Machine Learning Foundations

(機器學習基石)



Lecture 12: Nonlinear Transformation

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Roadmap

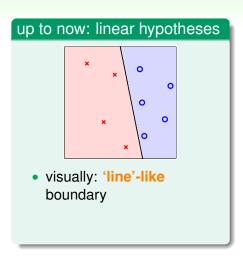
- 1 When Can Machines Learn?
- 2 Why Can Machines Learn?
- **3 How Can Machines Learn?**

Lecture 11: Linear Models for Classification

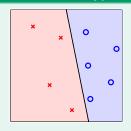
binary classification via (logistic) regression; multiclass via OVA/OVO decomposition

Lecture 12: Nonlinear Transformation

- Quadratic Hypotheses
- Nonlinear Transform
- Price of Nonlinear Transform
- Structured Hypothesis Sets
- 4 How Can Machines Learn Better?

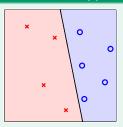


up to now: linear hypotheses



- visually: 'line'-like boundary
- mathematically: linear scores s = w^Tx

up to now: linear hypotheses

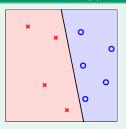


- visually: 'line'-like boundary
- mathematically: linear scores s = w^Tx

but limited ...

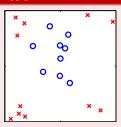
theoretically: d_{VC} under control:-)

up to now: linear hypotheses



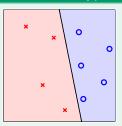
- visually: 'line'-like boundary
- mathematically: linear scores $s = \mathbf{w}^T \mathbf{x}$

but limited ...



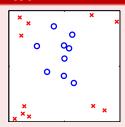
- theoretically: d_{VC} under control:-)
- practically: on some D,
 large E_{in} for every line :-(

up to now: linear hypotheses



- visually: 'line'-like boundary
- mathematically: linear scores s = w^Tx

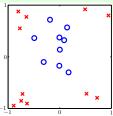
but limited . . .



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- practically: on some D,
 large E_{in} for every line :-(

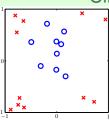
how to break the limit of linear hypotheses

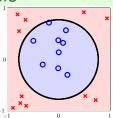
Circular Separable



• \mathcal{D} not linear separable

Circular Separable

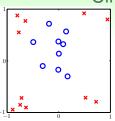


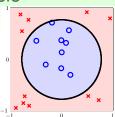


- \mathcal{D} not linear separable
- but circular separable by a circle of radius $\sqrt{0.6}$ centered at origin:

$$h_{\text{SEP}}(\mathbf{x}) = \text{sign}\left(-x_1^2 - x_2^2 + 0.6\right)$$

Circular Separable





- ullet ${\cal D}$ not linear separable
- but circular separable by a circle of radius $\sqrt{0.6}$ centered at origin:

$$h_{\text{SEP}}(\mathbf{x}) = \text{sign}\left(-x_1^2 - x_2^2 + 0.6\right)$$

re-derive Circular-PLA, Circular-Regression, blahblah . . . all over again? :-)

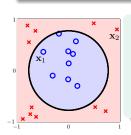
$$h(\mathbf{x}) = \text{sign} \left(\begin{array}{ccc} 0.6 & -1 \cdot x_1^2 & -1 \cdot x_2^2 \end{array} \right)$$

$$h(\mathbf{x}) = \operatorname{sign}\left(\underbrace{\begin{array}{ccc} 0.6 \\ \tilde{w}_0 \end{array}} \cdot \underbrace{\begin{array}{ccc} 1 \\ \tilde{z}_0 \end{array}} + \underbrace{\begin{pmatrix} -1 \\ \tilde{w}_1 \end{array}} \cdot \underbrace{\begin{array}{ccc} x_1^2 \\ \tilde{z}_1 \end{array}} + \underbrace{\begin{pmatrix} -1 \\ \tilde{w}_2 \end{array}} \cdot \underbrace{\begin{array}{ccc} x_2^2 \\ \tilde{z}_2 \end{array}} \right)$$

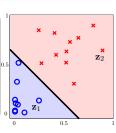
$$\begin{array}{lcl} \boldsymbol{h}(\mathbf{x}) & = & \operatorname{sign}\left(\underbrace{\begin{array}{ccc} 0.6 \\ \tilde{w}_0 \end{array}} \cdot \underbrace{\begin{array}{ccc} 1 \\ \tilde{z}_0 \end{array}} & + \underbrace{\begin{pmatrix} -1 \\ \tilde{w}_1 \end{array}} \cdot \underbrace{\begin{array}{ccc} x_1^2 \\ \tilde{z}_1 \end{array}} & + \underbrace{\begin{pmatrix} -1 \\ \tilde{w}_2 \end{array}} \cdot \underbrace{\begin{array}{ccc} x_2^2 \\ \tilde{z}_2 \end{array}} \right) \\ & = & \operatorname{sign}\left(\tilde{\mathbf{w}}^T \mathbf{z}\right) \end{array}$$

$$h(\mathbf{x}) = \operatorname{sign}\left(\underbrace{\begin{array}{ccc} 0.6 \\ \tilde{w}_0 \end{array}} \cdot \underbrace{\begin{array}{ccc} 1 \\ \tilde{z}_0 \end{array}} + \underbrace{\begin{pmatrix} -1 \\ \tilde{w}_1 \end{pmatrix}} \cdot \underbrace{\begin{array}{ccc} \chi_1^2 \\ \tilde{z}_1 \end{array}} + \underbrace{\begin{pmatrix} -1 \\ \tilde{w}_2 \end{pmatrix}} \cdot \underbrace{\begin{array}{ccc} \chi_2^2 \\ \tilde{z}_2 \end{array}} \right)$$

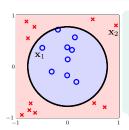
$$= \operatorname{sign}\left(\widetilde{\mathbf{w}}^T \mathbf{z}\right)$$



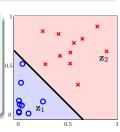
• $\{(\mathbf{x}_n, y_n)\}$ circular separable $\Longrightarrow \{(\mathbf{z}_n, y_n)\}$ linear separable



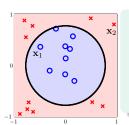
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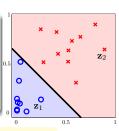
- $\{(\mathbf{x}_n, y_n)\}$ circular separable $\Rightarrow \{(\mathbf{z}_n, y_n)\}$ linear separable
- $\mathbf{x} \in \mathcal{X} \stackrel{\Phi}{\longmapsto} \mathbf{z} \in \mathcal{Z}$: (nonlinear) feature transform Φ



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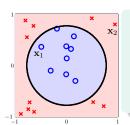


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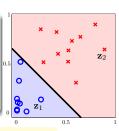


circular separable in $\mathcal{X} \Longrightarrow$ linear separable in \mathcal{Z}

$$h(\mathbf{x}) = \operatorname{sign}\left(\underbrace{\begin{array}{ccc} \underline{0.6} & \underbrace{1} & \underbrace{+(-1)} & \underbrace{x_1^2} & \underbrace{+(-1)} & \underbrace{x_2^2} \\ & & = \operatorname{sign}\left(\tilde{\mathbf{w}}^{\mathsf{T}}\mathbf{z}\right) \end{array}\right)$$



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circular separable in $\mathcal{X} \Longrightarrow$ linear separable in \mathcal{Z} vice versa?

$$(z_0, z_1, z_2) = \mathbf{z} = \mathbf{\Phi}(\mathbf{x}) = (1, x_1^2, x_2^2)$$

$$h(\mathbf{x}) = \tilde{h}(\mathbf{z}) = \operatorname{sign}\left(\tilde{\mathbf{w}}^T \mathbf{\Phi}(\mathbf{x})\right) = \operatorname{sign}\left(\tilde{\mathbf{w}}_0 + \tilde{\mathbf{w}}_1 x_1^2 + \tilde{\mathbf{w}}_2 x_2^2\right)$$

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$\tilde{\mathbf{w}} = (\tilde{w}_0, \tilde{w}_1, \tilde{w}_2)$

• (0.6, −1, −1): circle (∘ inside)

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- (0.6, -1, -2): ellipse

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lines in \mathcal{Z} -space

 \iff **special** quadratic curves in \mathcal{X} -space

a 'bigger'
$$\mathcal{Z}\text{-space}$$
 with $\Phi_2(\boldsymbol{x})=(1,x_1,x_2,x_1^2,x_1x_2,x_2^2)$

perceptrons in \mathcal{Z} -space \iff quadratic hypotheses in \mathcal{X} -space

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$$\mathcal{H}_{\Phi_2} = \left\{ h(\mathbf{x}) \colon h(\mathbf{x}) = \tilde{h}(\Phi_2(\mathbf{x})) \text{ for some linear } \tilde{h} \text{ on } \mathcal{Z} \right\}$$

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• can implement all possible quadratic curve boundaries: circle, ellipse, rotated ellipse, hyperbola, parabola, ...

ellipse
$$2(x_1 + x_2 - 3)^2 + (x_1 - x_2 - 4)^2 = 1$$

$$\iff \tilde{\mathbf{w}}^T =$$

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$$\mathcal{Z}\text{-space}$$
 with $\Phi_2(\mathbf{x})=(1,x_1,x_2,x_1^2,x_1x_2,x_2^2)$

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$$2(x_1 + x_2 - 3)^2 + (x_1 - x_2 - 4)^2 = 1$$

 $\iff \tilde{\mathbf{w}}^T = \begin{bmatrix} 33, -20, -4, 3, 2, 3 \end{bmatrix}$

a 'bigger'
$$\mathcal{Z}\text{-space}$$
 with $\Phi_2(\mathbf{x})=(1,x_1,x_2,x_1^2,x_1x_2,x_2^2)$

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include lines and constants as degenerate cases

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include lines and constants as degenerate cases

next: **learn** a good quadratic hypothesis *g*

Fun Time

Using the transform $\Phi_2(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_1 x_2, x_2^2)$, which of the following weights $\tilde{\mathbf{w}}^T$ in the \mathbb{Z} -space implements the parabola $2x_1^2 + x_2 = 1$?

- 1 [-1,2,1,0,0,0]
- 2 [0,2,1,0,-1,0]
- **3** [-1, 0, 1, 2, 0, 0]
- 4 [-1,2,0,0,0,1]

Fun Time

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- [0,2,1,0,-1,0]
- (3) [-1,0,1,2,0,0]
- 4 [-1,2,0,0,0,1]

Reference Answer: (3)

Too simple, uh? :-) Flexibility to implement arbitrary quadratic curves opens new possibilities for minimizing E_{in} !

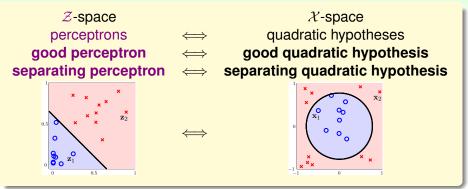
 \mathcal{Z} -space perceptrons

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 $\mathcal{X} ext{-space}$ quadratic hypotheses

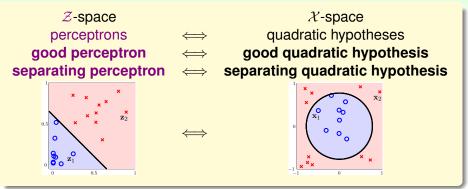
 \mathcal{Z} -space perceptrons \iff good perceptron

 $\mathcal{X}\text{-space}$ quadratic hypotheses good quadratic hypothesis



want: get good perceptron in Z-space

Good Quadratic Hypothesis



- want: get good perceptron in Z-space
- known: get **good perceptron** in \mathcal{X} -space with data $\{(\mathbf{x}_n, y_n)\}$

Good Quadratic Hypothesis

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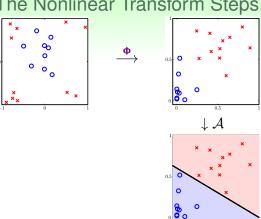
todo: get **good perceptron** in \mathbb{Z} -space with data $\{(\mathbf{z}_n = \Phi_2(\mathbf{x}_n), y_n)\}$

The Nonlinear Transform Steps



1 transform original data $\{(\mathbf{x}_n, y_n)\}$ to $\{(\mathbf{z}_n = \mathbf{\Phi}(\mathbf{x}_n), y_n)\}$ by $\mathbf{\Phi}$

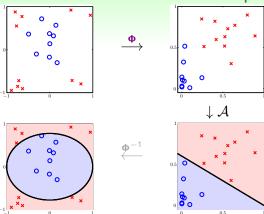
The Nonlinear Transform Steps



- transform original data $\{(\mathbf{x}_n, y_n)\}$ to $\{(\mathbf{z}_n = \mathbf{\Phi}(\mathbf{x}_n), y_n)\}$ by $\mathbf{\Phi}$
- 2 get a good perceptron $\tilde{\mathbf{w}}$ using $\{(\mathbf{z}_n, \mathbf{y}_n)\}$ and your favorite linear classification algorithm A

Nonlinear Transform

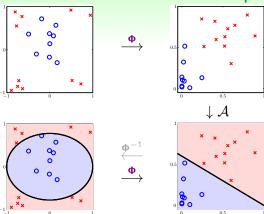
The Nonlinear Transform Steps



- **1** transform original data $\{(\mathbf{x}_n, y_n)\}$ to $\{(\mathbf{z}_n = \mathbf{\Phi}(\mathbf{x}_n), y_n)\}$ by $\mathbf{\Phi}$
- 2 get a good perceptron $\tilde{\mathbf{w}}$ using $\{(\mathbf{z}_n, y_n)\}$ and your favorite linear classification algorithm \mathcal{A}
- 3 return $g(\mathbf{x}) = \operatorname{sign}\left(\tilde{\mathbf{w}}^{\mathsf{T}}\mathbf{\Phi}(\mathbf{x})\right)$

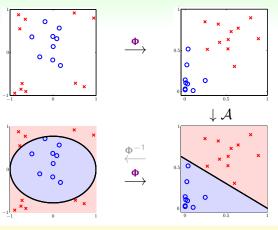
Nonlinear Transform

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Nonlinear Model via Nonlinear Φ + Linear Models



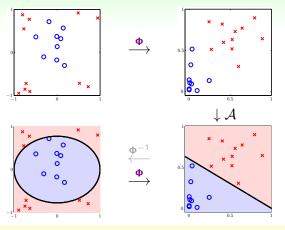
two choices:

feature transform

Pandora's box :-):

can now freely do quadratic PLA, quadratic regression, cubic regression, ..., polynomial regression

Nonlinear Model via Nonlinear Φ + Linear Models



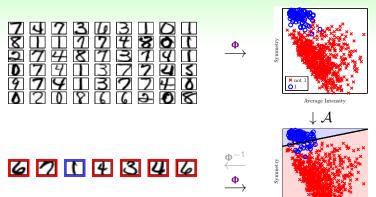
two choices:

- feature transformΦ
- linear model A, not just binary classification

Pandora's box :-):

can now freely do quadratic PLA, quadratic regression, cubic regression, ..., polynomial regression

Feature Transform **Φ**



not new, not just polynomial:

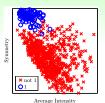
raw (pixels) domain knowledge

concrete (intensity, symmetry)

Average Intensity

Feature Transform •







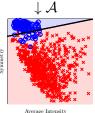












not new, not just polynomial:

raw (pixels)

concrete (intensity, symmetry)

the force, too good to be true? :-)

Fun Time

Consider the quadratic transform $\Phi_2(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^d$ instead of in \mathbb{R}^2 . The transform should include all different quadratic, linear, and constant terms formed by (x_1, x_2, \dots, x_d) . What is the number of dimensions of $\mathbf{z} = \Phi_2(\mathbf{x})$?

- 1 0
- $\frac{d^2}{2} + \frac{3d}{2} + 1$
- 3 $d^2 + d + 1$
- 4 2^d

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- 10
- $\frac{d^2}{2} + \frac{3d}{2} + 1$
- 3 $d^2 + d + 1$
- 4 2^d

Reference Answer: (2)

Number of different quadratic terms is $\binom{d}{2} + d$; number of different linear terms is d; number of different constant term is 1.

Q-th order polynomial transform:
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$$\underbrace{1}_{\widetilde{w}_0} + \underbrace{\widetilde{d}}_{\text{others}}$$
 dimensions

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$$- \# \text{ ways of } \leq O \text{-combination from } d \text{ k}$$

= # ways of $\leq Q$ -combination from d kinds with repetitions

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 dimensions

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$$= \binom{Q+d}{Q} = \binom{Q+d}{d} = {\color{red}O} \left({\color{red}Q^d} \right)$$

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 $Q \text{ large} \Longrightarrow \text{difficult to compute/store}$

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any $\tilde{d}+2$ inputs not shattered in \mathcal{Z} \Longrightarrow any $\tilde{d}+2$ inputs not shattered in \mathcal{X}

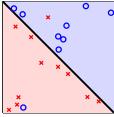
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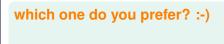
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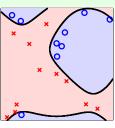
any $\tilde{d} + 2$ inputs not shattered in \mathcal{Z} \Longrightarrow any $\tilde{d} + 2$ inputs not shattered in \mathcal{X}

 $Q \text{ large} \Longrightarrow \text{large } d_{VC}$

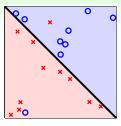


 Φ_1 (original \mathbf{x})





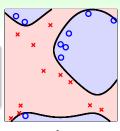
 Φ_4



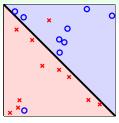
 $\Phi_1 \; (\text{original} \; \boldsymbol{x})$

which one do you prefer? :-)

Φ₁ 'visually' preferred



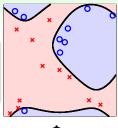
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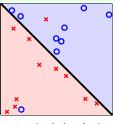


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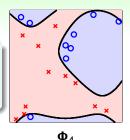
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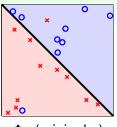


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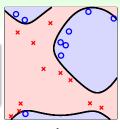


- Φ_1 (original \mathbf{x})
- 1 can we make sure that $E_{out}(g)$ is close enough to $E_{in}(g)$?
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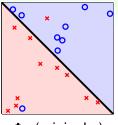
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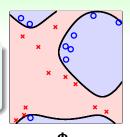
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trade-off:	$\tilde{d}(Q)$	1	2
	higher	:-(:-D
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how to pick Q? visually, maybe?

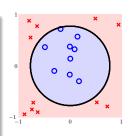
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Visualize $\mathcal{X} = \mathbb{R}^2$

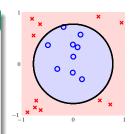
• full Φ_2 : $\mathbf{z} = (1, x_1, x_2, x_1^2, x_1 x_2, x_2^2), d_{VC} = 6$



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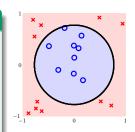
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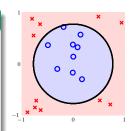
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- or $\mathbf{z} = (1, x_1^2, x_2^2), d_{VC} = 3, after visualizing?$
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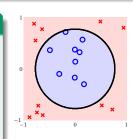
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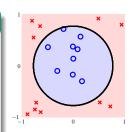
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for VC-safety, Φ shall be decided without 'peeking' data

Fun Time

Consider the Q-th order polynomial transform $\Phi_Q(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^2$. Recall that $\tilde{d} = \binom{Q+2}{2} - 1$. When Q = 50, what is the value of \tilde{d} ?

- 1126
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- 3 2651
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Reference Answer: 2

It's just a simple calculation, but shows you how \tilde{d} becomes hundreds of times of d=2 after the transform.

$$\Phi_0(\mathbf{x}) = (1), \Phi_1(\mathbf{x}) = (\Phi_0(\mathbf{x}), \qquad x_1, x_2, \dots, x_d)$$

$$\begin{aligned} \boldsymbol{\Phi}_0(\mathbf{x}) &= \Big(1\Big), \boldsymbol{\Phi}_1(\mathbf{x}) = \Big(\boldsymbol{\Phi}_0(\mathbf{x}), \quad x_1, x_2, \dots, x_d\Big) \\ \boldsymbol{\Phi}_2(\mathbf{x}) &= \Big(\boldsymbol{\Phi}_1(\mathbf{x}), \quad x_1^2, x_1 x_2, \dots, x_d^2\Big) \end{aligned}$$

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$$\Phi_3(\mathbf{x}) = (\Phi_2(\mathbf{x}), \quad x_1^3, x_1^2 x_2, \dots, x_d^3)$$

$$\dots \dots$$

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$$\mathcal{H}_{\Phi_0} \subset \mathcal{H}_{\Phi_1} \subset \mathcal{H}_{\Phi_2} \subset \mathcal{H}_{\Phi_3} \subset \ldots \subset \mathcal{H}_{\Phi_Q}$$

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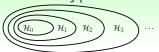
$$\dots$$

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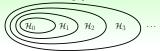
structure: nested \mathcal{H}_i

Structured Hypothesis Sets



 $\mathcal{H}_0 \quad \ \subset \quad \ \mathcal{H}_1 \quad \ \subset \quad \ \mathcal{H}_2 \quad \ \subset \quad \ \mathcal{H}_3 \quad \ \subset \quad \ldots$

Structured Hypothesis Sets



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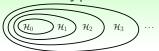


Structured Hypothesis Sets



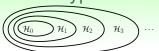
Let
$$g_i = \operatorname{argmin}_{h \in \mathcal{H}_i} E_{\operatorname{in}}(h)$$
:

Structured Hypothesis Sets

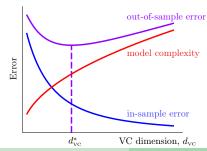


Let $g_i = \operatorname{argmin}_{h \in \mathcal{H}_i} E_{\operatorname{in}}(h)$:

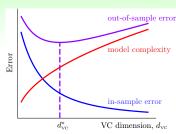
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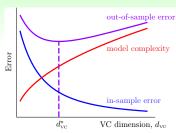
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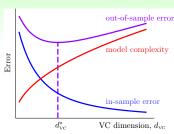
use \mathcal{H}_{1126} won't be good! :-(



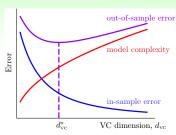
• tempting sin: use \mathcal{H}_{1126} , low $E_{in}(g_{1126})$ to fool your boss



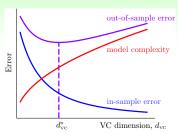
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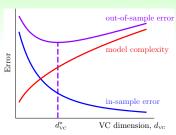
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linear model first: simple, efficient, safe, and workable!

Fun Time

Consider two hypothesis sets, \mathcal{H}_1 and \mathcal{H}_{1126} , where $\mathcal{H}_1 \subset \mathcal{H}_{1126}$. Which of the following relationship between $d_{VC}(\mathcal{H}_1)$ and $d_{VC}(\mathcal{H}_{1126})$ is not possible?

- $\mathbf{0} d_{VC}(\mathcal{H}_1) = d_{VC}(\mathcal{H}_{1126})$
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- **3** $d_{VC}(\mathcal{H}_1) < d_{VC}(\mathcal{H}_{1126})$
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Reference Answer: 4

Every input combination that \mathcal{H}_1 shatters can be shattered by \mathcal{H}_{1126} , so d_{VC} cannot decrease.

Summary

- 1 When Can Machines Learn?
- 2 Why Can Machines Learn?
- 3 How Can Machines Learn?

Lecture 11: Linear Models for Classification

Lecture 12: Nonlinear Transformation

Quadratic Hypotheses

linear hypotheses on quadratic-transformed data

- Nonlinear Transform happy linear modeling after $\mathcal{Z} = \Phi(\mathcal{X})$
- Price of Nonlinear Transform
 computation/storage/[model complexity]
- Structured Hypothesis Sets
 linear/simpler model first
- next: dark side of the force :-)
- 4 How Can Machines Learn Better?