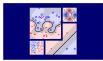
Machine Learning Techniques

(機器學習技法)



Lecture 3: Kernel Support Vector Machine

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Roadmap

1 Embedding Numerous Features: Kernel Models

Lecture 2: Dual Support Vector Machine

dual SVM: another QP with valuable geometric messages and almost no dependence on \tilde{d}

Lecture 3: Kernel Support Vector Machine

- Kernel Trick
- Polynomial Kernel
- Gaussian Kernel
- Comparison of Kernels
- 2 Combining Predictive Features: Aggregation Models
- 3 Distilling Implicit Features: Extraction Models

Dual SVM Revisited

goal: SVM without dependence on \tilde{d}

half-way done:

高維度的矩陣內積仍然藏在Qd矩陣裡面!

$$\begin{split} \min_{\pmb{\alpha}} & \quad \frac{1}{2} \pmb{\alpha}^T \mathbf{Q}_{\mathrm{D}} \pmb{\alpha} - \mathbf{1}^T \pmb{\alpha} \\ \text{subject to} & \quad \pmb{y}^T \pmb{\alpha} = \mathbf{0}; \\ & \quad \alpha_n \geq 0, \text{for } n = 1, 2, \dots, N \end{split}$$

- $q_{n,m} = y_n y_m \mathbf{z}_n^T \mathbf{z}_m$: inner product in $\mathbb{R}^{\tilde{d}}$
- need: $\mathbf{z}_n^\mathsf{T} \mathbf{z}_m = \mathbf{\Phi}(\mathbf{x}_n)^\mathsf{T} \mathbf{\Phi}(\mathbf{x}_m)$ calculated faster than $O(\tilde{d})$

簡化inner product in R^n

can we do so?

我們能不能簡化Q矩陣裡面的高維度特徵內積運算?

Fast Inner Product for Φ_2

2nd order polynomial transform 二次多項式轉換:

$$\mathbf{\Phi}_{2}(\mathbf{x}) = (1, x_{1}, x_{2}, \dots, x_{d}, x_{1}^{2}, x_{1}x_{2}, \dots, x_{1}x_{d}, x_{2}x_{1}, x_{2}^{2}, \dots, x_{2}x_{d}, \dots, x_{d}^{2})$$

—include both $x_1x_2 \& x_2x_1$ for 'simplicity':-)

我們現在來看看先用這個\phi轉換、再做內積,會不會算得比較快:

$$\Phi_{2}(\mathbf{x})^{T}\Phi_{2}(\mathbf{x}') = 1 + \sum_{i=1}^{d} x_{i}x'_{i} + \sum_{i=1}^{d} \sum_{j=1}^{d} x_{i}x'_{j}x'_{i}x'_{j}$$

$$= 1 + \sum_{i=1}^{d} x_{i}x'_{i} + \sum_{i=1}^{d} x_{i}x'_{i} \sum_{j=1}^{d} x_{j}x'_{j}$$

$$= 1 + \mathbf{x}^{T}\mathbf{x}' + (\mathbf{x}^{T}\mathbf{x}')(\mathbf{x}^{T}\mathbf{x}')$$

只需要花d的力氣就好、不需要花到d^2的力氣

for Φ_2 , transform + inner product can be carefully done in O(d) instead of $O(d^2)$

Kernel: Transform + Inner Product

transform
$$\Phi \iff \text{kernel function}$$
: $\mathcal{K}_{\Phi}(\mathbf{x}, \mathbf{x}') \equiv \Phi(\mathbf{x})^T \Phi(\mathbf{x}')$
 $\Phi_2 \iff \mathcal{K}_{\Phi_2}(\mathbf{x}, \mathbf{x}') = 1 + (\mathbf{x}^T \mathbf{x}') + (\mathbf{x}^T \mathbf{x}')^2$

- quadratic coefficient $q_{n,m} = y_n y_m \mathbf{z}_n^{\mathsf{T}} \mathbf{z}_m = y_n y_m K(\mathbf{x}_n, \mathbf{x}_m)$
- optimal bias b? from SV (\mathbf{x}_s, y_s) ,

$$b = y_s - \mathbf{w}^T \mathbf{z}_s = y_s - \left(\sum_{n=1}^N \alpha_n y_n \mathbf{z}_n \right)^T \mathbf{z}_s = y_s - \sum_{n=1}^N \alpha_n y_n \left(K(\mathbf{x}_n, \mathbf{x}_s) \right)$$

有了kernal,不需要算到z空間裡面那麼多向量的維度

• optimal hypothesis g_{SVM} : for test input **x**,

$$g_{\text{SVM}}(\mathbf{x}) = \text{sign}\left(\mathbf{w}^{\mathsf{T}}\mathbf{\Phi}(\mathbf{x}) + b\right) = \text{sign}\left(\sum_{n=1}^{N} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + b\right)$$

kernel trick: plug in efficient kernel function to avoid dependence on \tilde{d}

Kernel SVM with QP

Kernel Hard-Margin SVM Algorithm

- $\mathbf{q}_{n,m} = y_n y_m K(\mathbf{x}_n, \mathbf{x}_m); \mathbf{p} = -\mathbf{1}_N; (A, \mathbf{c})$ for equ./bound constraints
- 3 $b \leftarrow \left(y_s \sum_{\text{SV indices } n} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}_s) \right) \text{ with SV } (\mathbf{x}_s, y_s)$
- 4 return SVs and their α_n as well as b such that for new \mathbf{x} , $g_{\text{SV indices }n} \left(\sum_{\text{SV indices }n} \alpha_n \mathbf{y}_n K(\mathbf{x}_n, \mathbf{x}) + b \right)$
- (1): time complexity $O(N^2)$ · (kernel evaluation)
- (2): QP with N variables and N + 1 constraints
- (3) & (4): time complexity O(#SV) · (kernel evaluation)

kernel SVM:

use computational shortcut to avoid \tilde{d} & predict with SV only

Consider two examples \mathbf{x} and \mathbf{x}' such that $\mathbf{x}^T\mathbf{x}'=10$. What is

$$K_{\Phi_2}(x,x')$$
?

- 1
- **2** 11
- **3** 111
- **4** 1111

Consider two examples \mathbf{x} and \mathbf{x}' such that $\mathbf{x}^T\mathbf{x}'=10$. What is $K_{\Phi_2}(\mathbf{x},\mathbf{x}')$?

- 0
- **2** 11
- **3** 111
- 4 1111

Reference Answer: (3)

Using the derivation in previous slides,

$$K_{\mathbf{\Phi}_2}(\mathbf{x},\mathbf{x}') = 1 + \mathbf{x}^T \mathbf{x}' + (\mathbf{x}^T \mathbf{x}')^2.$$

在每個次項前面的 係數做放縮的動作

General Poly-2 Kernel 常用的二次多項式kernal轉換

$$\begin{aligned} & \mathbf{\Phi}_{2}(\mathbf{x}) = (1, x_{1}, \dots, x_{d}, x_{1}^{2}, \dots, x_{d}^{2}) & \Leftrightarrow & \mathcal{K}_{\mathbf{\Phi}_{2}}(\mathbf{x}, \mathbf{x}') = 1 + \mathbf{x}^{T} \mathbf{x}' + (\mathbf{x}^{T} \mathbf{x}')^{2} \\ & \mathbf{\Phi}_{2}(\mathbf{x}) = (1, \sqrt{2}x_{1}, \dots, \sqrt{2}x_{d}, x_{1}^{2}, \dots, x_{d}^{2}) & \Leftrightarrow & \mathcal{K}_{2}(\mathbf{x}, \mathbf{x}') = 1 + 2\mathbf{x}^{T} \mathbf{x}' + (\mathbf{x}^{T} \mathbf{x}')^{2} \end{aligned}$$

$$\Phi_2(\mathbf{x}) = (1, \sqrt{2\gamma}x_1, \dots, \sqrt{2\gamma}x_d, \gamma x_1^2, \dots, \gamma x_d^2)$$

$$\Leftrightarrow \mathcal{K}_2(\mathbf{x}, \mathbf{x}') = 1 + \frac{2\gamma}{2}\mathbf{x}^T\mathbf{x}' + \gamma^2(\mathbf{x}^T\mathbf{x}')^2$$

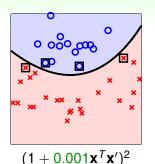
$$K_2(\mathbf{x}, \mathbf{x}') = (1 + \gamma \mathbf{x}^T \mathbf{x}')^2 \text{ with } \gamma > 0$$

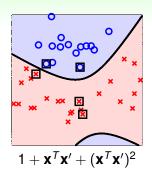
- K₂: somewhat 'easier' to calculate than K_{Φ2}
- Φ₂ and Φ₂: equivalent power, different inner product ⇒ different geometry

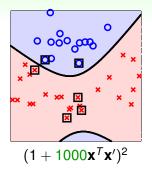
藍色跟綠色的其實對應到的是同樣的空間,所以其實有對等的power,只是幾何解看起來會有點不一樣而已

K₂ commonly used

Poly-2 Kernels in Action







- g_{SVM} different, SVs different 出來的margin可能有所差異,但對於模型表現不影響—fhard' to say which is better before learning
- change of kernel ⇔ change of margin definition

need selecting K, just like selecting Φ

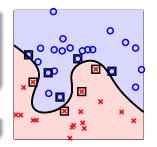
General Polynomial Kernel

$$\mathcal{K}_{2}(\mathbf{x}, \mathbf{x}') = (\zeta + \gamma \mathbf{x}^{T} \mathbf{x}')^{2} \text{ with } \gamma > 0, \zeta \geq 0
\mathcal{K}_{3}(\mathbf{x}, \mathbf{x}') = (\zeta + \gamma \mathbf{x}^{T} \mathbf{x}')^{3} \text{ with } \gamma > 0, \zeta \geq 0
\vdots
\mathcal{K}_{Q}(\mathbf{x}, \mathbf{x}') = (\zeta + \gamma \mathbf{x}^{T} \mathbf{x}')^{Q} \text{ with } \gamma > 0, \zeta \geq 0$$

- embeds Φ_Q specially with parameters (γ,ζ) 因為有large margin的幫助,可以多少避免over-fitting的問題
- allows computing large-margin polynomial classification without dependence on d

模型的複雜度可由\zeta跟Q來做調整!

SVM + Polynomial Kernel: Polynomial SVM

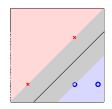


10-th order polynomial with margin 0.1

Special Case: Linear Kernel

$$\begin{split} \mathcal{K}_{1}(\mathbf{x}, \mathbf{x}') &= (\mathbf{0} + \mathbf{1} \cdot \mathbf{x}^{T} \mathbf{x}')^{1} \\ &\vdots \\ \mathcal{K}_{\mathbf{Q}}(\mathbf{x}, \mathbf{x}') &= (\zeta + \gamma \mathbf{x}^{T} \mathbf{x}')^{\mathbf{Q}} \text{ with } \gamma > 0, \zeta \geq 0 \end{split}$$

- K₁: just usual inner product, called linear kernel
- 'even easier': can be solved (often in primal form) efficiently



linear first, remember? :-)

Consider the general 2-nd polynomial kernel $K_2(\mathbf{x}, \mathbf{x}') = (\zeta + \gamma \mathbf{x}^T \mathbf{x}')^2$. Which of the following transform can be used to derive this kernel?

- $\Phi(\mathbf{x}) = (\zeta, \sqrt{2\gamma\zeta}x_1, \dots, \sqrt{2\gamma\zeta}x_d, \gamma x_1^2, \dots, \gamma x_d^2)$

Consider the general 2-nd polynomial kernel $K_2(\mathbf{x}, \mathbf{x}') = (\zeta + \gamma \mathbf{x}^T \mathbf{x}')^2$. Which of the following transform can be used to derive this kernel?

$$\bullet (\mathbf{x}) = (1, \sqrt{2\gamma}x_1, \dots, \sqrt{2\gamma}x_d, \gamma x_1^2, \dots, \gamma x_d^2)$$

$$\mathbf{\Phi}(\mathbf{x}) = (\zeta, \sqrt{2\gamma\zeta}x_1, \dots, \sqrt{2\gamma\zeta}x_d, \gamma x_1^2, \dots, \gamma x_d^2)$$

Reference Answer: (4)

We need to have ζ^2 from the 0-th order terms, $2\gamma\zeta\mathbf{x}^T\mathbf{x}'$ from the 1-st order terms, and $\gamma^2(\mathbf{x}^T\mathbf{x}')^2$ from the 2-nd order terms.

Kernel of Infinite Dimensional Transform

infinite dimensional $\Phi(\mathbf{x})$? Yes, if $K(\mathbf{x}, \mathbf{x}')$ efficiently computable!

when
$$\mathbf{x} = (x)$$
, $K(x, x')$ = $\exp(-(x - x')^2)$ exponential的泰勒展開
= $\exp(-(x)^2)\exp(-(x')^2)\exp(2xx')$
Taylor $= \exp(-(x)^2)\exp(-(x')^2)\left(\sum_{i=0}^{\infty}\frac{(2xx')^i}{i!}\right)$
= $\sum_{i=0}^{\infty}\left(\exp(-(x)^2)\exp(-(x')^2)\sqrt{\frac{2^i}{i!}}\sqrt{\frac{2^i}{i!}}(x)^i(x')^i\right)$
= $\Phi(x)^T\Phi(x')$

with infinite dimensional $\Phi(x) = \exp(-x^2) \cdot \left(1, \sqrt{\frac{2}{1!}}x, \sqrt{\frac{2^2}{2!}}x^2, \dots\right)$

more generally, Gaussian kernel $K(\mathbf{x}, \mathbf{x}') = \exp(-\gamma ||\mathbf{x} - \mathbf{x}'||^2)$ with $\gamma > 0$

Hypothesis of Gaussian SVM

Gaussian kernel
$$K(\mathbf{x}, \mathbf{x}') = \exp(-\gamma ||\mathbf{x} - \mathbf{x}'||^2)$$

$$\begin{split} g_{\text{SVM}}(\mathbf{x}) &= \text{sign}\left(\sum_{\text{SV}} \alpha_{n} y_{n} K(\mathbf{x}_{n}, \mathbf{x}) + b\right) \\ &= \text{sign}\left(\sum_{\text{SV}} \alpha_{n} y_{n} \text{exp}\left(-\gamma \|\mathbf{x} - \mathbf{x}_{n}\|^{2}\right) + b\right) \end{split}$$

- linear combination of Gaussians centered at SVs xn
- also called Radial Basis Function (RBF) kernel

Gaussian SVM:

find α_n to combine Gaussians centered at \mathbf{x}_n & achieve large margin in infinite-dim. space

Support Vector Mechanism

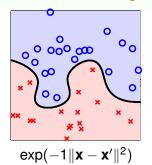
	large-margin hyperplanes higher-order transforms with kernel trick
#	not many
boundary	sophisticated

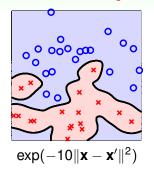
- transformed vector $\mathbf{z} = \mathbf{\Phi}(\mathbf{x}) \Longrightarrow$ efficient kernel $K(\mathbf{x}, \mathbf{x}')$
- store optimal w ⇒ store a few SVs and α_n

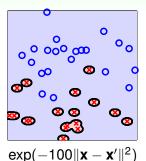
new possibility by Gaussian SVM: infinite-dimensional linear classification, with generalization 'guarded by' large-margin:-)

Gaussian SVM in Action

最後的圖形g_svm(x)其實是很多gaussian的線性組合,所以如果\gamma越大代表是越多很尖很細的gaussian的線性組合







- large $\gamma \Longrightarrow$ sharp Gaussians \Longrightarrow 'overfit'?
- warning: SVM can still overfit :-(

Gaussian SVM: need careful selection of γ

Consider the Gaussian kernel $K(\mathbf{x}, \mathbf{x}') = \exp(-\gamma ||\mathbf{x} - \mathbf{x}'||^2)$. What function does the kernel converge to if $\gamma \to \infty$?

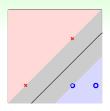
- **4** $K_{lim}(\mathbf{x}, \mathbf{x}') = 1$

Consider the Gaussian kernel $K(\mathbf{x}, \mathbf{x}') = \exp(-\gamma ||\mathbf{x} - \mathbf{x}'||^2)$. What function does the kernel converge to if $\gamma \to \infty$?

Reference Answer: (2)

If $\mathbf{x} = \mathbf{x}'$, $K(\mathbf{x}, \mathbf{x}') = 1$ regardless of γ . If $\mathbf{x} \neq \mathbf{x}'$, $K(\mathbf{x}, \mathbf{x}') = 0$ when $\gamma \to \infty$. Thus, K_{lim} is an impulse function, which is an extreme case of how the Gaussian gets sharper when $\gamma \to \infty$.

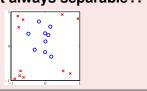
Linear Kernel: Cons and Pros



$$\mathcal{K}(\boldsymbol{x},\boldsymbol{x}') = \boldsymbol{x}^T\boldsymbol{x}'$$

Cons

restricted—not always separable?!

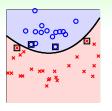


Pros

- safe—linear first, remember? :-)
- fast—with special QP solver in primal
- very explainable—w and SVs say something

linear kernel: an important basic tool

Polynomial Kernel: Cons and Pros



$$K(\mathbf{x}, \mathbf{x}') = (\zeta + \gamma \mathbf{x}^T \mathbf{x}')^Q$$

Cons

- numerical difficulty for large Q
 - $|\zeta + \gamma \mathbf{x}^T \mathbf{x}'| < 1$: $K \to 0$ • $|\zeta + \gamma \mathbf{x}^T \mathbf{x}'| > 1$: $K \to \text{big}$
- three parameters (γ, ζ, Q) -more difficult to select

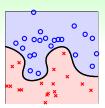
Pros

- less restricted than linear
- strong physical control —'knows' degree Q

主觀認定會是幾次方關係?

polynomial kernel: perhaps small-Q only —sometimes efficiently done by linear on $\Phi_{\mathcal{O}}(\mathbf{x})$

Gaussian Kernel: Cons and Pros



$$K(\mathbf{x}, \mathbf{x}') = \exp(-\gamma \|\mathbf{x} - \mathbf{x}'\|^2)$$

Cons

- mysterious—no w
- slower than linear
- too powerful?!



Pros

- more powerful than linear/poly.
- bounded—less numerical difficulty than poly.
- one parameter only—easier to select than poly.

實務上,Gaussian Kernel表現得挺不錯的

Gaussian kernel: one of most popular but shall be used with care

Other Valid Kernels

- kernel represents special similarity: $\Phi(\mathbf{x})^T \Phi(\mathbf{x}')$
- any similarity ⇒ valid kernel? not really
- necessary & sufficient conditions for valid kernel:
 Mercer's condition
 - symmetric
 - let $k_{ij} = K(\mathbf{x}_i, \mathbf{x}_i)$, the matrix K

$$= \begin{bmatrix} \mathbf{\Phi}(\mathbf{x}_1)^T \mathbf{\Phi}(\mathbf{x}_1) & \mathbf{\Phi}(\mathbf{x}_1)^T \mathbf{\Phi}(\mathbf{x}_2) & \dots & \mathbf{\Phi}(\mathbf{x}_1)^T \mathbf{\Phi}(\mathbf{x}_N) \\ \mathbf{\Phi}(\mathbf{x}_2)^T \mathbf{\Phi}(\mathbf{x}_1) & \mathbf{\Phi}(\mathbf{x}_2)^T \mathbf{\Phi}(\mathbf{x}_2) & \dots & \mathbf{\Phi}(\mathbf{x}_2)^T \mathbf{\Phi}(\mathbf{x}_N) \\ \dots & \dots & \dots & \dots \\ \mathbf{\Phi}(\mathbf{x}_N)^T \mathbf{\Phi}(\mathbf{x}_1) & \mathbf{\Phi}(\mathbf{x}_N)^T \mathbf{\Phi}(\mathbf{x}_2) & \dots & \mathbf{\Phi}(\mathbf{x}_N)^T \mathbf{\Phi}(\mathbf{x}_N) \end{bmatrix}$$

$$= \begin{bmatrix} \mathbf{z}_1 & \mathbf{z}_2 & \dots & \mathbf{z}_N \end{bmatrix}^T \begin{bmatrix} \mathbf{z}_1 & \mathbf{z}_2 & \dots & \mathbf{z}_N \end{bmatrix}$$

$$= \mathbf{Z} \mathbf{Z}^T \text{ must always be positive semi-definite}$$

define your own kernel: possible, but hard

Which of the following is not a valid kernel? (*Hint: Consider two* 1-dimensional vectors $\mathbf{x}_1 = (1)$ and $\mathbf{x}_2 = (-1)$ and check Mercer's

- 1-dimensional vectors $\mathbf{x}_1 = (1)$ and $\mathbf{x}_2 = (-1)$ and check Mercer's condition.)

 - 2 $K(\mathbf{x}, \mathbf{x}') = (0 + \mathbf{x}^T \mathbf{x}')^2$
 - **3** $K(\mathbf{x}, \mathbf{x}') = (1 + \mathbf{x}^T \mathbf{x}')^2$
 - **4** $K(\mathbf{x}, \mathbf{x}') = (-1 \mathbf{x}^T \mathbf{x}')^2$

Which of the following is not a valid kernel? (*Hint: Consider two* 1-dimensional vectors $\mathbf{x}_1 = (1)$ and $\mathbf{x}_2 = (-1)$ and check Mercer's condition.)

$$\mathbf{1} K(\mathbf{x}, \mathbf{x}') = (-1 + \mathbf{x}^T \mathbf{x}')^2$$

2
$$K(\mathbf{x}, \mathbf{x}') = (0 + \mathbf{x}^T \mathbf{x}')^2$$

3
$$K(\mathbf{x}, \mathbf{x}') = (1 + \mathbf{x}^T \mathbf{x}')^2$$

4
$$K(\mathbf{x}, \mathbf{x}') = (-1 - \mathbf{x}^T \mathbf{x}')^2$$

Reference Answer: (1)

The kernels in 2 and 3 are just polynomial kernels. The kernel in 4 is equivalent to the kernel in 3. For 1, the matrix K formed from the kernel and the two examples is not positive semi-definite. Thus, the underlying kernel is not a valid one.

Summary

1 Embedding Numerous Features: Kernel Models

Lecture 3: Kernel Support Vector Machine

Kernel Trick

kernel as shortcut of transform + inner product

- Polynomial Kernel
- embeds specially-scaled polynomial transform
- Gaussian Kernel
 embeds infinite dimensional transform
- Comparison of Kernels

 linear for efficiency or Gaussian for power
- next: avoiding overfitting in Gaussian (and other kernels)
- 2 Combining Predictive Features: Aggregation Models
- 3 Distilling Implicit Features: Extraction Models