Kernels for Structured Data

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Outline

Structured Data

Ubiquitous in important application domains

- **Bioinfomatics**
  e.g. DNA sequences and evolutionary trees
- **Natural language processing**
  e.g. textual documents and parse trees
- **Computer security**
  e.g. network packets and program behavior
- **Chemoinformatics**
  e.g. molecule structures and relations

How to incorporate structure into learning methods?

What is a Kernel?

- A positive semi-definite function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$
- Similarity measure for objects in a domain $\mathcal{X}$
- Basic building block for many learning algorithms

Definition

A symmetric function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a *Kernel* if and only if for any subset $\{x_1, \dots, x_l\} \subset \mathcal{X}$ k is positive semi-definite, that is

$$\sum_{i,j=1}^{l} c_i c_j k(x_i, x_j) \geq 0 \quad \text{with} \quad c_1, \dots, c_l \in \mathbb{R}.$$

Classic Kernels

Let $\mathcal{X} \subseteq \mathbb{R}^d$. Then kernels $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ are given by

- Linear kernel $k(x, y) := \langle x, y \rangle = \sum_{i=1}^{d} x_i y_i$
- Polynomial kernel $k(x, y) := (\langle x, y \rangle + \theta)^p$
- Gaussian kernel $k(x, y) := \exp\left(\frac{||x-y||^2}{\gamma}\right)$
- $\ldots$

But: type of domain $\mathcal{X}$ not restricted to vectorial data.

Induced Feature Space

Theorem

A kernel k induces a feature map $\psi : \mathcal{X} \to \mathcal{H}$ to a Hilbert space, such that for all $x, y \in \mathcal{X}$

$$k(x, y) = \langle \psi(x), \psi(y) \rangle$$

corresponds to an inner product in $\mathcal{H}$.

- Access to inner products, vector norms and distances, e.g.,

$$||\psi(x)||_2 = \sqrt{k(x, x)}$$

$$||\psi(x) - \psi(y)||_2 = \sqrt{k(x, x) + k(y, y) - 2k(x, y)}$$

Why use Kernels for Learning?

Advantages

- Efficient computation in high-dimensional feature spaces
- Non-linear feature maps for complex decision surfaces
- Abstraction from data representation and learning methods
  $\Rightarrow$ application of learning methods to structured data

Kernel-based learning

- Classification (Support Vector Machines, Kernel Peceptron)
- Clustering (Kernel k-means, Spectral Clustering)
- Data projection (Kernel PCA, Kernel ICA)

Kernels for Sequences

Sequences

Alphabet

An alphabet $\mathcal{A}$ is a finite set of discrete symbols

- DNA, $\mathcal{A} = \{A, C, G, T\}$
- Natural language text, $\mathcal{A} = \{a, b, c, \ldots A, B, C, \ldots\}$

Sequence

A sequence x is concatenation of symbols from $\mathcal{A}$, i.e., $x \in \mathcal{A}^*$

- $\mathcal{A}^n$ = all sequences of length n
- $\mathcal{A}^*$ = all sequences of arbitary length
- $|x|$ = length of a sequence

Embedding Sequences

- Characterize sequences using a *language* $L \subseteq \mathcal{A}^*$.
- Feature space spanned by frequencies of words $w \in L$

Feature map

A function $\phi : \mathcal{A}^* \to \mathbb{R}^{|L|}$ mapping sequences to $\mathbb{R}^{|L|}$ given by

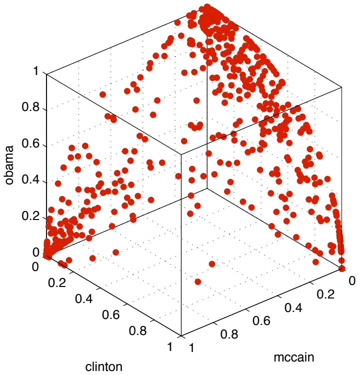
$$x \mapsto \left(\#_w(x) \cdot \sqrt{N_w}\right)_{w \in L}$$

where $\#_w(x)$ returns the frequency of w in sequence x.

- Refinement of embeddung using weighting constants N_w
- Normalization, often $||\phi(x)||_1 = 1$ or $||\phi(x)||_2 = 1$.

Example: Embedding

Embedding of new articles using the exemplary language
$L = \{\text{McCain}, \text{Clinton}, \text{Obama}\}$



Vectorial representation of sequence content via language L

Data lies on quarter-sphere due to $||\phi(x)||_2 = 1$ normalization

Source: news.google.com on 15. April 2008

Sequence Kernels

Generic Sequence Kernel

A sequence kernel $k : \mathcal{A}^* \times \mathcal{A}^* \to \mathbb{R}$ over ϕ is defined by

$$k(x,y) = \langle \phi(x), \phi(y) \rangle = \sum_{w \in L} \#_w(x) \cdot \#_w(y) \cdot N_w$$

Proof.

By definition k is an inner product in $\mathbb{R}^{|L|}$ and thus symmetric and positive semi-definite. □

- Feature space induced by ϕ *explicit* but *sparse*.
- Naive running time $\mathcal{O}(|x|^2 + |y|^2)$

Bag-of-Words

Characterization of sequences by non-overlapping words.

$x =$"Hasta la vista, baby." $\longrightarrow$ { "Hasta", "la", "vista", "baby" }

Bag-of-Words Kernel

Sequence kernel using embedding language containing words

$$L = \text{Dictionary (explicit)} \quad \text{or} \quad L = (\mathcal{A} \backslash D)^* \text{ (implicit)}$$

with $D \subset \mathcal{A}$ delimiter symbols, e.g., punctation and space.

- Extension using stemming techniques, "helping" $\Rightarrow$ "help"
- Weighting to control contribution of words

Implementing Bag-of-Words

- Efficient realization using sorted arrays or hash tables

$$x = \text{“to be or not to be”}$$
$$\phi(x) = [\text{“be”} : 2] \to [\text{“not”} : 1] \to [\text{“or”} : 1] \to [\text{“to”} : 2]$$

- Kernel computation similar to merging lists

$$\phi(x) = [\text{“be”} : 2] \to [\text{“not”} : 1] \to [\text{“or”} : 1] \to [\text{“to”} : 2]$$
$$\phi(y) = [\text{“be”} : 1] \to [\text{“free”} : 1] \to [\text{“to”} : 1]$$
$$\longrightarrow \quad 2 \cdot 1 \quad + \quad 2 \cdot 1$$

- Run-time $\mathcal{O}(n|x| + n|y|)$ for words of length n.

N-grams

Characterization of sequences by subsequences of length n

$$x = \text{“Hasta la vista, baby.”} \longrightarrow \{\text{ “Has”, “ast”, “sta”, } \ldots \}$$

Spectrum Kernel

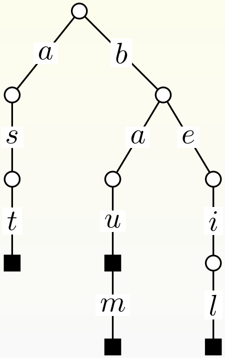
Sequence kernel using embedding language containing all sequences of length n (n-grams):

$$L = \mathcal{A}^n \text{ (normal)} \quad \text{or} \quad L = \bigcup_{i=1}^{n} \mathcal{A}^i \text{ (blended)}$$

- No prior knowledge of application domain required
- Note: n-grams have fixed overlap of $n-1$ symbols

Tries

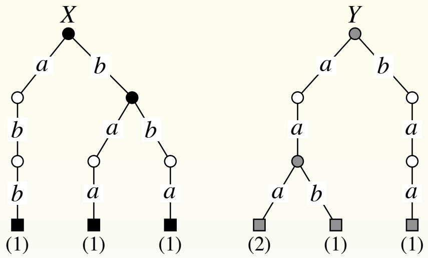
Efficient data structure for storage of sequences



- "Trie" = Re**trie**val tree (also dictionary or keyword tree)
- Path from root to marked node represents stored sequence
- Example sequences: {"ast", "bau", "baum", "beil"}

Implementation of N-grams

Efficient realization using Trie representation



Tries of 3-grams for $x =$“abbaa” and $y =$“baaaab”

- Kernel computation via parallel traversal of matching nodes
- Run-time $\mathcal{O}(n \cdot \min(|x|, |y|))$ for n-grams
- Blended n-grams by storing $\#_w(x)$ in inner nodes.

Positional N-grams

Incorporation of positional information into *n*-gram concept

x = "Hasta la vista, baby." $\rightarrow$ { "$\mathrm{H_1a_2s_3}$", "$\mathrm{a_2s_3t_4}$", "$\mathrm{s_5t_6a_7}$", ... }

Weighted Degree Kernel

Sequence kernel using *n*-grams and extended alphabet

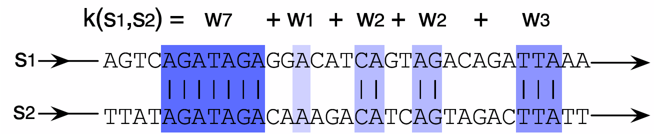
$$\tilde{\mathcal{A}} = \mathcal{A} \times \mathbb{N},$$

where for $(a, p) \in \tilde{\mathcal{A}}$, a encodes a symbol and p its position

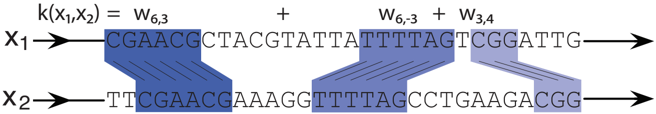
- Extension by incorporating minor positional shifts

Implementation of Positional N-grams

Efficient realization by looping over sequences



Implementation with shifts via multiple looping



Run-time $\mathcal{O}(s \cdot \max(|x|, |y|))$ with shift s

Contiguous Subsequences

Characterization using all possible subsequences

$$x = \text{“Hasta la vista, baby.”} \longrightarrow \{\text{“H”}, \text{“Ha”}, \text{“Has”}, \ldots\}$$

Contiguous Subsequence Kernel

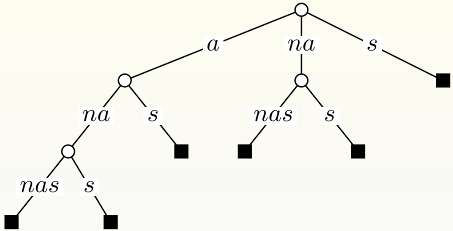
Sequence kernel using embedding language containing all possible sequences

$$L = \mathcal{A}^* = \bigcup_{i=1}^{\infty} \mathcal{A}^i$$

- Arbitary overlap ⇒ quadratic amount of subsequences
- Weighting to control contribution of subsequences, e.g. length-dependent $N_w = \lambda^{|-w|}$ with $0 < \lambda \leq 1$

Suffix Trees

- Efficient and versatile sequence representation
- Suffix Tree = Trie containing all suffixes of a sequence

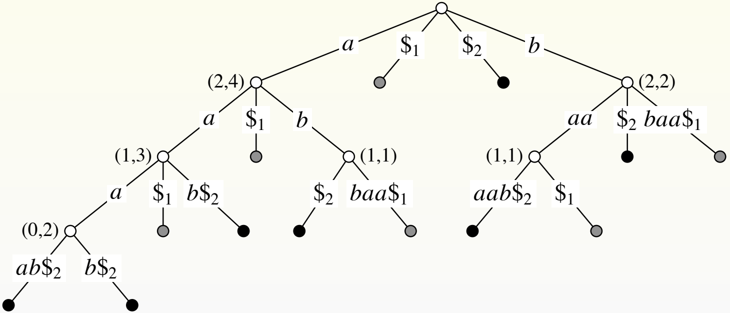


- Compact storage by edge compression, e.g. *nas* $\Rightarrow [4, 6]$
- Example sequence: "ananas"

Implementation of Subsequences

Efficient realization using generalized suffix trees (GST)

GST for x ="abbaa" and y ="baaaab" using z ="abaa$\$_1$baaab$\$_2$"



- Kernel computation via depth-first search in suffix tree
- $\mathcal{O}(|z|)$ inner nodes $\Rightarrow$ run-time $\mathcal{O}(|z|) = \mathcal{O}(|x| + |y|)$

Kernels for Trees

Trees and Parse Trees

Tree

A tree $x = (V, E, v^*)$ is an acyclic graph (V, E) rooted at $v^* \in V$.

Parse tree

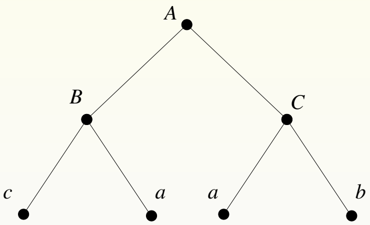
A tree x derived from a context-free grammar, such that each node $v \in V$ is associated with a production rule $p(v)$.

Further notation

- v_i = i-th child of node $v \in V$,
- $|v|$ = number of children of $v \in V$
- and the set $\mathcal{T}$ of all parse trees

Parse Trees

Tree representation of "sentences" derived from a grammar



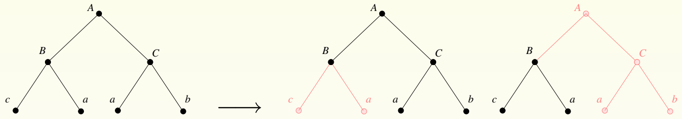
Parse tree for *caab* using grammar over $\{A, B, C, a, b, c\}$ and productions

- $p_1 : A \longrightarrow B\ C$
- $p_2 : B \longrightarrow c\ a$
- $p_3 : C \longrightarrow a\ b$

Common data structure in natural language processing and design of programming languages, compilers, etc.

Embedding subtrees

Characterization of parse trees by contained subtrees



Feature map

A function $\phi : \mathcal{T} \rightarrow \mathbb{R}^{|\mathcal{T}|}$ mapping trees to $\mathbb{R}^{|\mathcal{T}|}$ given by

$$x \mapsto (\mathbb{I}_t(x))_{t \in \mathcal{T}}$$

where $\mathbb{I}_t(x)$ indicates if t is a subtree of parse tree x.

- Binary feature space spanned by indicator for subtrees

Parse Tree Kernel

Parse Tree Kernel

A tree kernel $k : \mathcal{T} \times \mathcal{T} \to \mathbb{R}$ is given by

$$k(x, y) = \langle \phi(x), \phi(y) \rangle = \sum_{t \in T} \mathbb{I}_t(x) \mathbb{I}_t(y)$$

Proof.

By definition k is an inner product in the space of all trees $\mathcal{T}$ and thus is symmetric and positive semi-definite. □

- $\mathcal{T}$ has infinite size $\Rightarrow$ naive computation infeasible

Counting shared subtrees

- Parse tree kernel counts the number of shared subtrees
- For each pair (v, w) determine shared subtrees at v and w.

$$k(x, y) = \sum_{t \in T} \mathbb{I}_t(x)\mathbb{I}_t(y) = \sum_{v \in V_x} \sum_{w \in V_y} c(v, w)$$

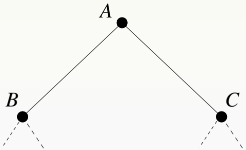
Counting function

- $c(v, w) = 0 \;\text{ if } p(v) \neq p(w)$ (different)
- $c(v, w) = 1 \;\text{ if } |v| = |w| = 0$ (leaves)
- otherwise

$$c(v, w) = \prod_{i=1}^{|v|} (1 + c(v_i, w_i))$$

Counting function in Detail

- First base case: $c(v,w) = 0$ if $p(v) \neq p(w)$
  $\Rightarrow$ trivial, no match = no shared subtrees
- Second base case: $c(v,w) = 1$ if $|v| = |w| = 0$
  $\Rightarrow$ trivial, one leave = one subtree
- Recursion: $c(v,w) = \prod_{i=1}^{|v|}(1 + c(v_i, w_i))$

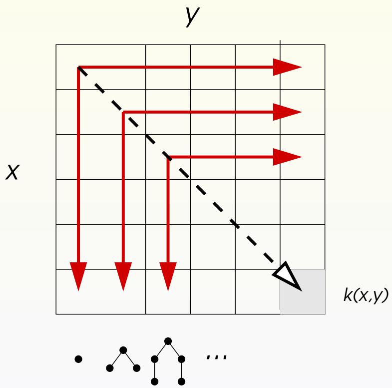


$$c(v_A, w_A) = (1 + c(v_B, w_B)) \cdot (1 + c(v_C, w_C))$$

Pair all shared subtrees in B with C including edges to A.

Implementation of Parse Tree Kernel

Realization using dynamic programming table.



Matrix of all $c(v, w)$ with $(v, w) \in V_x \times V_y$ ordered by descending depth

Run-time $\mathcal{O}(|V_x| \cdot |V_y|)$. Speed-up by skipping non-matching node pairs.

Shallow Tree Kernel

Idea: map trees to sequences and apply sequence kernels

Flattening

A function $f : \mathcal{T} \to \mathcal{A}^*$ mapping trees to sequences given by $f(x) \mapsto m(v^*)$ with

$$m(v) = \text{“}[\text{”} \circ m(v_1) \circ \cdots m(v_{|v|}) \circ \text{“}]\text{”}$$

Shallow tree kernel

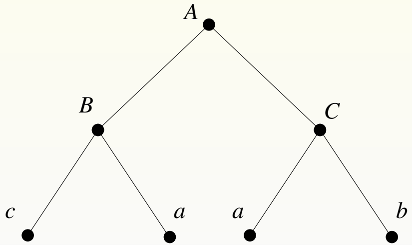
A kernel $k : \mathcal{T} \times \mathcal{T} \to \mathbb{R}$ based on a sequence kernel $\hat{k}$ given by

$$k(x, y) = \hat{k}(f(x), f(y)).$$

Flattening a Tree

Implementation of flattening

- Computation by depth-first traversal of tree
- Run-time dependent on traversal and sequence kernel



Example

- With labels $f(x) =$ "[A[B[c][a]][C[a][b]]]"
- Without labels $f(x) =$ "[[[][]][[][]]]"

Conclusions

Kernels for structured data

- Effective means for learning with structured data
- Various efficient kernels for sequences and trees

More on structured data and kernels

- Kernel for graphs, images, sounds
- . . .

Interesting applications (upcoming lectures)

- "Catching hackers": Network intrusion detection
- "Discovering genes": Analysis of DNA sequences

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