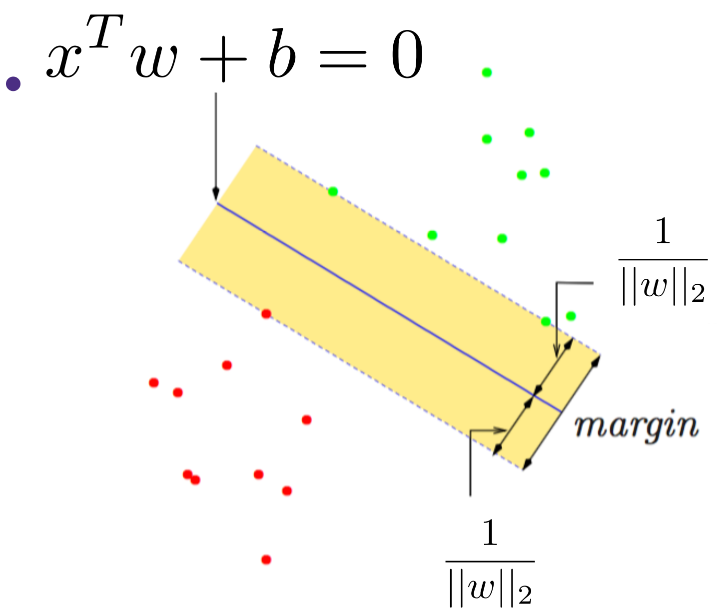
Kernels

What if the data is not linearly separable?



Some points do not satisfy margin constraint:

$$\min_{w,b} ||w||_2^2$$

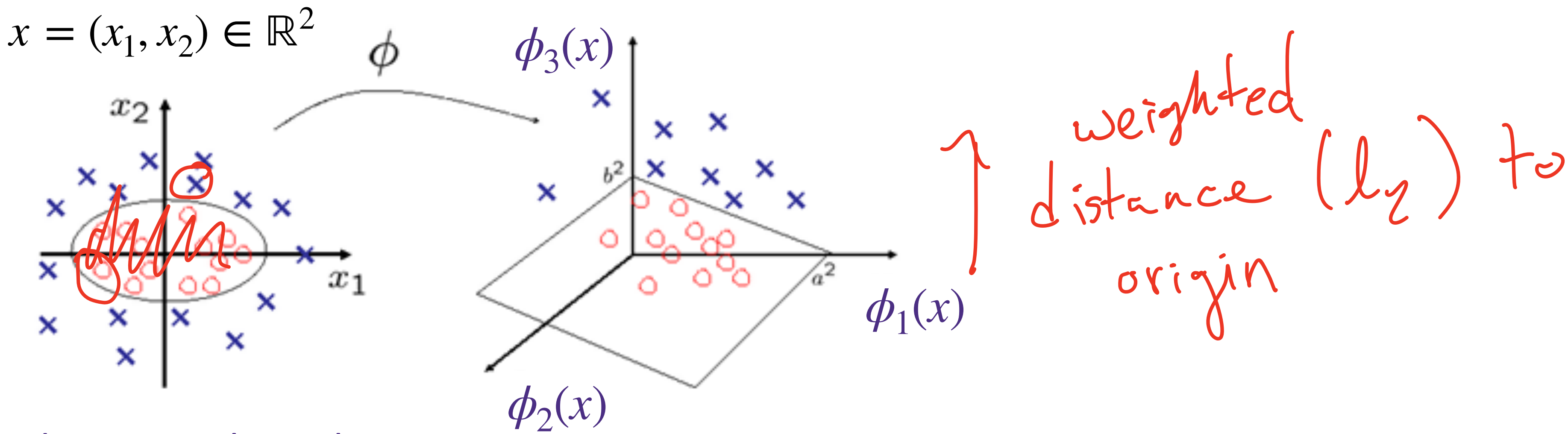
$$y_i(x_i^T w + b) \geq 1 \quad \forall i$$

Two options:

1. Introduce slack to this optimization problem (Support Vector Machine)
2. **Lift to higher dimensional space (Kernels)**

What if the data is not linearly separable?

- Use features, for example,

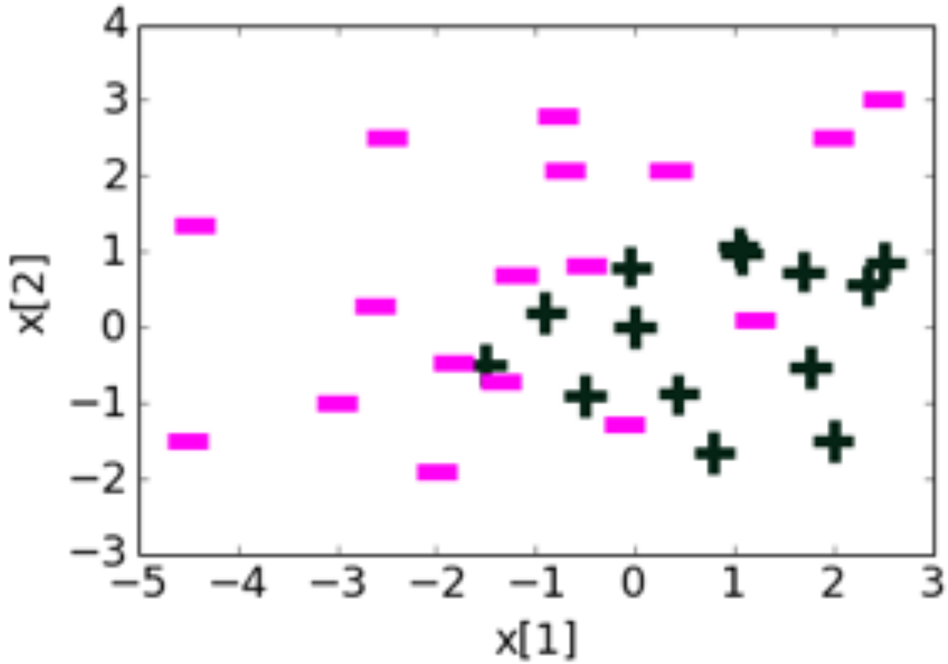


This data is not linearly separable

Can you suggest some features $\phi_1(x_1, x_2), \phi_2(x_1, x_2), \phi_3(x_1, x_2)$ such that this data is linearly separable in this 3-dimensional space?

- Generally, in high dimensional feature space, it is easier to linearly separate different classes
- However, it is hard to know which feature map will work for given data
- So the rule of thumb is to use high-dimensional features and hope that the algorithm will automatically pick the right set of features

Example: adding more polynomial features

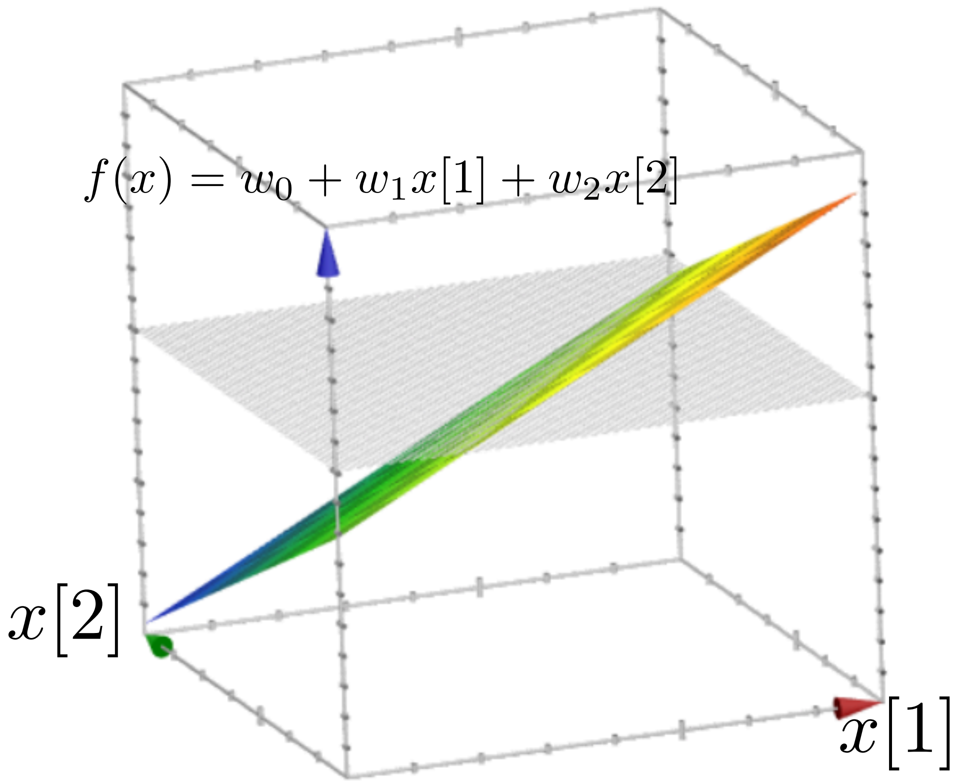


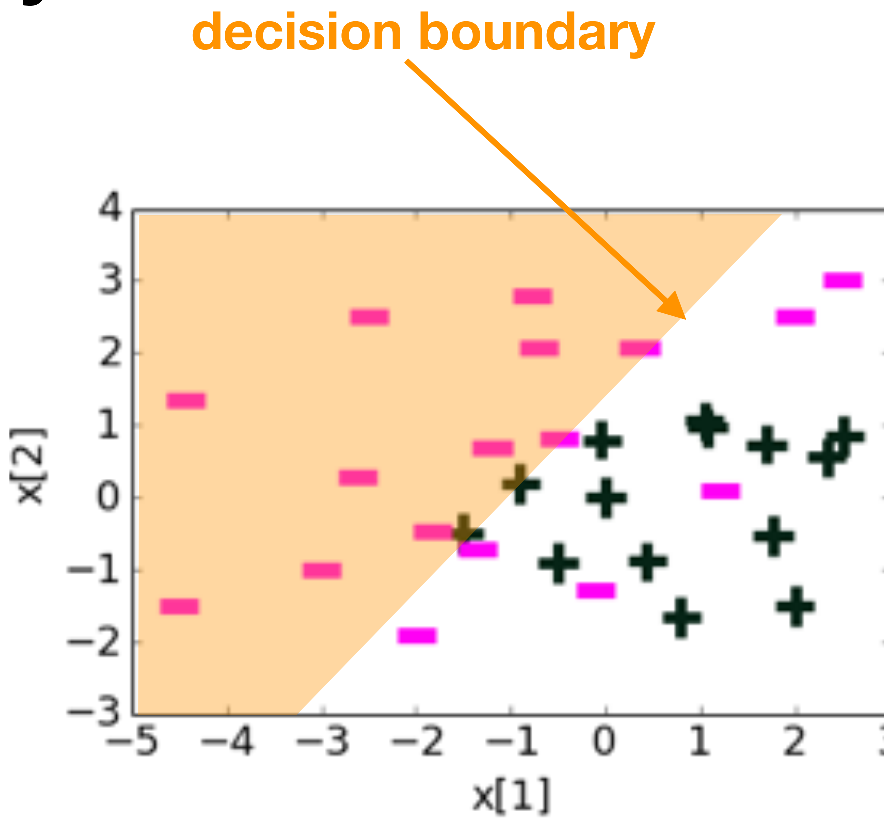
Polynomial features

$$\begin{bmatrix} h_0(x) = 1 \\ h_1(x) = x[1] \\ h_2(x) = x[2] \\ h_3(x) = x[1]^2 \\ h_4(x) = x[2]^2 \\ \vdots \end{bmatrix}$$

- data: ***x*** in 2-dimensions, ***y*** in {+1,-1}
- features: polynomials
- model: linear on polynomial features
- $$f(x) \ = \ w_0 h_0(x) + w_1 h_1(x) + w_2 h_2(x) + \cdots$$

Learned decision boundary





Feature	Value	Coefficient
$h_0(x)$	1	0.23
$h_1(x)$	x[1]	1.12
$h_2(x)$	x[2]	-1.07

- Simple **regression** models had **smooth** predictors
- Simple **classifier** models have **smooth** decision boundaries

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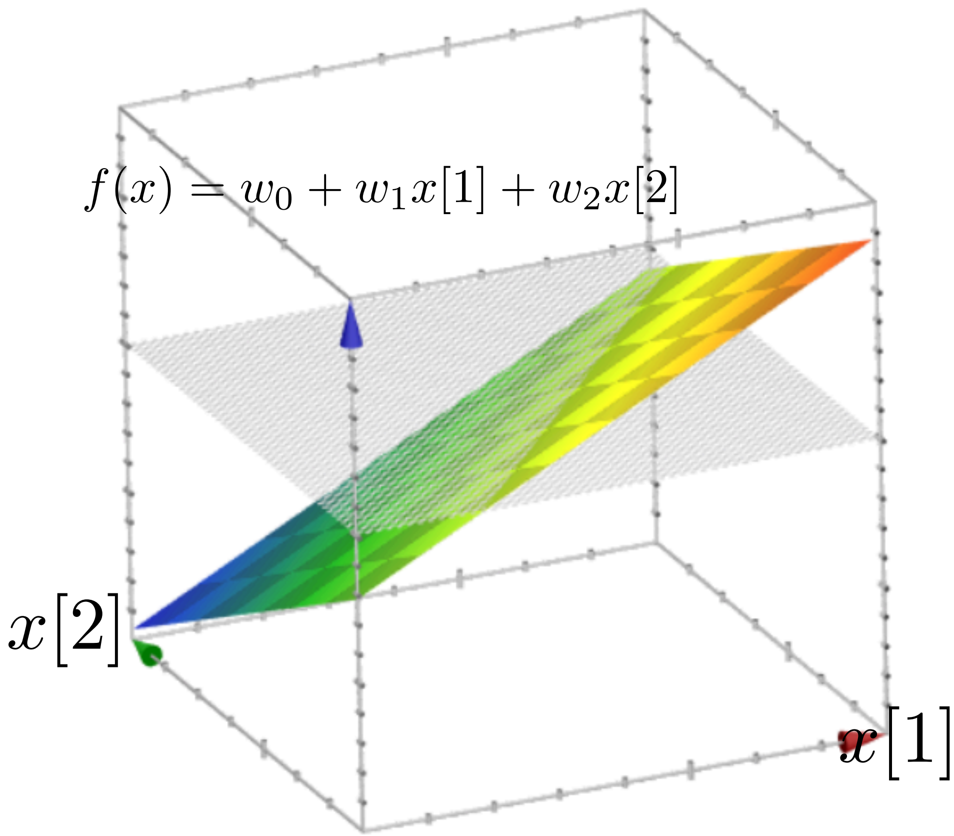

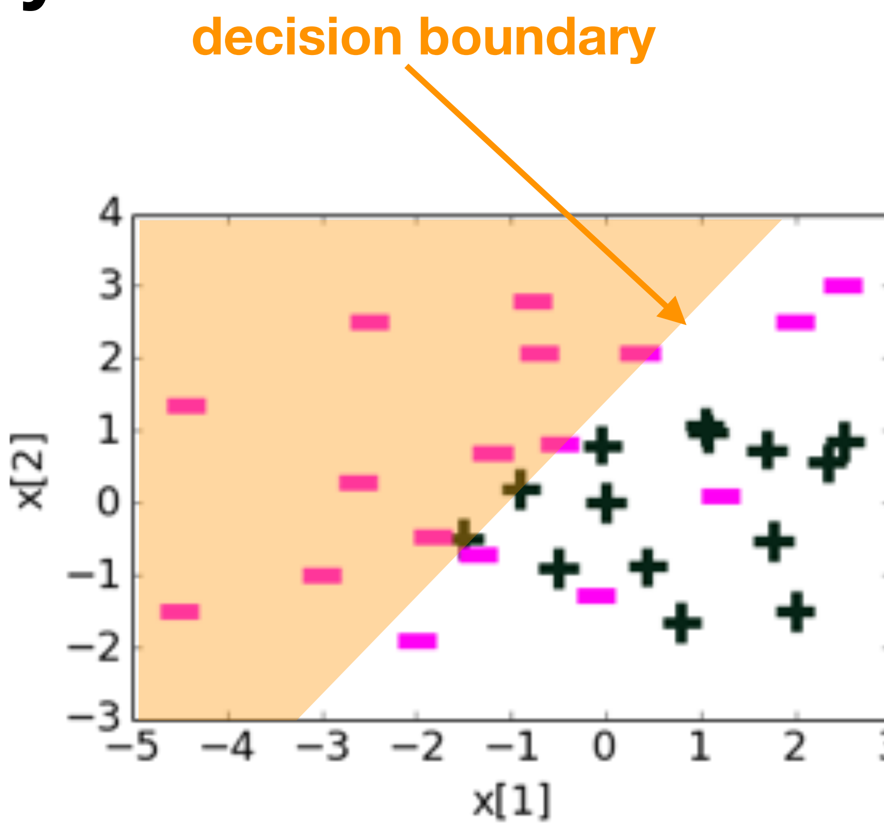

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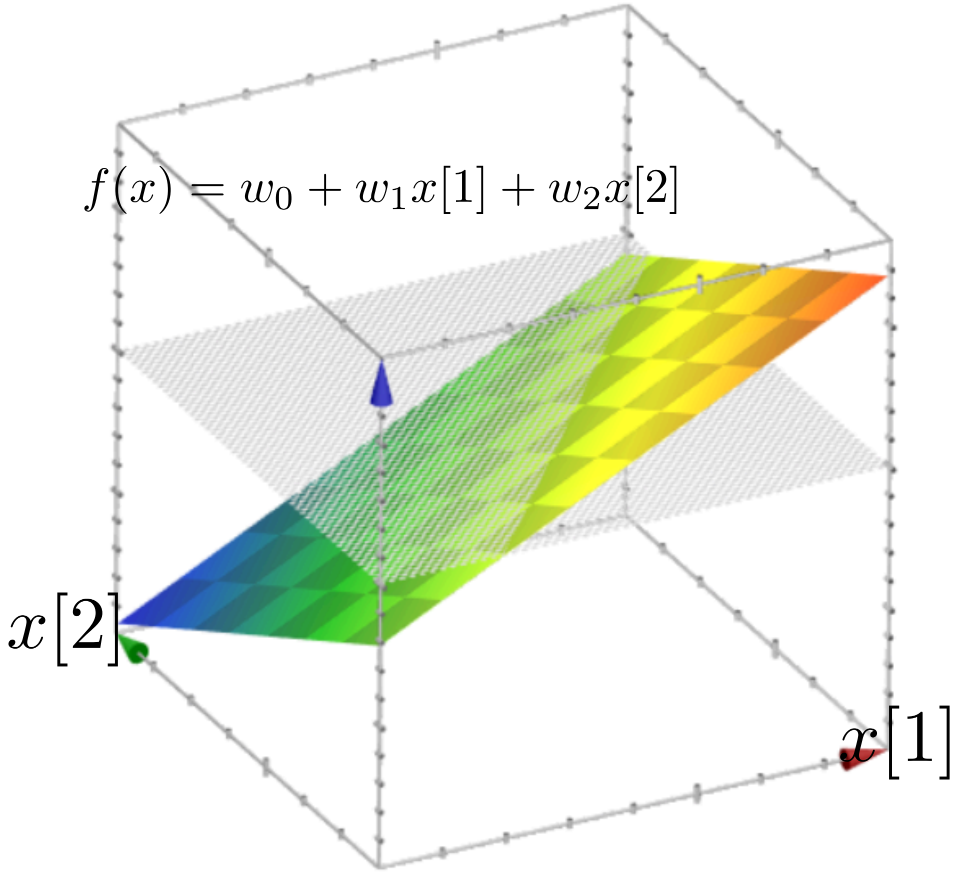

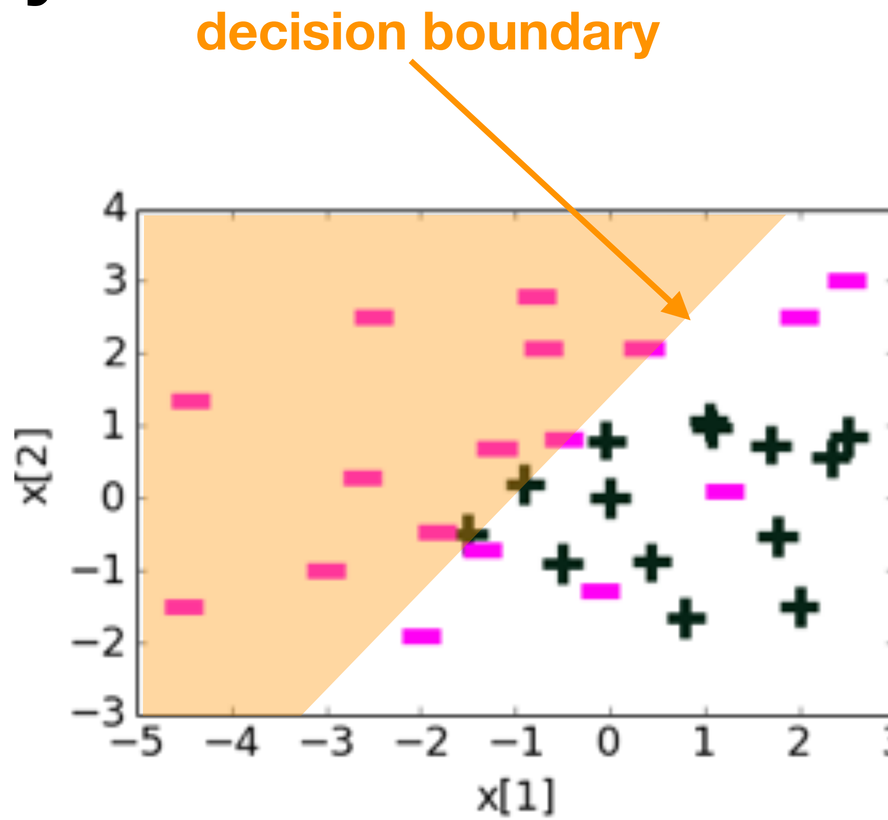

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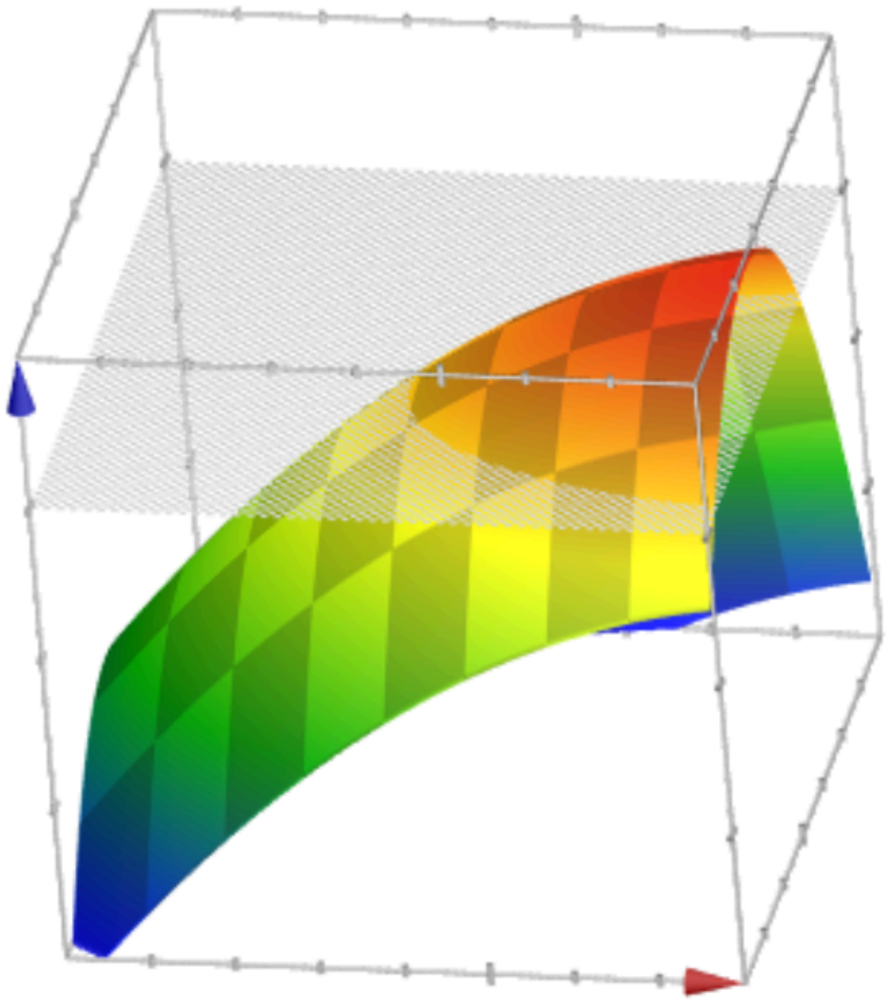
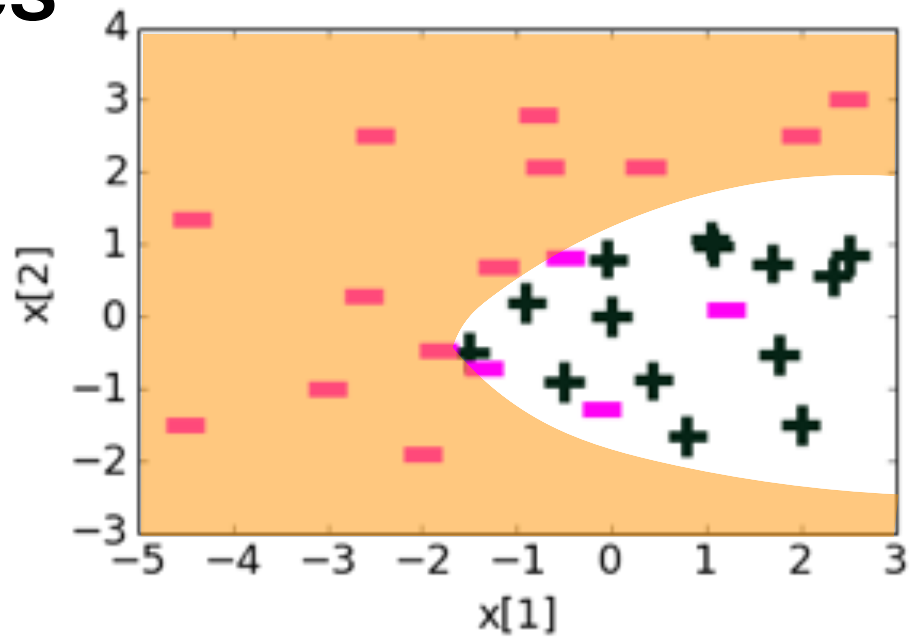
Adding quadratic features





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$h_1(x)$	x[1]	1.39
$h_2(x)$	x[2]	-0.59
$h_3(x)$	$(x[1])^2$	-0.17
$h_4(x)$	$(x[2])^2$	-0.96
$h_5(x)$	x[1]x[2]	Omitted

- Adding more features gives more complex models
- Decision boundary becomes more complex

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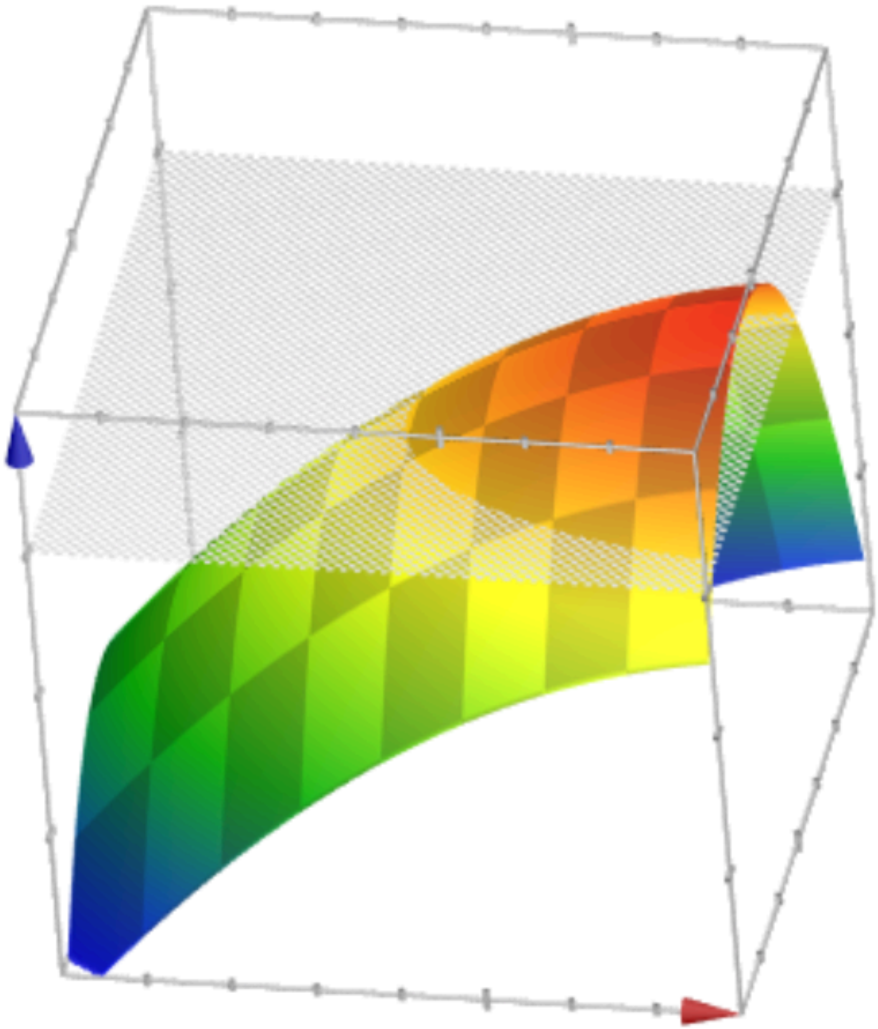

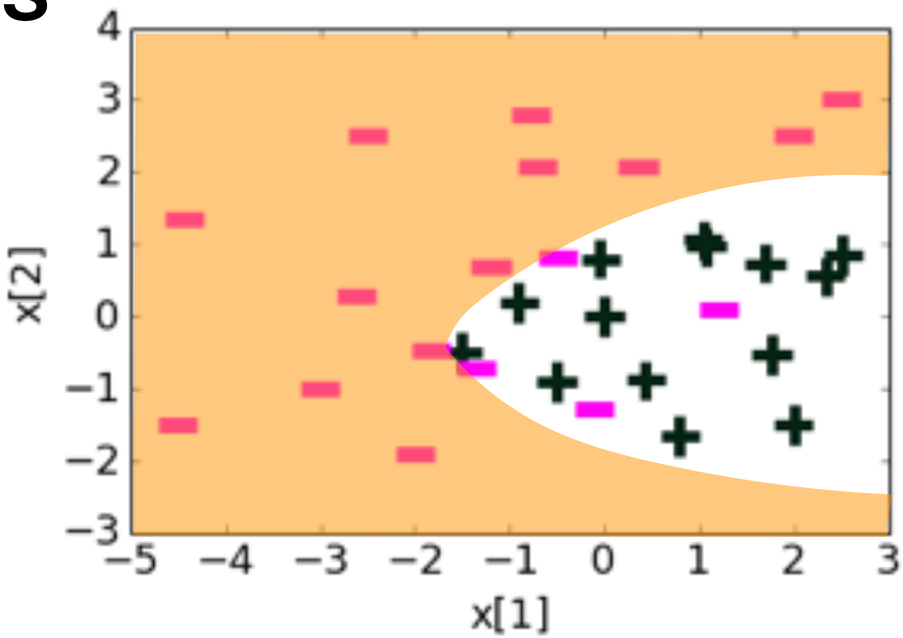

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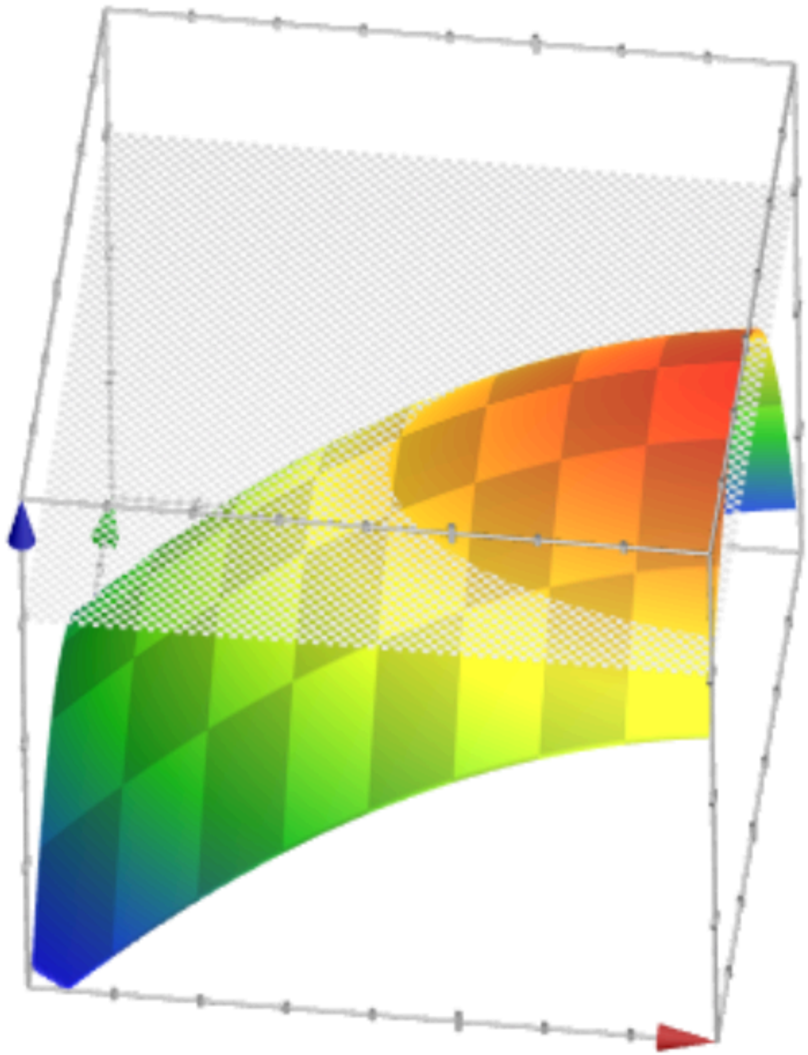

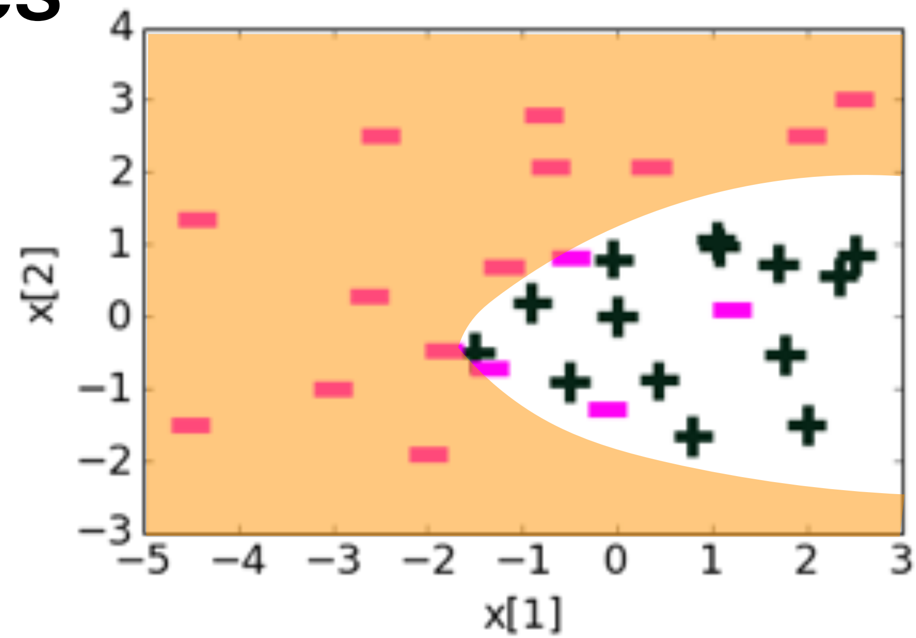

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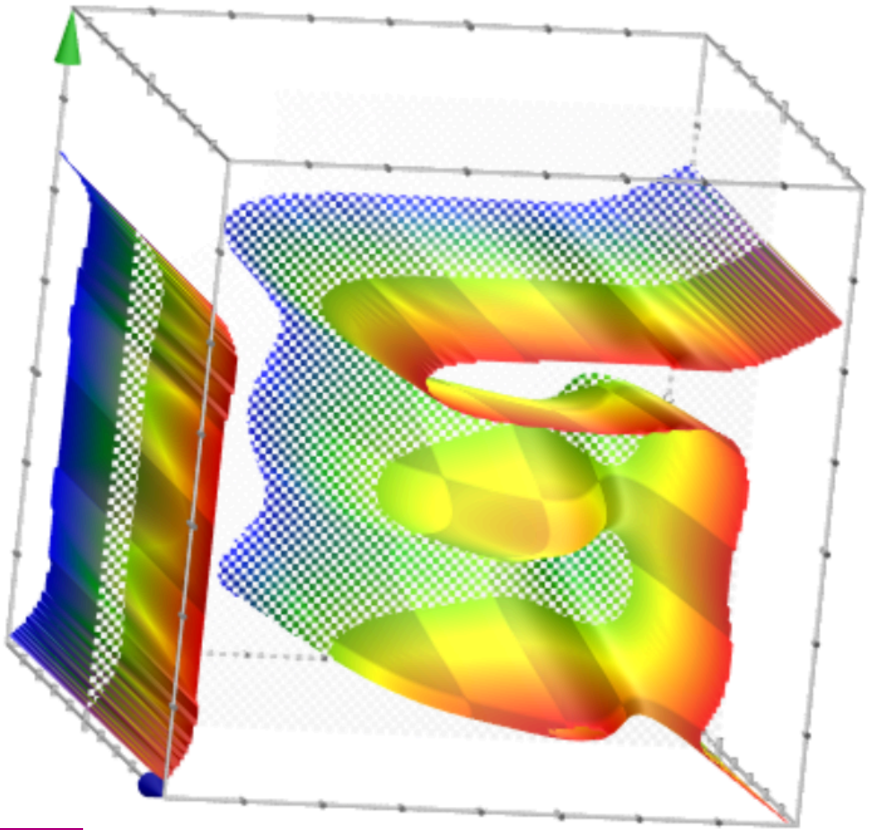
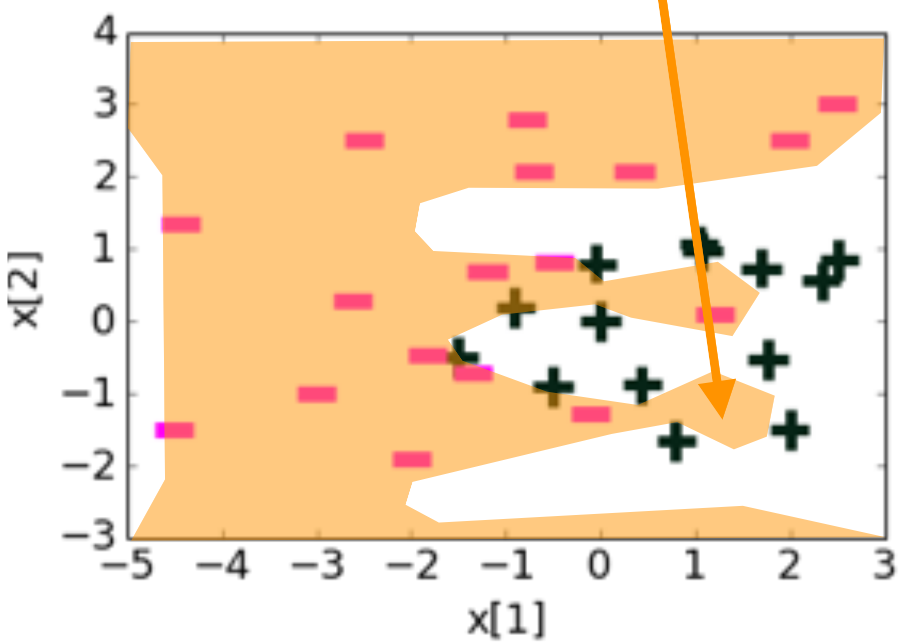


Overfitting leads to non-generalization



Feature	Value	Coefficient learned
$h_0(x)$	1	21.6
$h_1(x)$	x[1]	5.3
$h_2(x)$	x[2]	-42.7
$h_3(x)$	$(x[1])^2$	-15.9
$h_4(x)$	$(x[2])^2$	-48.6
$h_5(x)$	$(x[1])^3$	-11.0
$h_6(x)$	$(x[2])^3$	67.0
$h_7(x)$	$(x[1])^4$	1.5
$h_8(x)$	$(x[2])^4$	48.0
$h_9(x)$	$(x[1])^5$	4.4
$h_{10}(x)$	$(x[2])^5$	-14.2
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Coefficient values getting large

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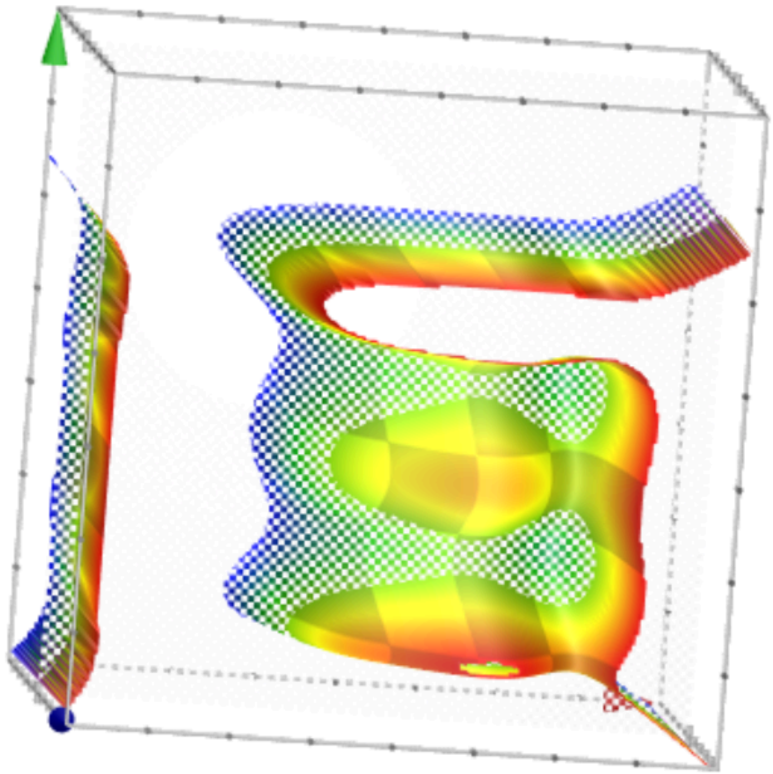

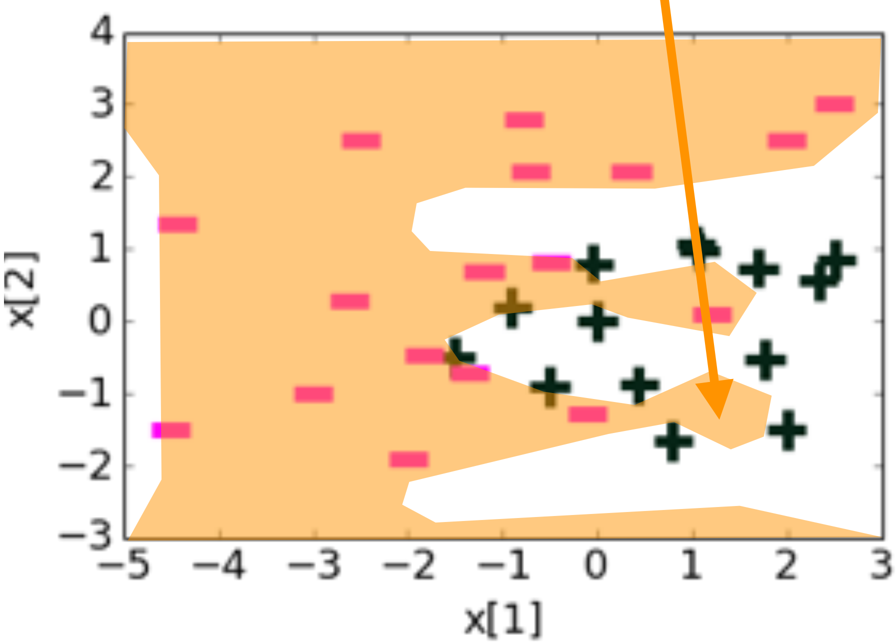

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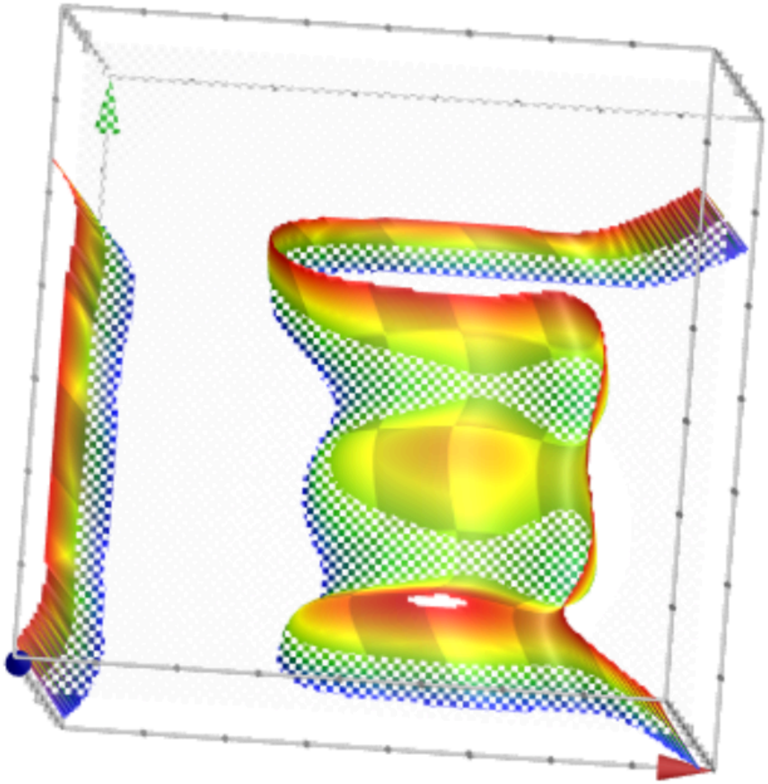

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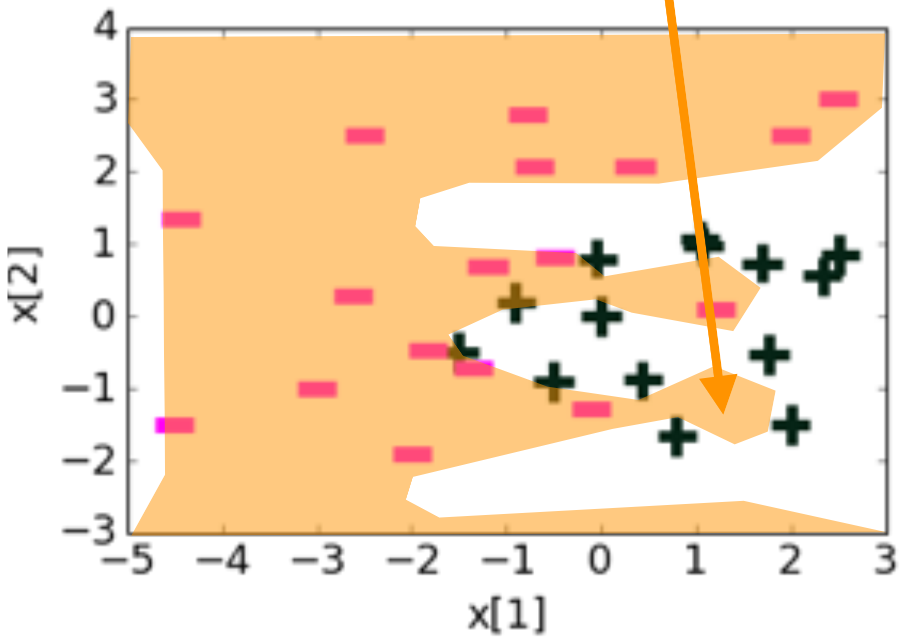

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- Overfitting leads to very large values of

$$f(x) = w_0 h_0(x) + w_1 h_1(x) + w_2 h_2(x) + \cdots$$

Creating Features

- Feature mapping $\phi : \mathbb{R}^d \to \mathbb{R}^p$ maps original data into a rich and high-dimensional feature space (usually $d \ll p$)

For example, in d=1, one can use

$$\phi(x) = \begin{bmatrix} \phi_1(x) \\ \phi_2(x) \\ \vdots \\ \phi_k(x) \end{bmatrix} = \begin{bmatrix} x \\ x^2 \\ \vdots \\ x^k \end{bmatrix}$$

For example, for d>1, one can generate vectors

and define features:

$$\phi_j(x) = \cos(u_j^T x)$$

$$\phi_j(x) = (u_j^T x)^2$$

$$\phi_j(x) = \frac{1}{1 + \exp(u_j^T x)}$$

- Feature space can get really large really quickly!
- How many coefficients/parameters are there for degree-k polynomials for $x = (x_1, \ldots, x_d) \in \mathbb{R}^d$?
- At a first glance, it seems inevitable that we need memory (to store the features $\{\phi(x_i) \in \mathbb{R}^p\}_{i=1}^n$) and run-time that increases with p where $d < n \ll p$

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How do we deal with high-dimensional lifts/data?

A fundamental trick in ML: use kernels

A function $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a *kernel* for a map ϕ if $K(x, x') = \phi(x) \cdot \phi(x')$ for all x, x'.

This notation is for dot product (which is the same as inner product)

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then we can avoid explicitly computing and storing (high-dimensional) $\{\phi(x_i)\}_{i=1}^n$ and instead only work with the kernel matrix of the training data $\{K(x_i, x_j)\}_{i,j\in\{1,\ldots,n\}}$

An example of a kernel

$x \in \mathbb{R}^2 \rightarrow \phi(x) \in \mathbb{R}^3$

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$$= x_1^3 \cdot {x'_1}^3 + \sqrt{3}x_1^2x_2 \cdot \sqrt{3}{x'_1}^2x'_2 + \sqrt{3}x_1x_2^2 \cdot \sqrt{3}x'_1{x'_2}^2 + x_2^3 \cdot {x'_2}^3$$

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$$= x_1^3 \cdot x_1'^3 + \sqrt{3}x_1^2x_2 \cdot \sqrt{3}x_1'^2x_2' + \sqrt{3}x_1x_2^2 \cdot \sqrt{3}x_1'x_2'^2 + x_2^3 \cdot x_2'^3$$

$$= x_1^3 \cdot x_1'^3 + 3x_1^2x_2x_1'^2x_2' + 3x_1x_2^2x_1'x_2'^2 + x_2^3 \cdot x_2'^3$$

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$$= x_1^3 \cdot {x'_1}^3 + 3x_1^2x_2{x'_1}^2x'_2 + 3x_1x_2^2x'_1{x'_2}^2 + x_2^3 \cdot {x'_2}^3$$

$$= ((x_1, x_2)^\top(x'_1, x'_2))^3$$

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An example of a kernel

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  - The features are **implicit** and accessed only via kernels, making it efficient

Ridge Linear Regression as Kernels

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(when $n < d$ via linear algebra)

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- Even if we run ridge linear regression on feature map $\phi(x) \in \mathbb{R}^p$, we only need to access the features via kernel $K(x_i, x_j)$ and $K(x_i, x_{\text{new}})$ and not the features $\phi(x_i)$

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4. Make prediction with $\widehat{y}_{\text{new}} = \sum_{i=1}^{n} \alpha_i K(x_i, x_{\text{new}})$

   (replacing $x_i^T x_{\text{new}}$ with $K(x_i, x_{\text{new}})$)

The Kernel Trick for regularized least squares

ℓ^2

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(transformed optimization)

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$$= \arg\min_\alpha \sum_{i=1}^n (y_i - \sum_{j=1}^n \alpha_j K(x_i, x_j))^2 + \lambda \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j K(x_i, x_j)$$

The Kernel Trick for regularized least squares

$$\widehat{w} = \arg\min_w \sum_{i=1}^n (y_i - w^T x_i)^2 + \lambda \|w\|_2^2$$

There exists an $\alpha \in \mathbb{R}^n$: $\widehat{w} = \sum_{i=1}^n \alpha_i x_i$ (Step 1. Use a linear predictor)

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(Step 2. Write an algorithm in terms of $\widehat{\alpha}$)

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$$= \arg\min_{\alpha} ||\mathbf{y} - \mathbf{P}\alpha||_2^2 + \lambda \alpha^{\top} \mathbf{P} \alpha$$

Where $\mathbf{P}_{ij} = K(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle$

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Thus, $\widehat{\alpha}_{\text{kernel}} = (\mathbf{P} + \lambda \mathbf{I}_{n \times n})^{-1} \mathbf{y}$

Examples of popular Kernels

- **Polynomials of degree exactly k**

$$K(x, x') = (x^T x')^k$$

- **Polynomials of degree up to k**

$$K(x, x') = (1 + x^T x')^k$$

- **Gaussian (squared exponential) kernel**
  (a.k.a RBF kernel for Radial Basis Function)

$$K(x, x') = \exp\left(- \frac{\|x - x'\|_2^2}{2\sigma^2} \right)$$

- **Sigmoid**

$$K(x, x') = \tanh(\gamma x^T x' + r)$$