CS 4824/ECE 4424: Kernels

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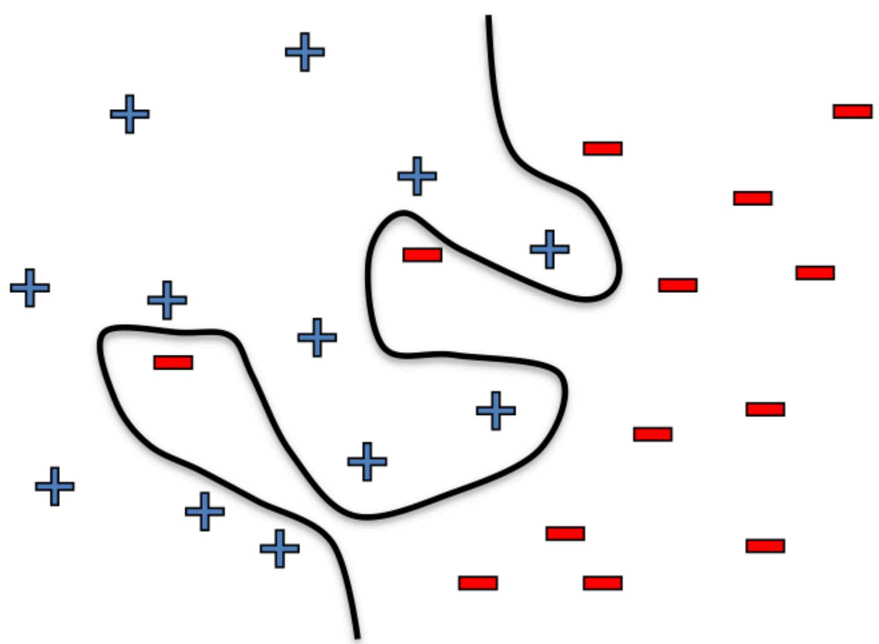
Generalized linear models vs. neural networks

- Generalized linear models (up to ~2010)
  - Fixed basis functions
  - Hypothesis space is limited
  - Easy to optimize (usually convex)

- Neural networks (2010 onwards)
  - Adaptive basis functions
  - Rich hypothesis space
  - Hard to optimize (usually non-convex)

How to extend generalized linear models to have richer hypothesis?

How to generalize linear models for linearly non-separable data?



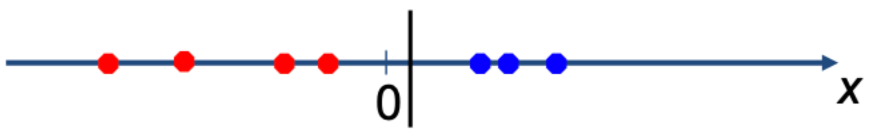
- Use features of features of features of features….

$$\phi(x) = \begin{pmatrix} x_1 \\ \vdots \\ x_n \\ x_1 x_2 \\ x_2 x_3 \\ \vdots \\ x_1^2 \\ x_2^2 \\ \vdots \end{pmatrix}$$

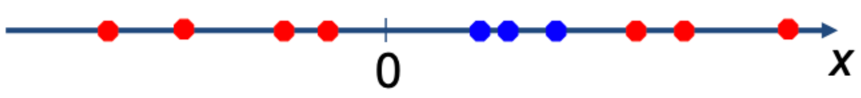
- **Challenge**: Feature space can get really large really quickly!

Non-linear features: 1D input

◦ Datasets that are linearly separable with some noise work out great:



◦ But what are we going to do if the dataset is just too hard?



Non-linear features: 1D input

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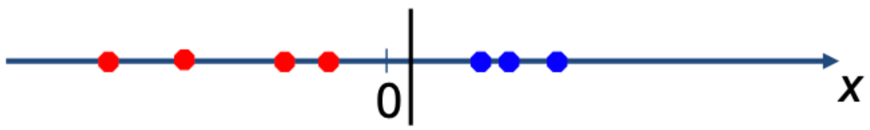

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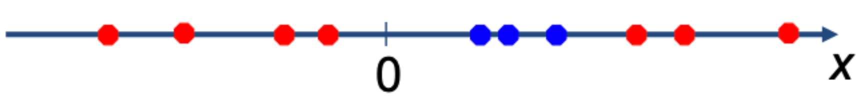
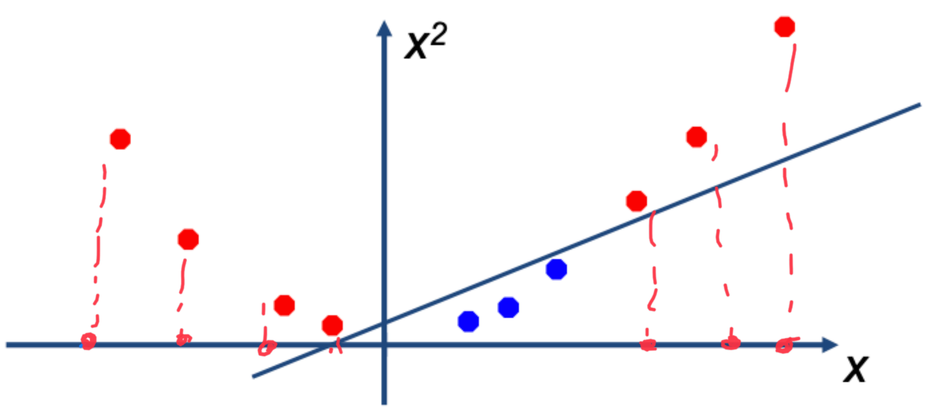
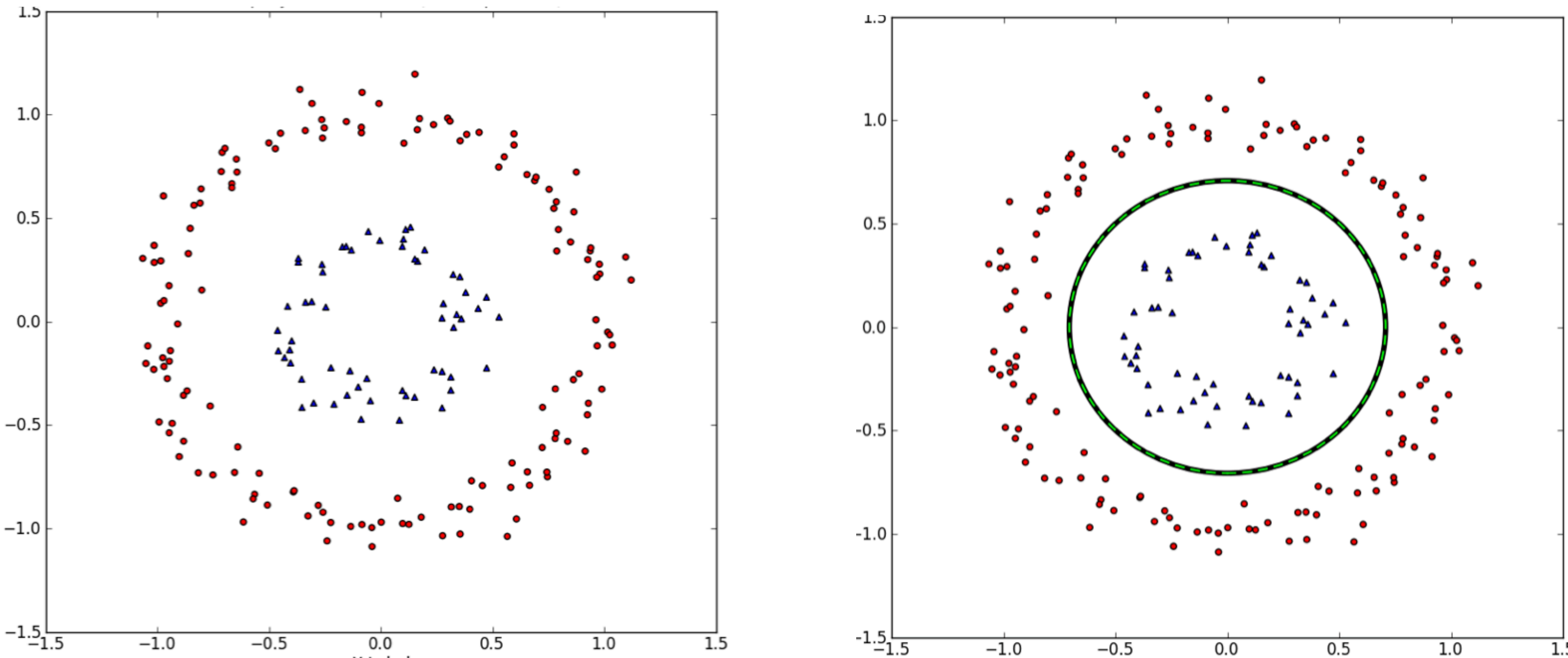


- How about… mapping data to a higher-dimensional space:

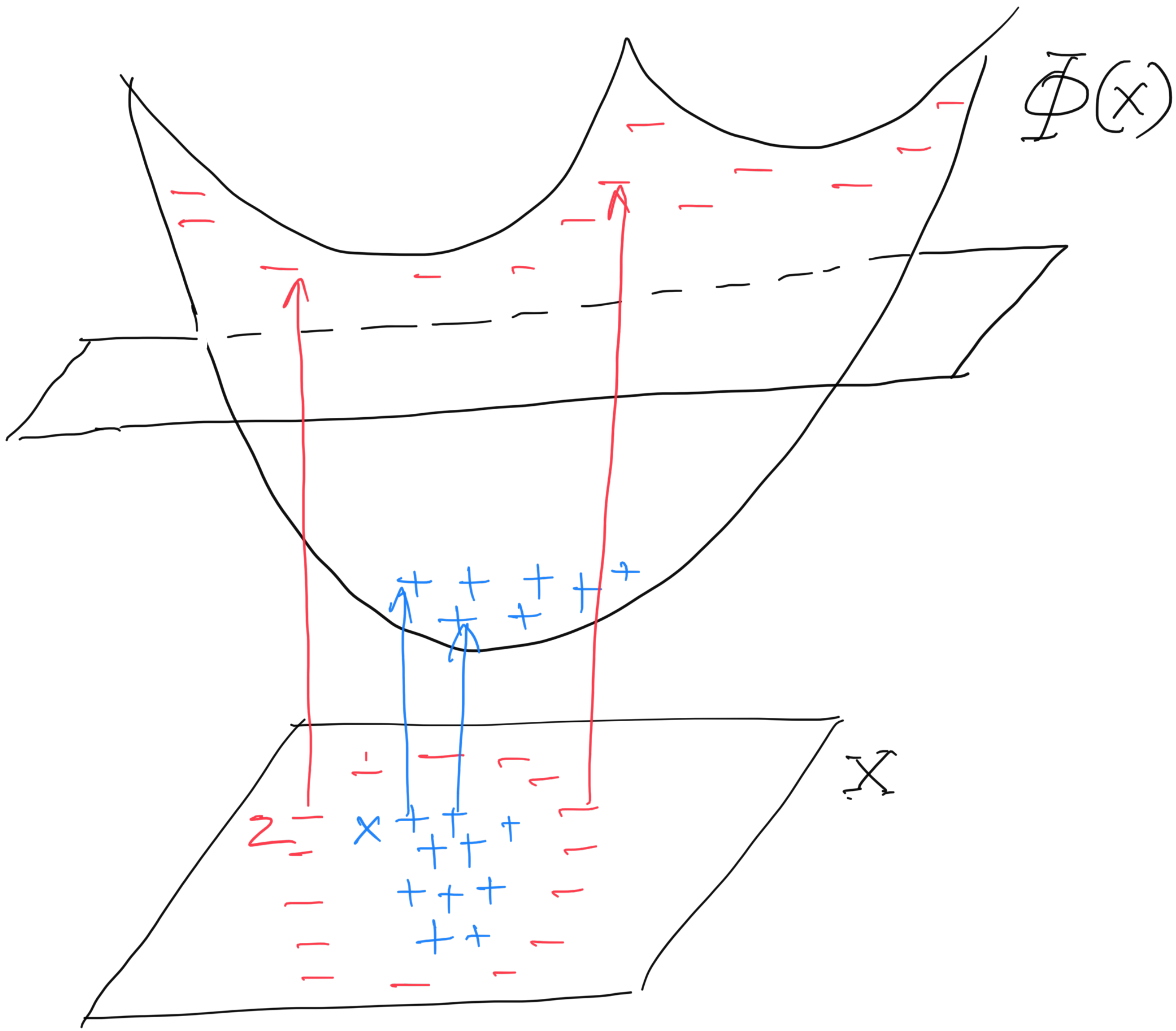


Mapping to higher dimensional space

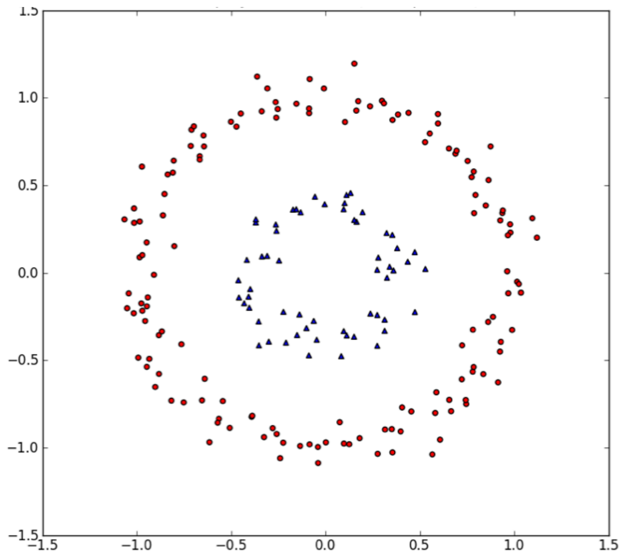


Linearly non-separable

Mapping to higher dimensional space

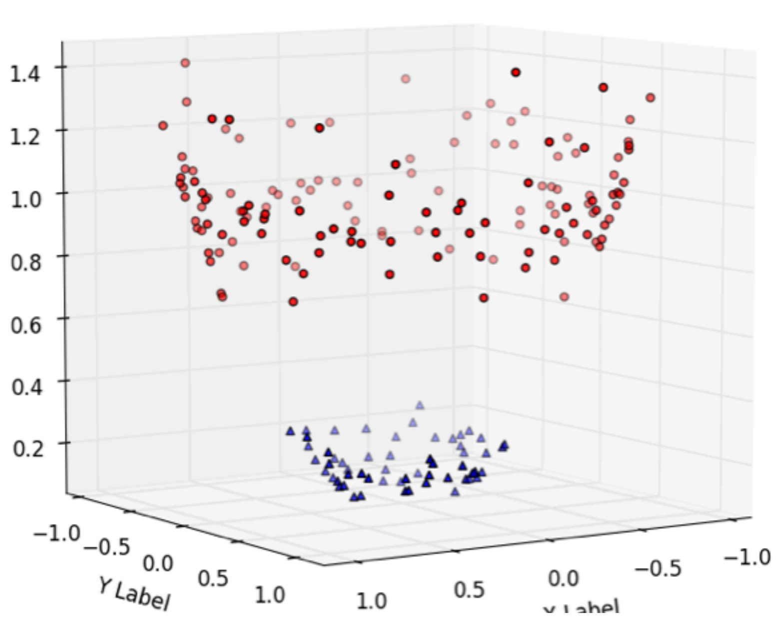


Mapping to higher dimensional space

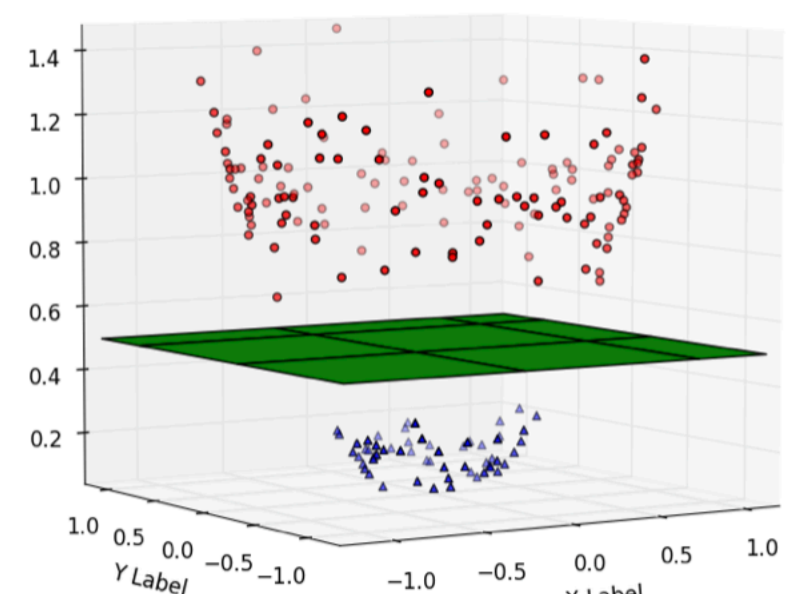


x

Map to 3D



$\Phi(x)$

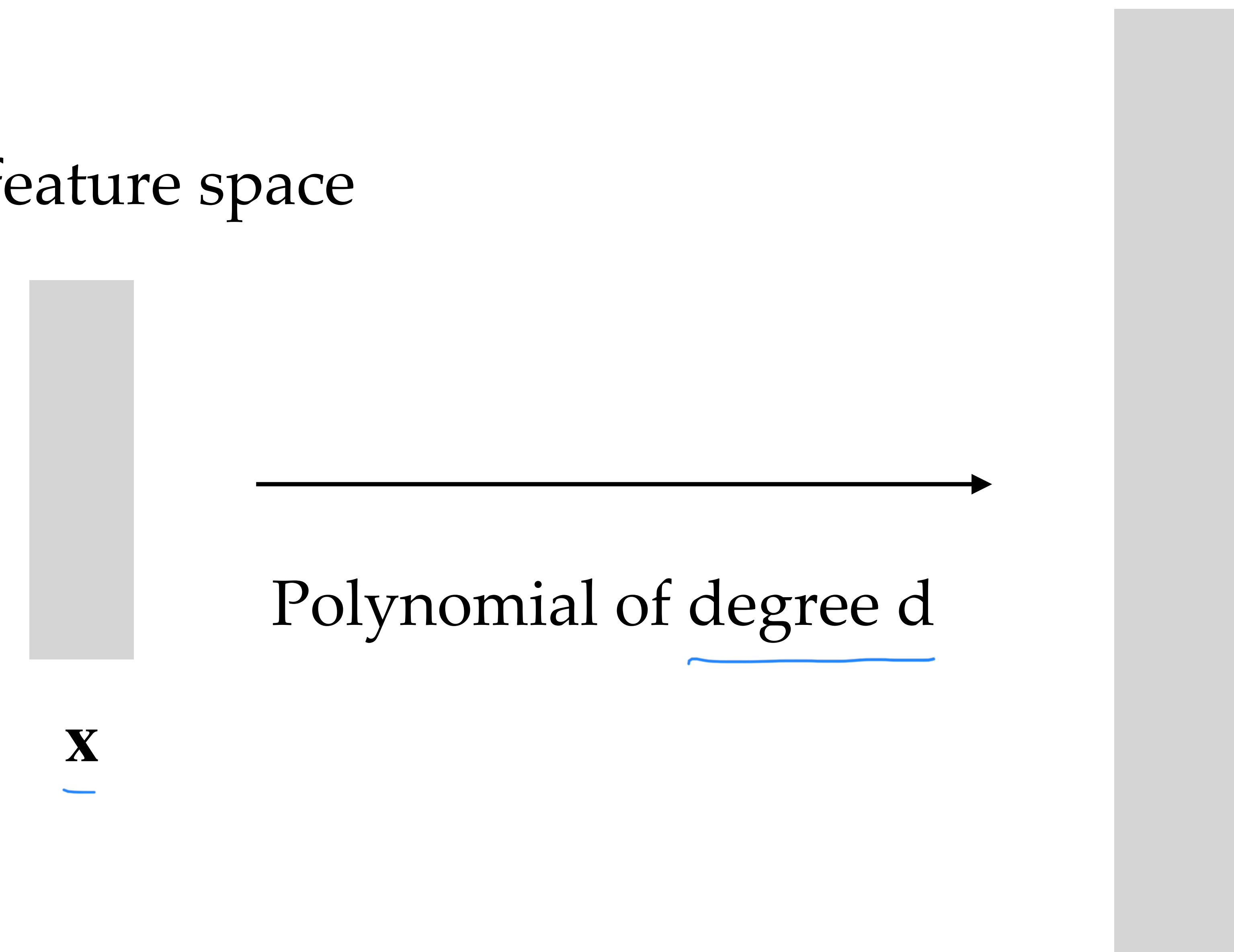


Linearly separable

Mapping to higher dimensional space

Higher dimensional space

Input feature space



Polynomial of degree d

$\mathbf{x}$

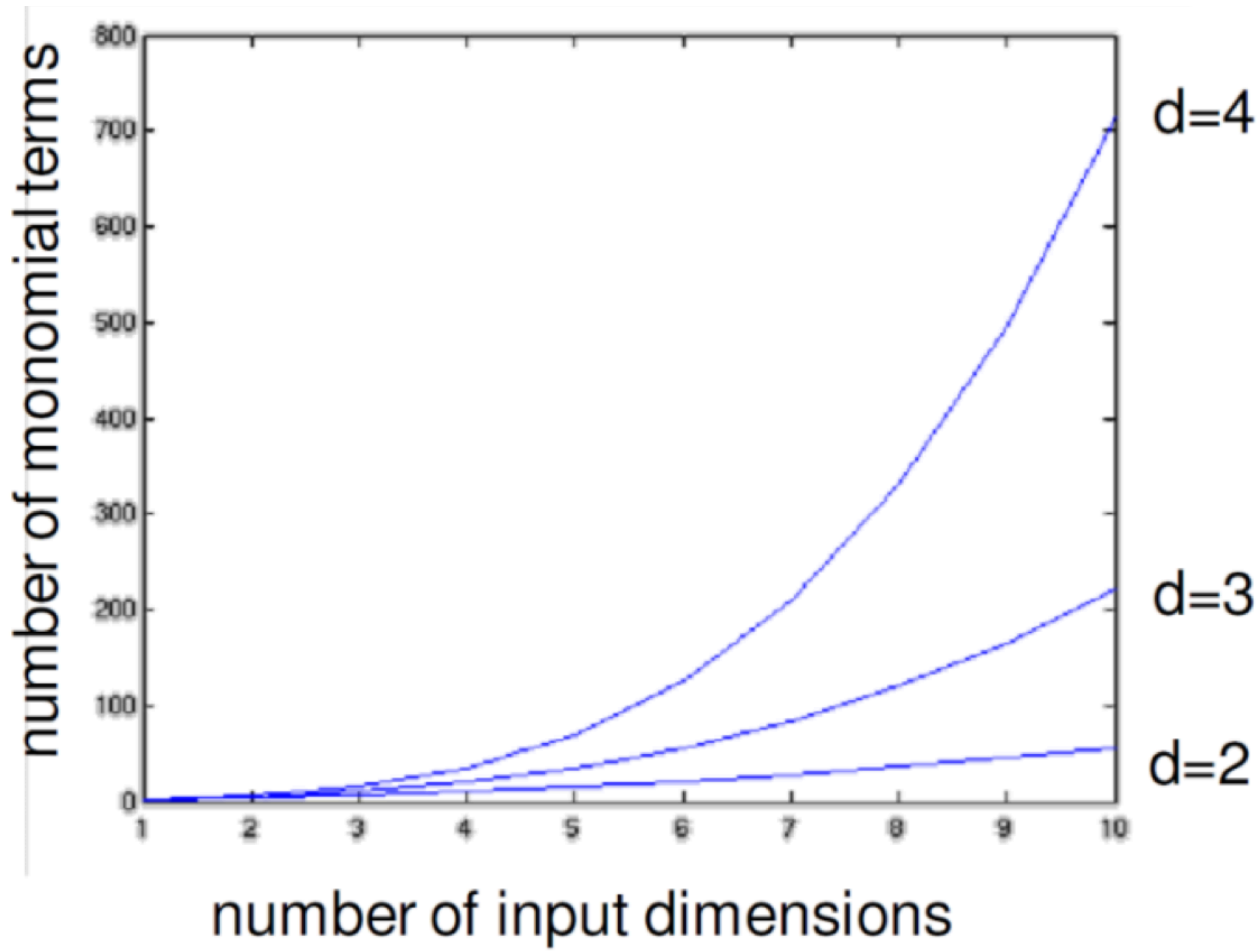
$\mathbf{w} \cdot \phi(\mathbf{x})$

$\phi(\mathbf{x})$

What can go wrong?

Higher order polynomials

- Number of terms $= \binom{d+m-1}{d} = \frac{(d+m-1)!}{d!(m-1)!}$
- where m = dimension of input features; d = degree of polynomial
- Grows fast!
  - m = 100, d = 6
  - ~1.6 billion terms



Feature Mappings

- **Pros**: can help turn non-linear classification problem into linear problem
- **Cons**: "feature explosion" creates issues when training linear classifier in new feature space
  - More computationally expensive to train
  - More training examples needed to avoid overfitting

Kernel Methods

- Goal: keep advantages of linear models, but make them capture non-linear patterns in data!

- **How?**
  - By mapping data to higher dimensions where it exhibits linear patterns

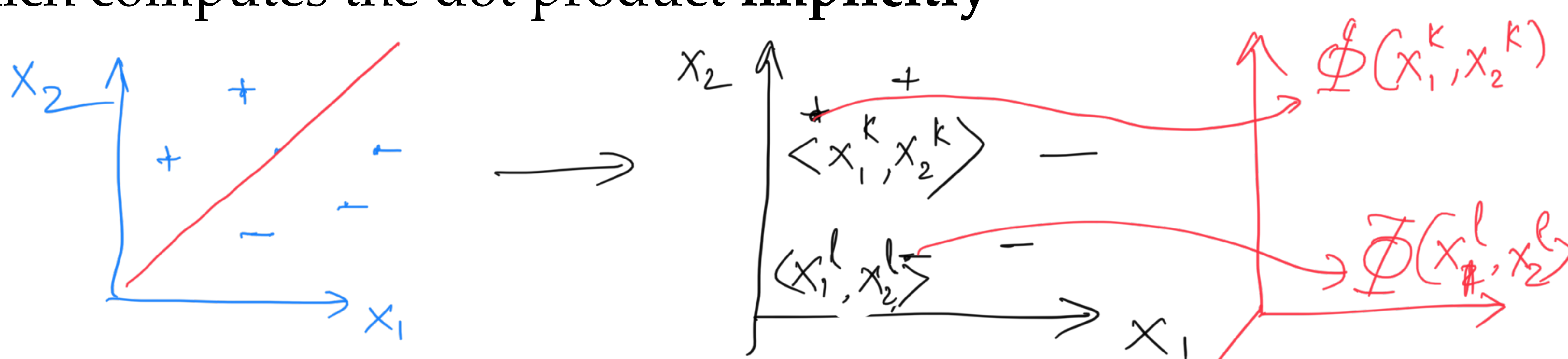
  - **By rewriting linear models so that the mapping never needs to be explicitly computed**

Convert the original linear model into a higher-dimensional model

The Kernel Trick

- Rewrite learning algorithms so they only depend on **dot products between two examples**

- Replace dot product $\phi(\mathbf{x}) \,.\, \phi(\mathbf{z})$
  by **kernel function** $k(\mathbf{x}, \mathbf{z})$
  which computes the dot product **implicitly**



Example of Kernel function

- Consider two examples $\mathbf{x} = \{x_1, x_2\}$ and $\mathbf{z} = \{z_1, z_2\}$
- Let's assume we are given a function k (kernel) that takes as inputs $\mathbf{x}$ and $\mathbf{z}$

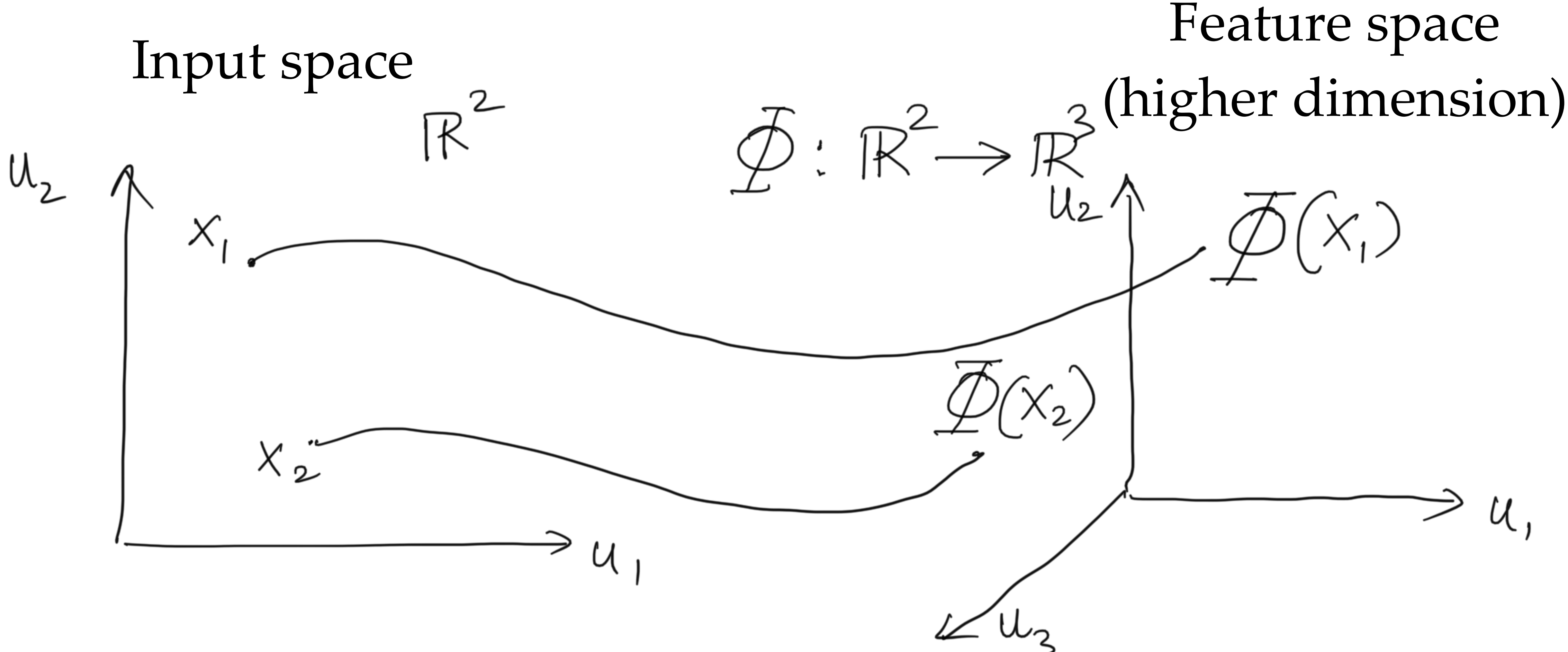
$$\phi(x) = \begin{bmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{bmatrix} \qquad \phi(z) = \begin{bmatrix} z_1^2 \\ \sqrt{2}z_1z_2 \\ z_2^2 \end{bmatrix}$$

$$\begin{aligned} K(x,z) &= (x \cdot z)^2 \\ &= (x_1z_1 + x_2z_2)^2 \\ &= x_1^2z_1^2 + x_2^2z_2^2 + 2x_1x_2z_1z_2 \\ &= (x_1^2, \sqrt{2}x_1x_2, x_2^2)^T(z_1^2, \sqrt{2}z_1z_2, z_2^2) \\ &= \phi(x) \cdot \phi(z) \end{aligned}$$

- **Cool!** taking a dot product and an exponential gives same results as mapping into high dimensional space and then taking dot product
- The above k **implicitly** defines a mapping ϕ to a higher dimensional space

Kernel function

It is a dot-product only business, $K(x_1 \cdot x_2) = \Phi(x_1) \cdot \Phi(x_2)$



- But, it isn't obvious yet how we will incorporate it into actual learning algorithms.

We will do that next…

"Kernelizing" learning algorithms

- **Key idea**: map to higher dimensional space
  - If **x** is in $\mathbb{R}^n$, then $\boldsymbol{\phi}(\mathbf{x})$ is in $\mathbb{R}^m$ for m > n
  - We can now learn feature weights **w** in R^m and
    - predict y by computing $\mathbf{w} \cdot \phi(\mathbf{x})$
  - Linear function in the higher dimensional space will be non-linear in the original space

Question to think about…

How can we “Kernelize” perceptron learning algorithm?