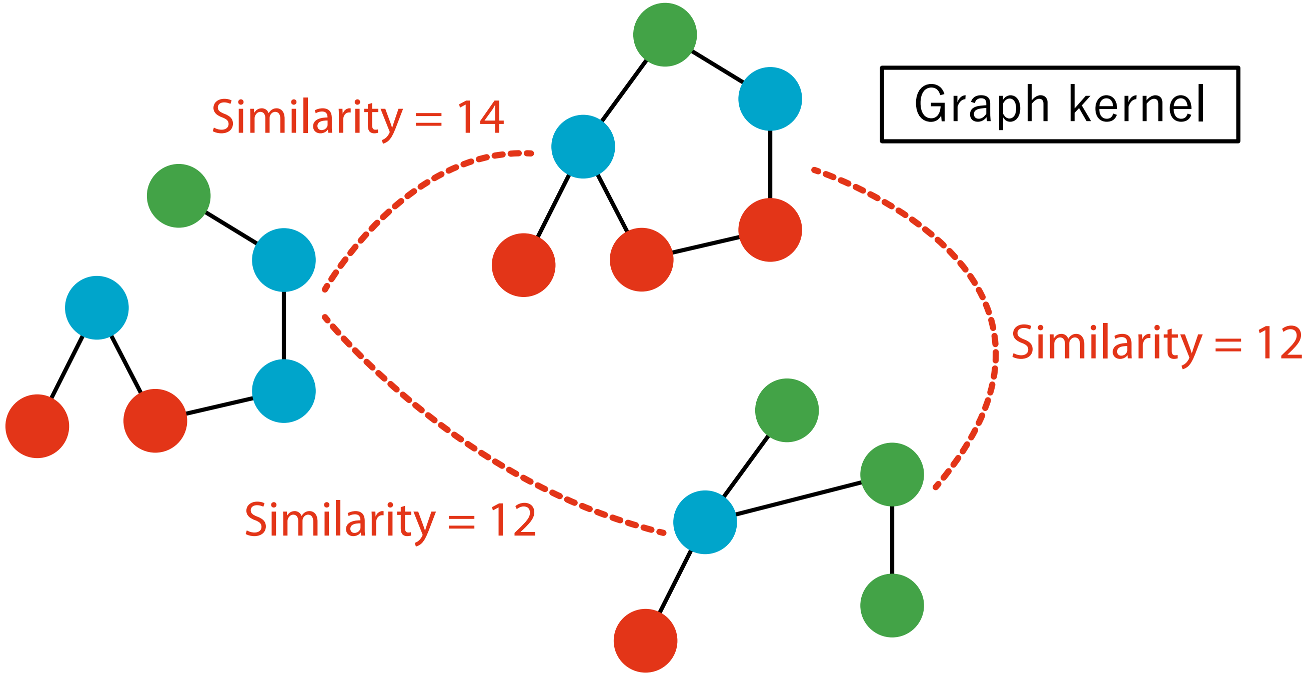
- The adjacency matrix

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

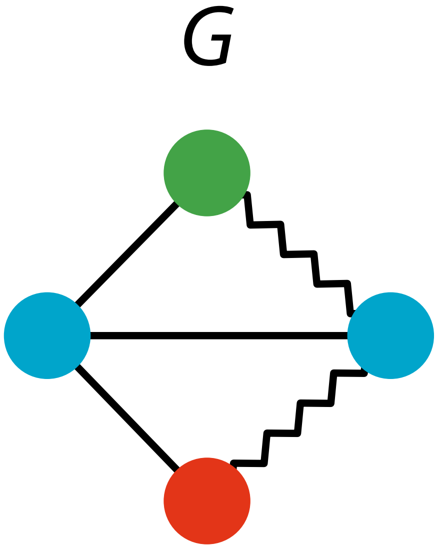
Similarity between Graphs

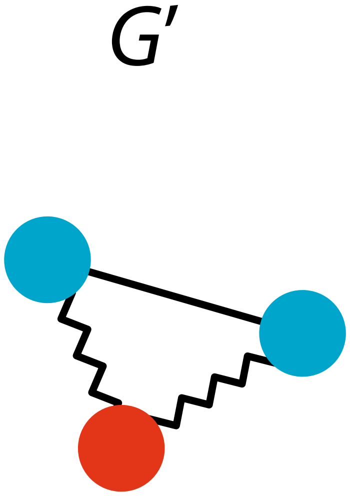


Similarity between Graphs



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

$$K_{EH}(G, G') = 3 \cdot 1 + 2 \cdot 2 = 7$$

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

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

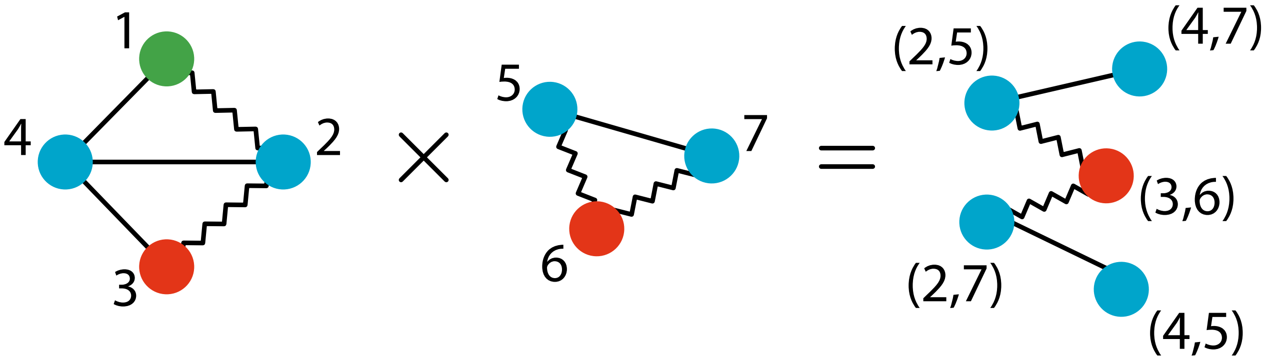
Product Graph

- The direct product $G_\times = (V_\times, E_\times, \phi_\times)$ of G and G':

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

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

  - 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 $\ell \in \{0, \dots, k\}$ (geometric series), resulting in the geometric random walk kernel:

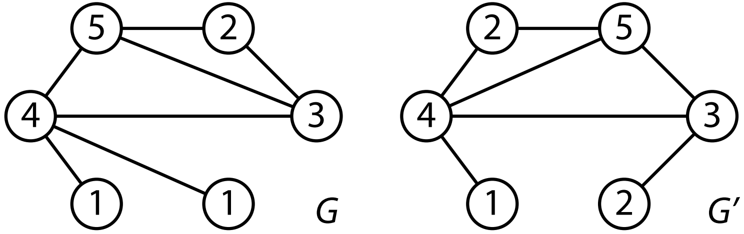
$$K_{\mathrm{GR}}(G, G') = \sum_{i,j=1}^{|V_\times|} \left[\lambda^0 A_\times^0 + \lambda^1 A_\times^1 + \lambda^2 A_\times^2 + \cdots\right]_{ij} = \sum_{i,j=1}^{|V_\times|} \left[\sum_{\ell=0}^{\infty} \lambda^\ell A_\times^\ell\right]_{ij}$$

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

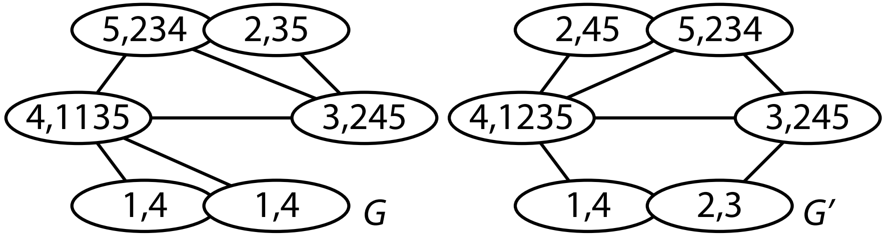
  - Well-defined only if $\lambda < 1/\mu_{\times,\max}$ ($\mu_{\times,\max}$ is the max. eigenvalue of $A_\times$)
  - $\delta_\times$ (min. degree) $\leq \overline{d}_\times$ (average degree) $\leq \mu_{\times,\max} \leq \Delta_\times$ (max. degree)

Weisfeiler–Lehman Kernel

Given graphs



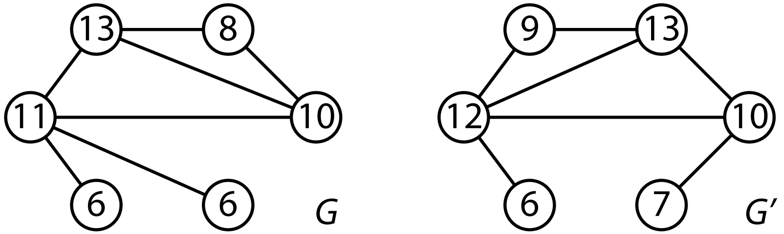
1st iteration



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



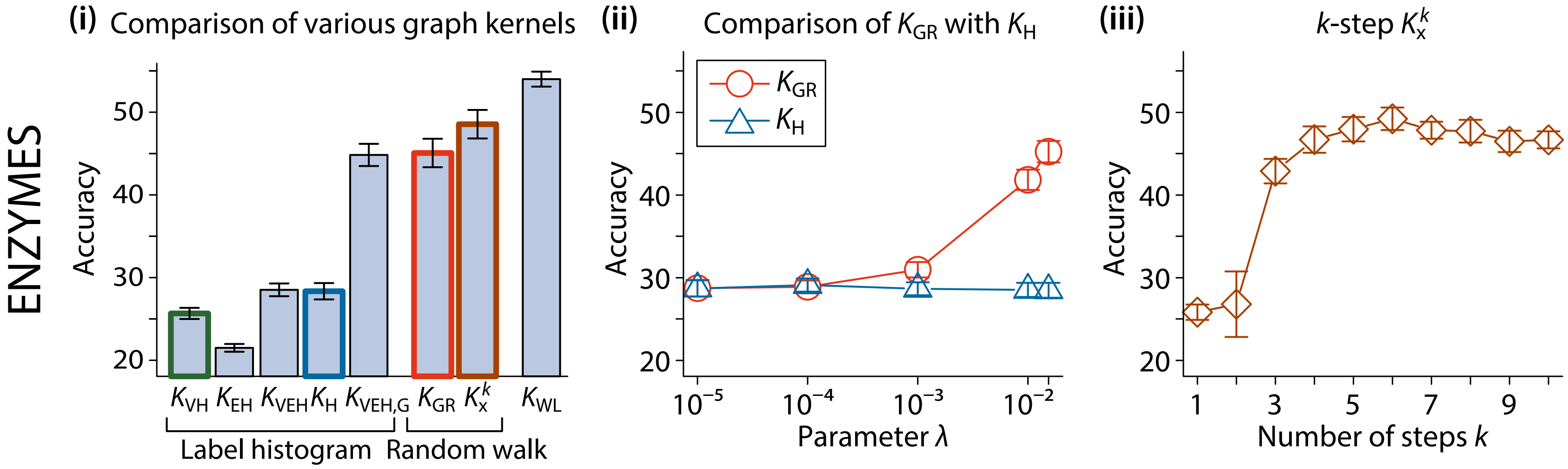
Weisfeiler–Lehman Kernel

- The kernel value becomes:

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

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

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

Summary

- SVM finds the “best” classification hyperplane
  - The margin is maximized
- Although the original SVM can perform only linear classification, it can be extended to nonlinear classification for structured data using kernels
- Gaussian kernel + C-SVM can be the first choice for numerical data
- WL kernel can be the first choice for graph data