

Foundations of Machine Learning

Lecture 5

Mehryar Mohri
Courant Institute and Google Research
mohri@cims.nyu.edu

Kernel Methods

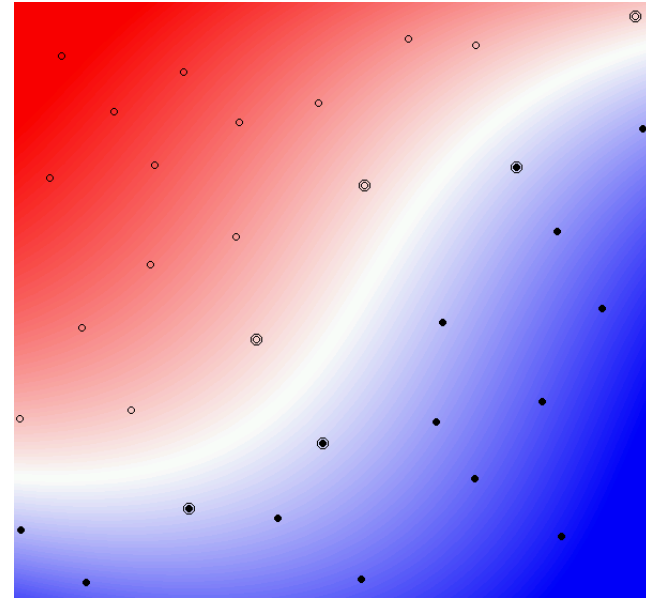
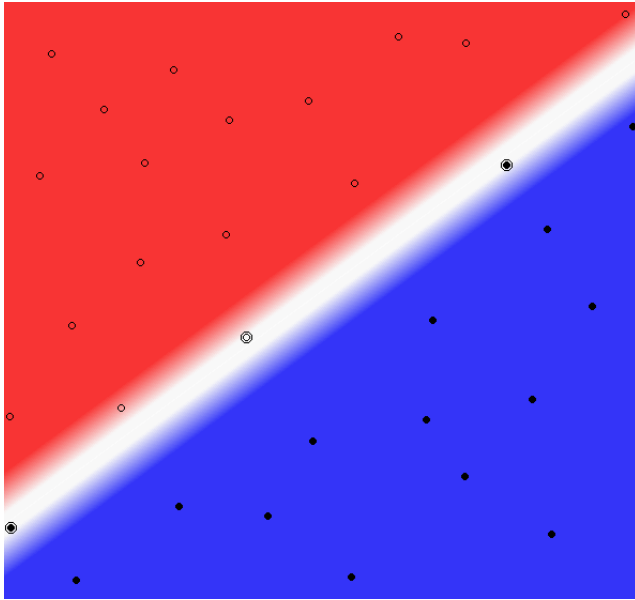
Motivation

- Non-linear decision boundary.
- Efficient computation of inner products in high dimension.
- Flexible selection of more complex features.

This Lecture

- Definitions
- SVMs with kernels
- Closure properties
- Sequence Kernels
- Negative kernels

Non-Linear Separation



- Linear separation impossible in most problems.
- Non-linear mapping from input space to high-dimensional feature space: $\Phi: X \rightarrow F$.
- Generalization ability: independent of $\dim(F)$, depends only on ρ and m .

Kernel Methods

■ Idea:

- Define $K : X \times X \rightarrow \mathbb{R}$, called **kernel**, such that:

$$\Phi(x) \cdot \Phi(y) = K(x, y).$$

- K often interpreted as a similarity measure.

■ Benefits:

- **Efficiency**: K is often more efficient to compute than Φ and the dot product.
- **Flexibility**: K can be chosen arbitrarily so long as the existence of Φ is guaranteed (PDS condition or Mercer's condition).

PDS Condition

- **Definition:** a kernel $K: X \times X \rightarrow \mathbb{R}$ is **positive definite symmetric** (PDS) if for any $\{x_1, \dots, x_m\} \subseteq X$, the matrix $\mathbf{K} = [K(x_i, x_j)]_{ij} \in \mathbb{R}^{m \times m}$ is symmetric positive semi-definite (SPSD).
- \mathbf{K} is SPD if symmetric and one of the 2 equiv. cond.'s:
 - its eigenvalues are non-negative.
 - for any $\mathbf{c} \in \mathbb{R}^{m \times 1}$, $\mathbf{c}^\top \mathbf{K} \mathbf{c} = \sum_{i,j=1}^m c_i c_j K(x_i, x_j) \geq 0$.
- **Terminology:** PDS for kernels, SPD for kernel matrices (see (Berg et al., 1984)).

Example - Polynomial Kernels

■ Definition:

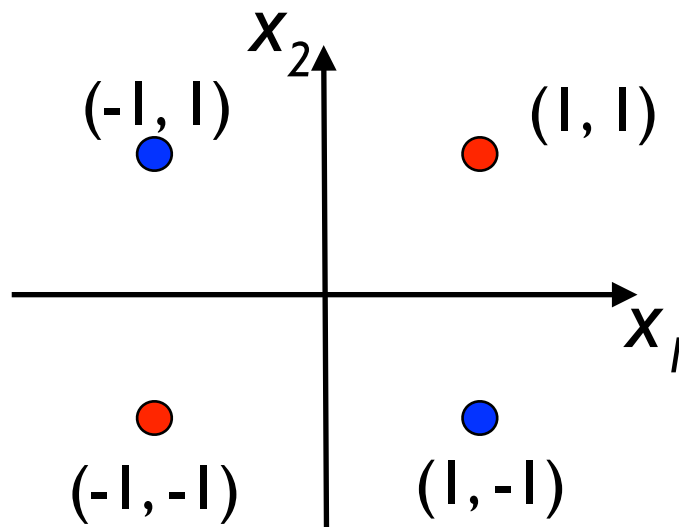
$$\forall x, y \in \mathbb{R}^N, \quad K(x, y) = (x \cdot y + c)^d, \quad c > 0.$$

■ Example: for $N=2$ and $d=2$,

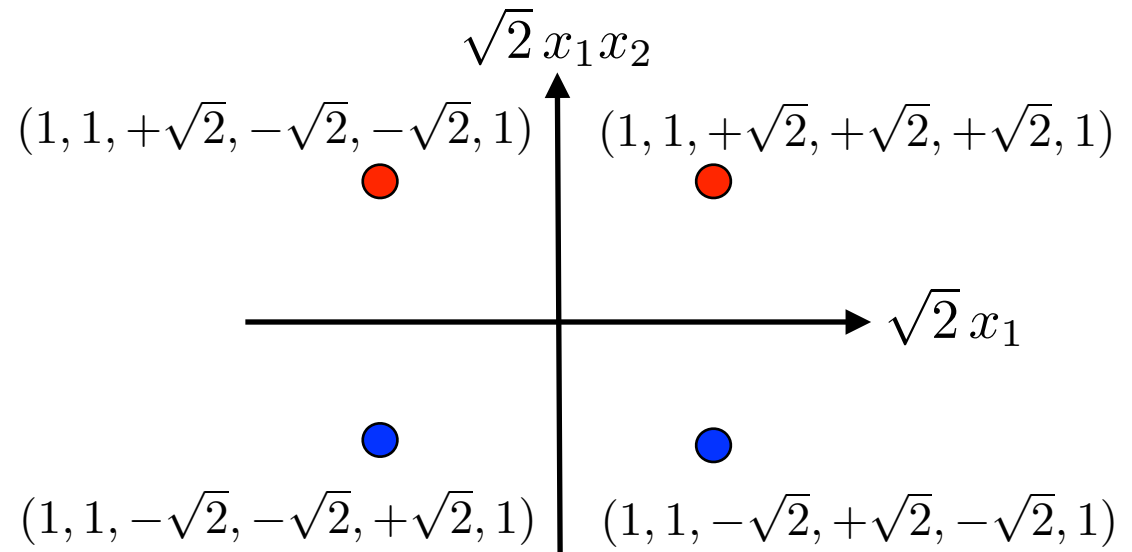
$$\begin{aligned} K(x, y) &= (x_1 y_1 + x_2 y_2 + c)^2 \\ &= \begin{bmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2} x_1 x_2 \\ \sqrt{2c} x_1 \\ \sqrt{2c} x_2 \\ c \end{bmatrix} \cdot \begin{bmatrix} y_1^2 \\ y_2^2 \\ \sqrt{2} y_1 y_2 \\ \sqrt{2c} y_1 \\ \sqrt{2c} y_2 \\ c \end{bmatrix}. \end{aligned}$$

XOR Problem

- Use second-degree polynomial kernel with $c = 1$:



Linearly non-separable



Linearly separable by
 $x_1x_2 = 0$.

Normalized Kernels

- **Definition:** the **normalized kernel** K' associated to a kernel K is defined by

$$\forall x, x' \in \mathcal{X}, K'(x, x') = \begin{cases} 0 & \text{if } (K(x, x) = 0) \vee (K(x', x') = 0) \\ \frac{K(x, x')}{\sqrt{K(x, x)K(x', x')}} & \text{otherwise.} \end{cases}$$

- If K is PDS, then K' is PDS:

$$\sum_{i,j=1}^m \frac{c_i c_j K(x_i, x_j)}{\sqrt{K(x_i, x_i)K(x_j, x_j)}} = \sum_{i,j=1}^m \frac{c_i c_j \langle \Phi(x_i), \Phi(x_j) \rangle}{\|\Phi(x_i)\|_H \|\Phi(x_j)\|_{\mathbb{H}}} = \left\| \sum_{i=1}^m \frac{c_i \Phi(x_i)}{\|\Phi(x_i)\|_H} \right\|_{\mathbb{H}}^2 \geq 0.$$

- By definition, for all x with $K(x, x) \neq 0$,

$$K'(x, x) = 1.$$

Other Standard PDS Kernels

■ Gaussian kernels:

$$K(x, y) = \exp \left(-\frac{\|x - y\|^2}{2\sigma^2} \right), \quad \sigma \neq 0.$$

- Normalized kernel of $(\mathbf{x}, \mathbf{x}') \mapsto \exp \left(\frac{\mathbf{x} \cdot \mathbf{x}'}{\sigma^2} \right)$.

■ Sigmoid Kernels:

$$K(x, y) = \tanh(a(x \cdot y) + b), \quad a, b \geq 0.$$

This Lecture

- Definitions
- SVMs with kernels
- Closure properties
- Sequence Kernels
- Negative kernels

Reproducing Kernel Hilbert Space

(Aronszajn, 1950)

- **Theorem:** Let $K: X \times X \rightarrow \mathbb{R}$ be a PDS kernel. Then, there exists a Hilbert space H and a mapping Φ from X to H such that

$$\forall x, y \in X, \quad K(x, y) = \Phi(x) \cdot \Phi(y).$$

- **Proof:** For any $x \in X$, define $\Phi(x): X \rightarrow \mathbb{R}^X$ as follows:

$$\forall y \in X, \quad \Phi(x)(y) = K(x, y).$$

- Let $H_0 = \left\{ \sum_{i \in I} a_i \Phi(x_i) : a_i \in \mathbb{R}, x_i \in X, \text{card}(I) < \infty \right\}$.
- We are going to define an inner product $\langle \cdot, \cdot \rangle$ on H_0 .

- **Definition:** for any $f = \sum_{i \in I} a_i \Phi(x_i)$, $g = \sum_{j \in J} b_j \Phi(y_j)$,

$$\langle f, g \rangle = \sum_{i \in I, j \in J} a_i b_j K(x_i, y_j) = \sum_{j \in J} b_j f(y_j) = \sum_{i \in I} a_i g(x_i).$$

does not depend on representations of f and g .

- $\langle \cdot, \cdot \rangle$ is bilinear and symmetric.
- $\langle \cdot, \cdot \rangle$ is positive semi-definite since K is PDS:

$$\text{for any } f, \langle f, f \rangle = \sum_{i, j \in I} a_i a_j K(x_i, x_j) \geq 0.$$

for any f_1, \dots, f_m and c_1, \dots, c_m ,

$$\sum_{i, j=1}^m c_i c_j \langle f_i, f_j \rangle = \left\langle \sum_{i=1}^m c_i f_i, \sum_{j=1}^m c_j f_j \right\rangle \geq 0.$$

→ $\langle \cdot, \cdot \rangle$ is a PDS kernel on H_0 .

- $\langle \cdot, \cdot \rangle$ is definite.

- first, **Cauchy-Schwarz** inequality for PDS kernels.
If K is PDS, $\mathbf{M} = \begin{pmatrix} K(x,x) & K(x,y) \\ K(y,x) & K(y,y) \end{pmatrix}$ is SPSPD for all $x, y \in X$
In particular, the product of its eigenvalues, $\det(\mathbf{M})$ is non-negative:

$$\det(\mathbf{M}) = K(x, x)K(y, y) - K(x, y)^2 \geq 0.$$

- since $\langle \cdot, \cdot \rangle$ is a PDS kernel, for any $f \in H_0$ and $x \in X$,

$$\langle f, \Phi(x) \rangle^2 \leq \langle f, f \rangle \langle \Phi(x), \Phi(x) \rangle.$$

- observe the **reproducing property** of $\langle \cdot, \cdot \rangle$:

$$\forall f \in H_0, \forall x \in X, f(x) = \langle f, \Phi(x) \rangle.$$

- Thus, $[f(x)]^2 \leq \langle f, f \rangle K(x, x)$ for all $x \in X$, which shows the definiteness of $\langle \cdot, \cdot \rangle$.

- Thus, $\langle \cdot, \cdot \rangle$ defines an inner product on H_0 , which thereby becomes a pre-Hilbert space.
- H_0 can be completed to form a Hilbert space H in which it is dense.

■ Notes:

- H is called the reproducing kernel Hilbert space (**RKHS**) associated to K .
- A Hilbert space such that there exists $\Phi: X \rightarrow H$ with $K(x, y) = \Phi(x) \cdot \Phi(y)$ for all $x, y \in X$ is also called a **feature space** associated to K . Φ is called a **feature mapping**.
- Feature spaces associated to K are in general **not unique**.

Consequence: SVMs with PDS Kernels

(Boser, Guyon, and Vapnik, 1992)

■ Constrained optimization:

$$\max_{\alpha} \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i,j=1}^m \alpha_i \alpha_j y_i y_j \underbrace{K(x_i, x_j)}_{\Phi(x_i) \cdot \Phi(x_j)}$$

$$\text{subject to: } 0 \leq \alpha_i \leq C \wedge \sum_{i=1}^m \alpha_i y_i = 0, i \in [1, m].$$

■ Solution:

$$h(x) = \text{sgn}\left(\sum_{i=1}^m \alpha_i y_i \underbrace{K(x_i, x)}_{\Phi(x_i) \cdot \Phi(x)} + b\right),$$

$$\text{with } b = y_i - \sum_{j=1}^m \alpha_j y_j \underbrace{K(x_j, x_i)}_{\Phi(x_j) \cdot \Phi(x_i)} \text{ for any } x_i \text{ with } 0 < \alpha_i < C.$$

Generalization: Representer Theorem

(Kimeldorf and Wahba, 1971)

■ **Theorem:** Let $K: X \times X \rightarrow \mathbb{R}$ be a PDS kernel with H the corresponding RKHS. Then, for any non-decreasing function $G: \mathbb{R} \rightarrow \mathbb{R}$ and any $L: \mathbb{R}^m \rightarrow \mathbb{R} \cup \{+\infty\}$ problem

$$\operatorname{argmin}_{h \in H} F(h) = \operatorname{argmin}_{h \in H} G(\|h\|_H) + L(h(x_1), \dots, h(x_m))$$

admits a solution of the form $h^* = \sum_{i=1}^m \alpha_i K(x_i, \cdot)$.

If G is further assumed to be increasing, then any solution has this form.

- **Proof:** let $H_1 = \text{span}(\{K(x_i, \cdot) : i \in [1, m]\})$. Any $h \in H$ admits the decomposition $h = h_1 + h^\perp$ according to $H = H_1 \oplus H_1^\perp$.
- Since G is non-decreasing,

$$G(\|h_1\|_H) \leq G\left(\sqrt{\|h_1\|_H^2 + \|h^\perp\|_H^2}\right) = G(\|h\|_H).$$
- By the reproducing property, for all $i \in [1, m]$,

$$h(x_i) = \langle h, K(x_i, \cdot) \rangle = \langle h_1, K(x_i, \cdot) \rangle = h_1(x_i).$$
- Thus, $L(h(x_1), \dots, h(x_m)) = L(h_1(x_1), \dots, h_1(x_m))$ and $F(h_1) \leq F(h)$.
- If G is increasing, then $F(h_1) < F(h)$ when $h^\perp \neq 0$ and any solution of the optimization problem must be in H_1 .

Rad. Complexity of Kernel-Based Hypotheses

■ **Theorem:** Let $K: X \times X \rightarrow \mathbb{R}$ be a PDS kernel and let $\Phi: X \rightarrow H$ be a feature mapping associated to K . Let $S \subseteq \{x: K(x, x) \leq R^2\}$ be a sample of size m , and let $H = \{\mathbf{x} \mapsto \mathbf{w} \cdot \Phi(x) : \|\mathbf{w}\|_H \leq \Lambda\}$. Then,

$$\hat{\mathfrak{R}}_S(H) \leq \frac{\Lambda \sqrt{\text{Tr}[\mathbf{K}]}}{m} \leq \sqrt{\frac{R^2 \Lambda^2}{m}}.$$

■ **Proof:**
$$\begin{aligned} \hat{\mathfrak{R}}_S(H) &= \frac{1}{m} \mathbb{E}_{\sigma} \left[\sup_{\|\mathbf{w}\| \leq \Lambda} \mathbf{w} \cdot \sum_{i=1}^m \sigma_i \Phi(x_i) \right] \leq \frac{\Lambda}{m} \mathbb{E}_{\sigma} \left[\left\| \sum_{i=1}^m \sigma_i \Phi(x_i) \right\| \right] \\ (\text{Jensen's ineq.}) &\leq \frac{\Lambda}{m} \left[\mathbb{E}_{\sigma} \left[\left\| \sum_{i=1}^m \sigma_i \Phi(x_i) \right\|^2 \right] \right]^{1/2} \leq \frac{\Lambda}{m} \left[\mathbb{E}_{\sigma} \left[\sum_{i=1}^m \|\Phi(x_i)\|^2 \right] \right]^{1/2} \\ &= \frac{\Lambda}{m} \left[\mathbb{E}_{\sigma} \left[\sum_{i=1}^m K(x_i, x_i) \right] \right]^{1/2} = \frac{\Lambda \sqrt{\text{Tr}[\mathbf{K}]}}{m} \leq \sqrt{\frac{R^2 \Lambda^2}{m}}. \end{aligned}$$

Kernel-Based Algorithms

- PDS kernels used to extend a variety of algorithms in classification and other areas:
 - regression.
 - ranking.
 - dimensionality reduction.
 - clustering.
- But, how do we define PDS kernels?

This Lecture

- Definitions
- SVMs with kernels
- Closure properties
- Sequence Kernels
- Negative kernels

Closure Properties of PDS Kernels

■ **Theorem:** Positive definite symmetric (PDS) kernels are closed under:

- sum,
- product,
- tensor product,
- pointwise limit,
- composition with a power series.

Closure Properties - Proof

■ **Proof:** closure under **sum**:

$$\mathbf{c}^\top \mathbf{K} \mathbf{c} \geq 0 \wedge \mathbf{c}^\top \mathbf{K}' \mathbf{c} \geq 0 \Rightarrow \mathbf{c}^\top (\mathbf{K} + \mathbf{K}') \mathbf{c} \geq 0.$$

● closure under **product**: $\mathbf{K} = \mathbf{M} \mathbf{M}^\top$,

$$\begin{aligned} \sum_{i,j=1}^m c_i c_j (\mathbf{K}_{ij} \mathbf{K}'_{ij}) &= \sum_{i,j=1}^m c_i c_j \left(\left[\sum_{k=1}^m \mathbf{M}_{ik} \mathbf{M}_{jk} \right] \mathbf{K}'_{ij} \right) \\ &= \sum_{k=1}^m \left[\sum_{i,j=1}^m c_i c_j \mathbf{M}_{ik} \mathbf{M}_{jk} \mathbf{K}'_{ij} \right] = \sum_{k=1}^m \mathbf{z}_k^\top \mathbf{K}' \mathbf{z}_k \geq 0, \end{aligned}$$

$$\text{with } \mathbf{z}_k = \begin{bmatrix} c_1 \mathbf{M}_{1k} \\ \vdots \\ c_m \mathbf{M}_{mk} \end{bmatrix}.$$

- Closure under **tensor product**:

- definition: for all $x_1, x_2, y_1, y_2 \in X$,

$$(K_1 \otimes K_2)(x_1, y_1, x_2, y_2) = K_1(x_1, x_2)K_2(y_1, y_2).$$

- thus, PDS kernel as product of the kernels

$$(x_1, y_1, x_2, y_2) \rightarrow K_1(x_1, x_2) \quad (x_1, y_1, x_2, y_2) \rightarrow K_2(y_1, y_2).$$

- Closure under **pointwise limit**: if for all $x, y \in X$,

$$\lim_{n \rightarrow \infty} K_n(x, y) = K(x, y),$$

$$\text{Then, } (\forall n, \mathbf{c}^\top \mathbf{K}_n \mathbf{c} \geq 0) \Rightarrow \lim_{n \rightarrow \infty} \mathbf{c}^\top \mathbf{K}_n \mathbf{c} = \mathbf{c}^\top \mathbf{K} \mathbf{c} \geq 0.$$

- Closure under **composition with power series**:
- assumptions: K PDS kernel with $|K(x, y)| < \rho$ for all $x, y \in X$ and $f(x) = \sum_{n=0}^{\infty} a_n x^n$, $a_n \geq 0$ power series with radius of convergence ρ .
- $f \circ K$ is a PDS kernel since K^n is PDS by closure under product, $\sum_{n=0}^N a_n K^n$ is PDS by closure under sum, and closure under pointwise limit.
- **Example**: for any PDS kernel K , $\exp(K)$ is PDS.

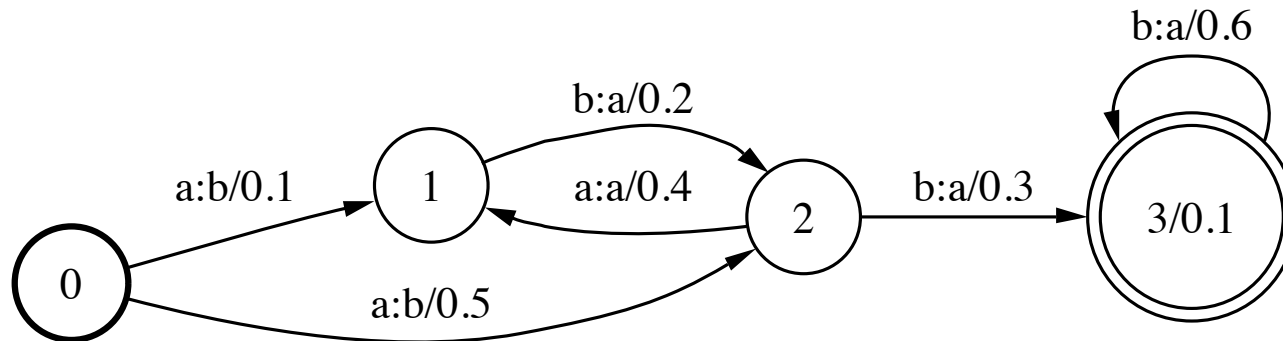
This Lecture

- Definitions
- SVMs with kernels
- Closure properties
- Sequence Kernels
- Negative kernels

Sequence Kernels

- **Definition:** Kernels defined over pairs of strings.
 - Motivation: computational biology, text and speech classification.
 - Idea: two sequences are related when they share some common substrings or subsequences.
 - Example: sum of the product of the counts of common substrings.

Weighted Transducers



$T(x, y)$ = Sum of the weights of all accepting paths with input x and output y .

$$T(abb, baa) = .1 \times .2 \times .3 \times .1 + .5 \times .3 \times .6 \times .1$$

Rational Kernels over Strings

(Cortes et al., 2004)

■ **Definition:** a kernel $K : \Sigma^* \times \Sigma^* \rightarrow \mathbb{R}$ is **rational** if $K = T$ for some weighted transducer T .

■ **Definition:** let $T_1 : \Sigma^* \times \Delta^* \rightarrow \mathbb{R}$ and $T_2 : \Delta^* \times \Omega^* \rightarrow \mathbb{R}$ be two weighted transducers. Then, the **composition** of T_1 and T_2 is defined for all $x \in \Sigma^*, y \in \Omega^*$ by

$$(T_1 \circ T_2)(x, y) = \sum_{z \in \Delta^*} T_1(x, z) T_2(z, y).$$

■ **Definition:** the **inverse** of a transducer $T : \Sigma^* \times \Delta^* \rightarrow \mathbb{R}$ is the transducer $T^{-1} : \Delta^* \times \Sigma^* \rightarrow \mathbb{R}$ obtained from T by swapping input and output labels.

Composition

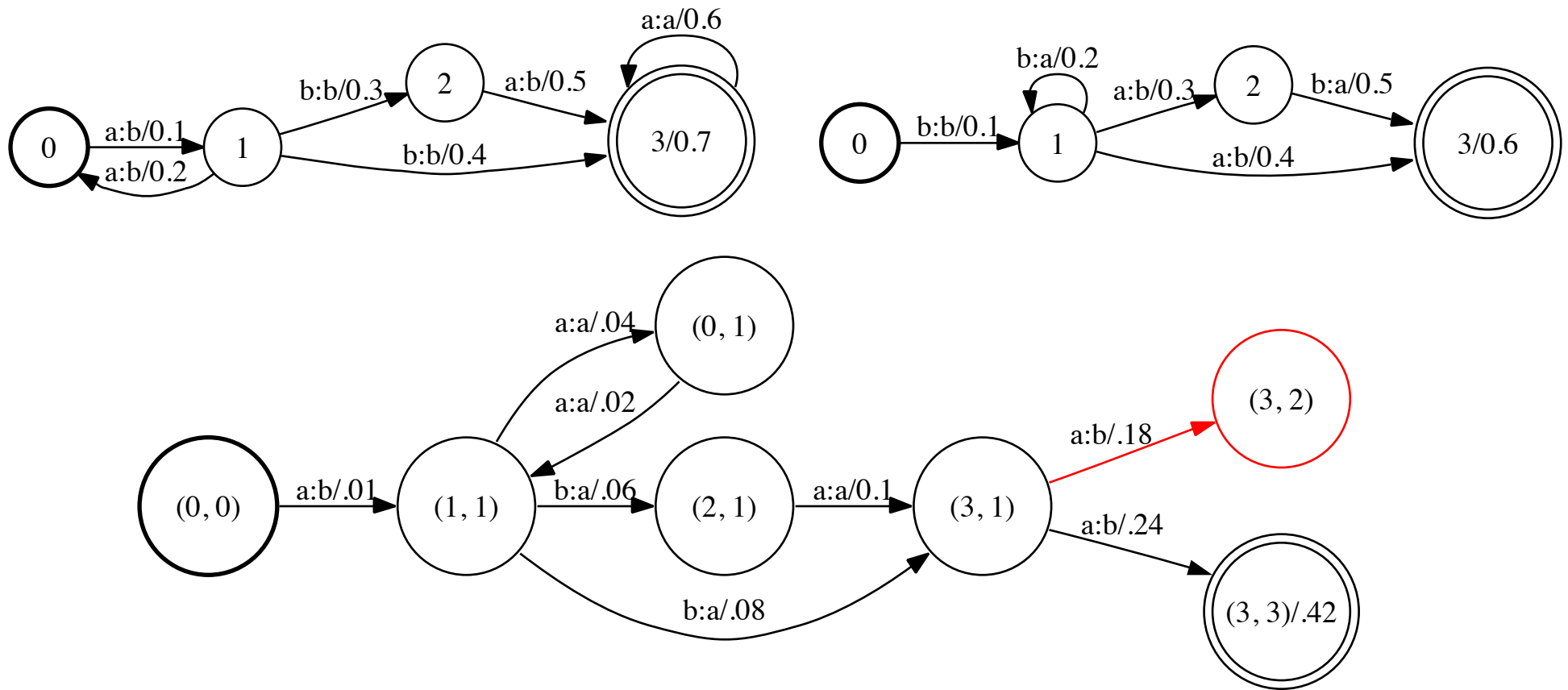
- **Theorem:** the composition of two weighted transducer is also a weighted transducer.
- **Proof:** constructive proof based on **composition algorithm**.
 - states identified with pairs.
 - ϵ -free case: transitions defined by

$$E = \bigcup_{\substack{(q_1, a, b, w_1, q_2) \in E_1 \\ (q'_1, b, c, w_2, q'_2) \in E_2}} \left\{ \left((q_1, q'_1), a, c, w_1 \times w_2, (q_2, q'_2) \right) \right\}.$$

- general case: use of intermediate ϵ -filter.

Composition Algorithm

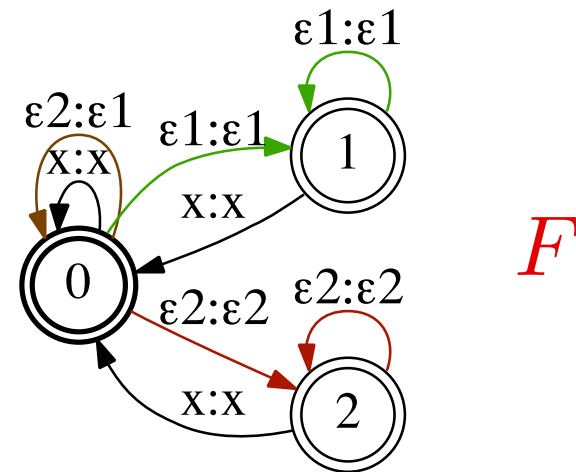
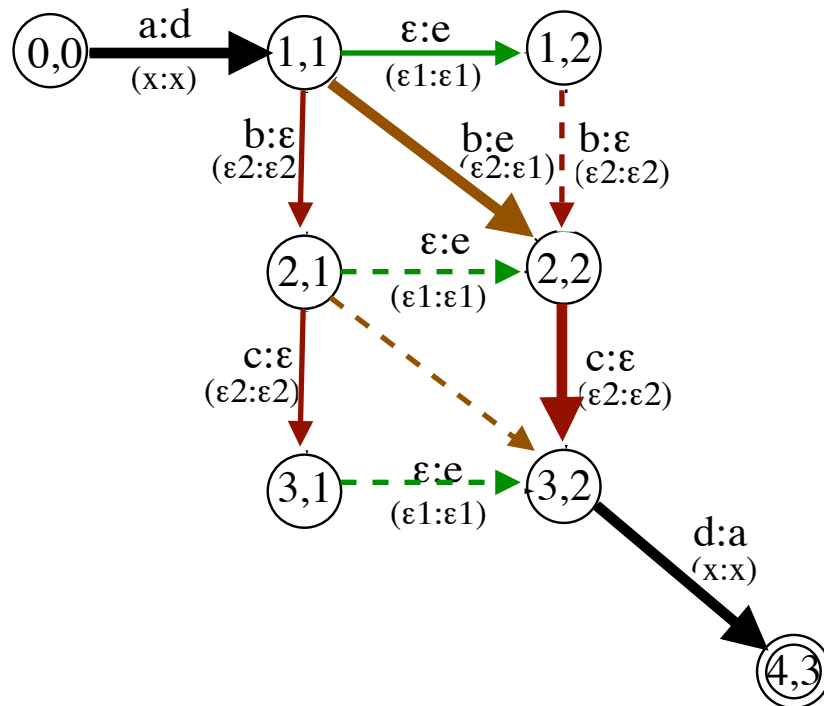
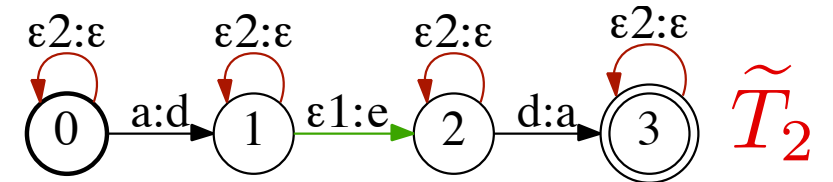
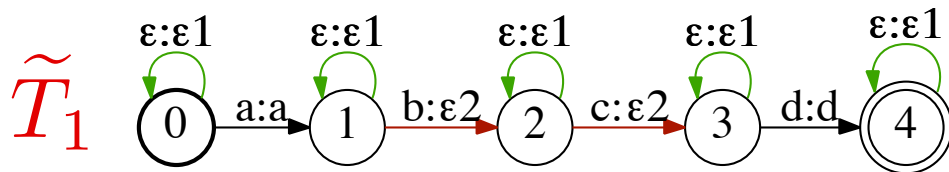
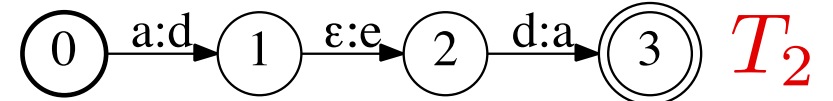
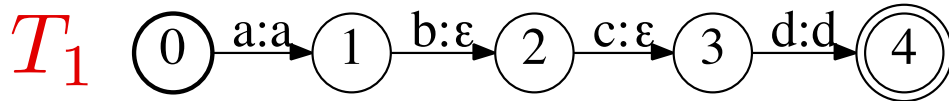
ϵ -Free Case



Complexity: $O(|T_1| |T_2|)$ in general, linear in some cases.

Redundant ϵ -Paths Problem

(MM, Pereira, and Riley, 1996; Pereira and Riley, 1997)



$$T = \tilde{T}_1 \circ F \circ \tilde{T}_2.$$

PDS Rational Kernels

General Construction

■ **Theorem:** for any weighted transducer $T: \Sigma^* \times \Sigma^* \rightarrow \mathbb{R}$, the function $K = T \circ T^{-1}$ is a PDS rational kernel.

■ **Proof:** by definition, for all $x, y \in \Sigma^*$,

$$K(x, y) = \sum_{z \in \Delta^*} T(x, z) T(y, z).$$

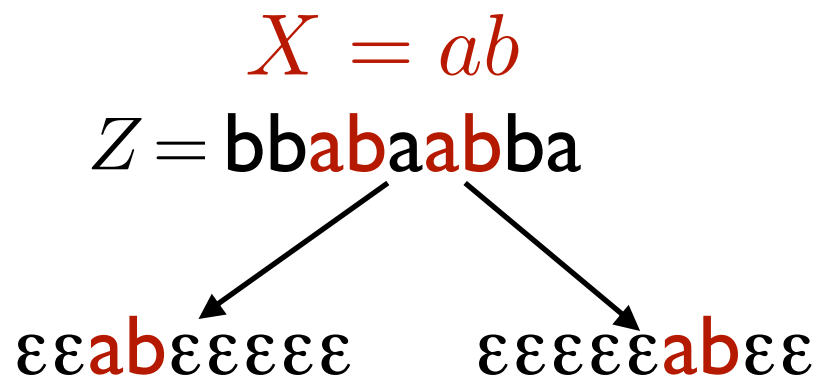
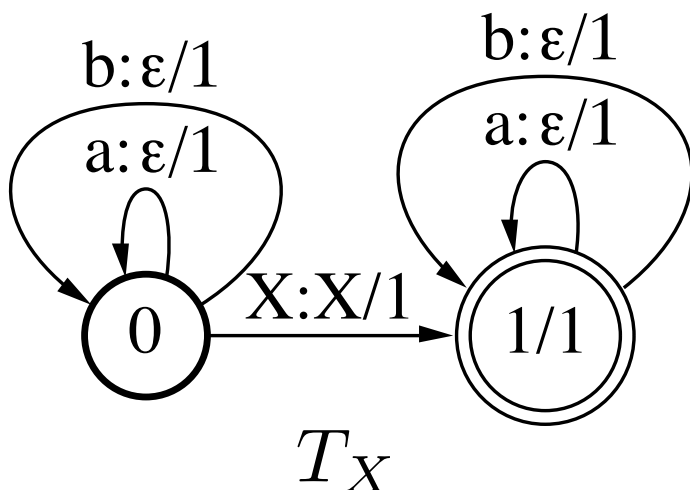
● K is pointwise limit of $(K_n)_{n \geq 0}$ defined by

$$\forall x, y \in \Sigma^*, \quad K_n(x, y) = \sum_{|z| \leq n} T(x, z) T(y, z).$$

● K_n is PDS since for any sample (x_1, \dots, x_m) ,

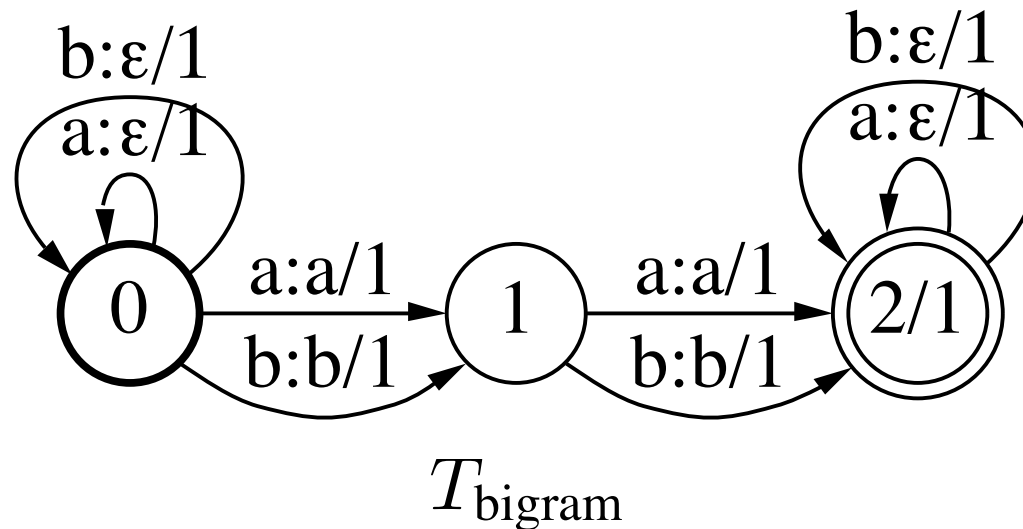
$$\mathbf{K}_n = \mathbf{A} \mathbf{A}^\top \text{ with } \mathbf{A} = (K_n(x_i, z_j))_{\substack{i \in [1, m] \\ j \in [1, N]}}.$$

Counting Transducers



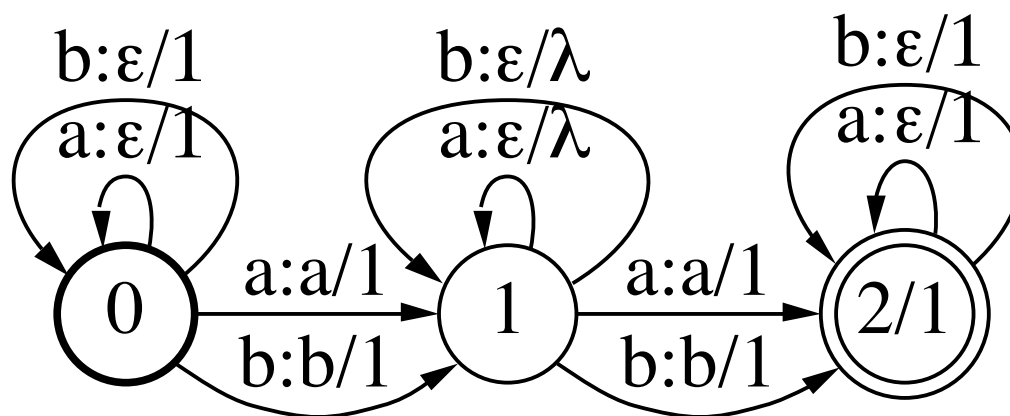
- X may be a string or an automaton representing a regular expression.
- Counts of Z in X : sum of the weights of accepting paths of $Z \circ T_X$.

Transducer Counting Bigrams



Counts of Z given by $Z \circ T_{\text{bigram}} \circ ab$.

Transducer Counting Gappy Bigrams



$T_{\text{gappy bigram}}$

Counts of Z given by $Z \circ T_{\text{gappy bigram}} \circ ab$,
gap penalty $\lambda \in (0, 1)$.

Kernels for Other Discrete Structures

- Similarly, PDS kernels can be defined on other discrete structures:
 - Images,
 - graphs,
 - parse trees,
 - automata,
 - weighted automata.

This Lecture

- Definitions
- SVMs with kernels
- Closure properties
- Sequence Kernels
- Negative kernels

Questions

- Gaussian kernels have the form $\exp(-d^2)$ where d is a metric.
- for what other functions d does $\exp(-d^2)$ define a PDS kernel?
- what other PDS kernels can we construct from a metric in a Hilbert space?

Negative Definite Kernels

(Schoenberg, 1938)

- **Definition:** A function $K: X \times X \rightarrow \mathbb{R}$ is said to be a **negative definite symmetric (NDS) kernel** if it is symmetric and if for all $\{x_1, \dots, x_m\} \subseteq X$ and $\mathbf{c} \in \mathbb{R}^{m \times 1}$ with $\mathbf{1}^\top \mathbf{c} = 0$,

$$\mathbf{c}^\top \mathbf{K} \mathbf{c} \leq 0.$$

- Clearly, if K is PDS, then $-K$ is NDS, but the converse does not hold in general.

Examples

- The squared distance $\|x - y\|^2$ in a Hilbert space H defines an NDS kernel. If $\sum_{i=1}^m c_i = 0$,

$$\begin{aligned}\sum_{i,j=1}^m c_i c_j \|\mathbf{x}_i - \mathbf{x}_j\|^2 &= \sum_{i,j=1}^m c_i c_j (\mathbf{x}_i - \mathbf{x}_j) \cdot (\mathbf{x}_i - \mathbf{x}_j) \\&= \sum_{i,j=1}^m c_i c_j (\|\mathbf{x}_i\|^2 + \|\mathbf{x}_j\|^2 - 2\mathbf{x}_i \cdot \mathbf{x}_j) \\&= \sum_{i,j=1}^m c_i c_j (\|\mathbf{x}_i\|^2 + \|\mathbf{x}_j\|^2) - 2 \sum_{i=1}^m c_i \mathbf{x}_i \cdot \sum_{j=1}^m c_j \mathbf{x}_j \\&\leq \sum_{i,j=1}^m c_i c_j (\|\mathbf{x}_i\|^2 + \|\mathbf{x}_j\|^2) \\&= \sum_{j=1}^m c_j \left(\sum_{i=1}^m c_i (\|\mathbf{x}_i\|^2) \right) + \sum_{i=1}^m c_i \left(\sum_{j=1}^m c_j \|\mathbf{x}_j\|^2 \right) = 0.\end{aligned}$$

NDS Kernels - Property

(Schoenberg, 1938)

■ **Theorem:** Let $K: X \times X \rightarrow \mathbb{R}$ be an NDS kernel such that for all $x, y \in X$, $K(x, y) = 0$ iff $x = y$. Then, there exists a Hilbert space H and a mapping $\Phi: X \rightarrow H$ such that

$$\forall x, y \in X, K(x, y) = \|\Phi(x) - \Phi(y)\|^2.$$

Thus, under the hypothesis of the theorem, \sqrt{K} defines a metric.

PDS and NDS Kernels

(Schoenberg, 1938)

- **Theorem:** let $K: X \times X \rightarrow \mathbb{R}$ be a symmetric kernel, then:
- K is NDS iff $\exp(-tK)$ is a PDS kernel for all $t > 0$.
 - Let K' be defined for any x_0 by
$$K'(x, y) = K(x, x_0) + K(y, x_0) - K(x, y) - K(x_0, x_0)$$
for all $x, y \in X$. Then, K is NDS iff K' is PDS.

Example

- The kernel defined by $K(x, y) = \exp(-t||x - y||^2)$ is PDS for all $t > 0$ since $||x - y||^2$ is NDS.
- The kernel $\exp(-|x - y|^p)$ is not PDS for $p > 2$.
Otherwise, for any $t > 0, \{x_1, \dots, x_m\} \subseteq X$ and $\mathbf{c} \in \mathbb{R}^{m \times 1}$
$$\sum_{i,j=1}^m c_i c_j e^{-t|x_i - x_j|^p} = \sum_{i,j=1}^m c_i c_j e^{-|t^{1/p} x_i - t^{1/p} x_j|^p} \geq 0.$$
- This would imply that $|x - y|^p$ is NDS for $p > 2$, but that cannot be (see past homework assignments).

References

- N. Aronszajn, Theory of Reproducing Kernels, *Trans. Amer. Math. Soc.*, 68, 337-404, 1950.
- Peter Bartlett and John Shawe-Taylor. Generalization performance of support vector machines and other pattern classifiers. In *Advances in kernel methods: support vector learning*, pages 43–54. MIT Press, Cambridge, MA, USA, 1999.
- Christian Berg, Jens Peter Reus Christensen, and Paul Ressel. *Harmonic Analysis on Semigroups*. Springer-Verlag: Berlin-New York, 1984.
- Bernhard Boser, Isabelle M. Guyon, and Vladimir Vapnik. A training algorithm for optimal margin classifiers. In proceedings of COLT 1992, pages 144-152, Pittsburgh, PA, 1992.
- Corinna Cortes, Patrick Haffner, and Mehryar Mohri. Rational Kernels: Theory and Algorithms. *Journal of Machine Learning Research (JMLR)*, 5:1035-1062, 2004.
- Corinna Cortes and Vladimir Vapnik, Support-Vector Networks, *Machine Learning*, 20, 1995.
- Kimeldorf, G. and Wahba, G. Some results on Tchebycheffian Spline Functions, *J. Mathematical Analysis and Applications*, 33, 1 (1971) 82-95.

References

- James Mercer. Functions of Positive and Negative Type, and Their Connection with the Theory of Integral Equations. In *Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character*, Vol. 83, No. 559, pp. 69-70, 1909.
- Mehryar Mohri, Fernando C. N. Pereira, and Michael Riley. *Weighted Automata in Text and Speech Processing*, In *Proceedings of the 12th biennial European Conference on Artificial Intelligence (ECAI-96), Workshop on Extended finite state models of language*. Budapest, Hungary, 1996.
- Fernando C. N. Pereira and Michael D. Riley. Speech Recognition by Composition of Weighted Finite Automata. In *Finite-State Language Processing*, pages 431-453. MIT Press, 1997.
- I. J. Schoenberg, Metric Spaces and Positive Definite Functions. *Transactions of the American Mathematical Society*, Vol. 44, No. 3, pp. 522-536, 1938.
- Vladimir N. Vapnik. *Estimation of Dependences Based on Empirical Data*. Springer, Berlin, 1982.
- Vladimir N. Vapnik. *The Nature of Statistical Learning Theory*. Springer, 1995.
- Vladimir N. Vapnik. *Statistical Learning Theory*. Wiley-Interscience, New York, 1998.

Appendix

Mercer's Condition

(Mercer, 1909)

■ **Theorem:** Let $X \times X$ be a compact subset of \mathbb{R}^N and let $K : X \times X \rightarrow \mathbb{R}$ be in $L_\infty(X \times X)$ and symmetric. Then, K admits a uniformly convergent expansion

$$K(x, y) = \sum_{n=0}^{\infty} a_n \phi_n(x) \phi_n(y), \text{ with } a_n > 0,$$


iff for any function c in $L_2(X)$,

$$\int \int_{X \times X} c(x) c(y) K(x, y) dx dy \geq 0.$$

SVMs with PDS Kernels

■ Constrained optimization:

$$\begin{aligned} \max_{\alpha} \quad & 2 \mathbf{1}^\top \alpha - (\alpha \circ \mathbf{y})^\top \mathbf{K}(\alpha \circ \mathbf{y}) \\ \text{subject to:} \quad & \mathbf{0} \leq \alpha \leq \mathbf{C} \wedge \alpha^\top \mathbf{y} = 0. \end{aligned}$$

Hadamard product 

■ Solution:

$$h = \text{sgn} \left(\sum_{i=1}^m \alpha_i y_i K(x_i, \cdot) + b \right),$$

with $b = y_i - (\alpha \circ \mathbf{y})^\top \mathbf{K} \mathbf{e}_i$ **for any** x_i **with**
 $0 < \alpha_i < C$.