Making Linear Models Nonlinear via Kernel Methods

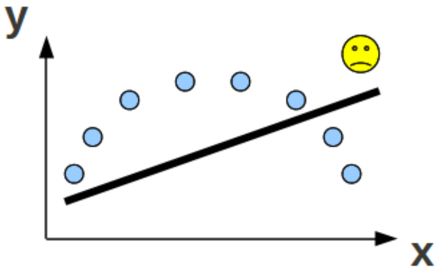
Piyush Rai

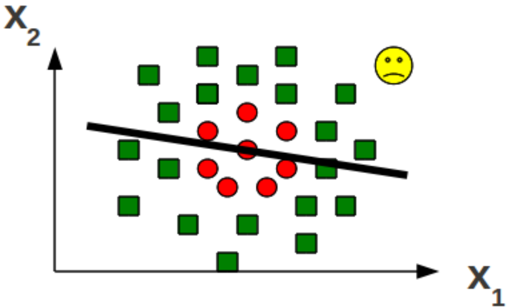
Introduction to Machine Learning (CS771A)

September 6, 2018

Linear Models

- Nice and interpretable but can't learn "difficult" nonlinear patterns





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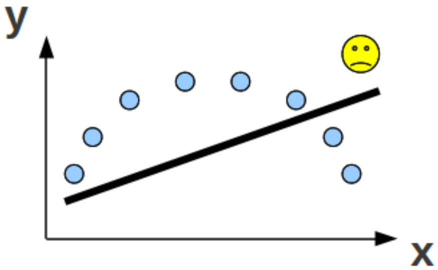

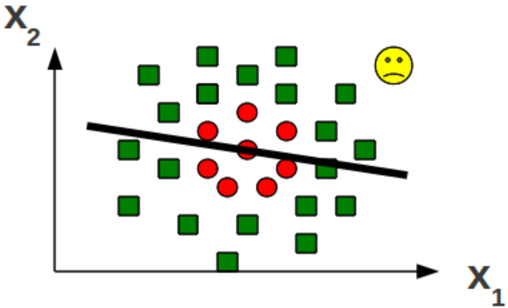

- So, are linear models useless for such problems?

Linear Models for Nonlinear Problems!

- Consider the following one-dimensional inputs from two classes

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- Can't separate using a linear hyperplane

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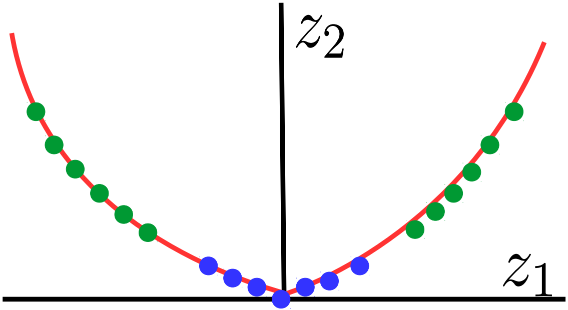

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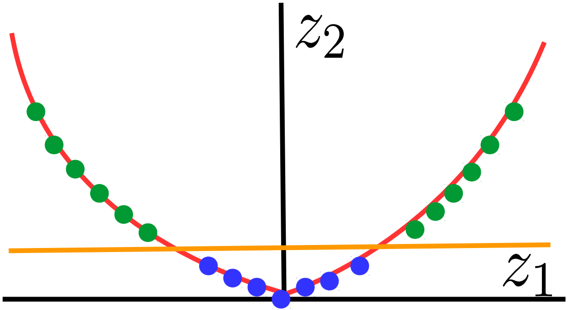
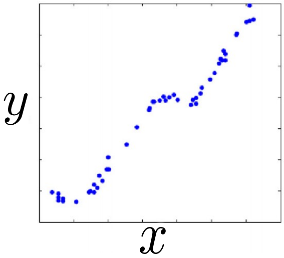


- Data now becomes linearly separable in the two-dimensional space

Linear Models for Nonlinear Problems!

- Consider this regression problem with one-dimensional inputs



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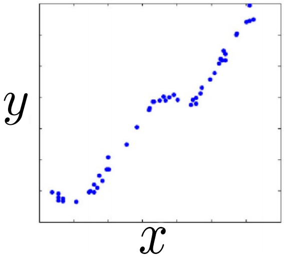

- Linear regression won't work well

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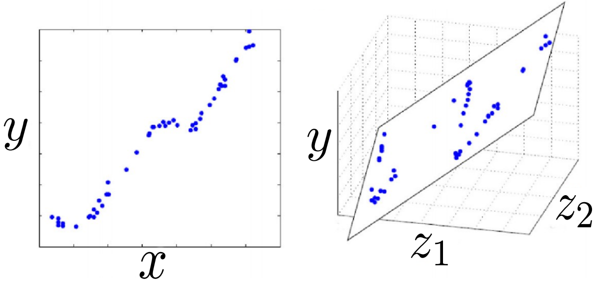

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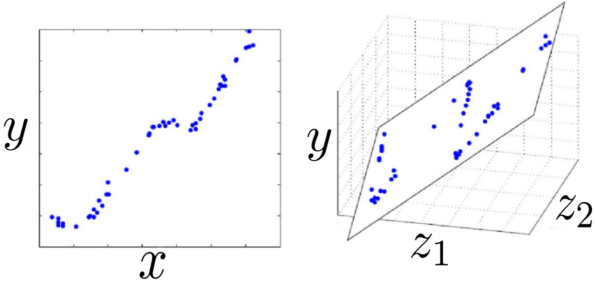

- Now we can fit a linear regression model in two-dimensional input space

Linear Models for Nonlinear Problems!

- Essentially, can use some function ϕ to map/transform inputs to a "nice" space

$$\phi : \mathbb{R}^2 \rightarrow \mathbb{R}^3$$

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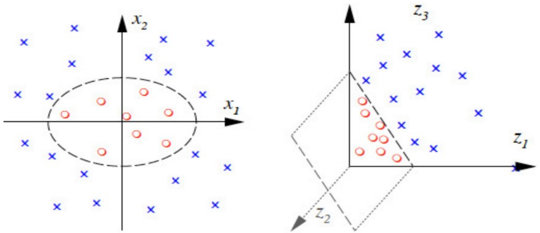

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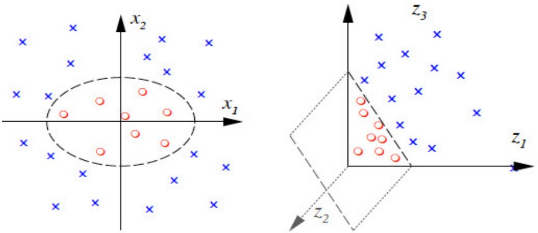

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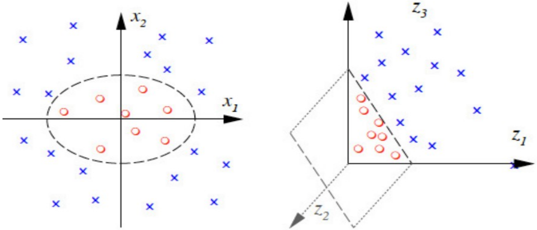
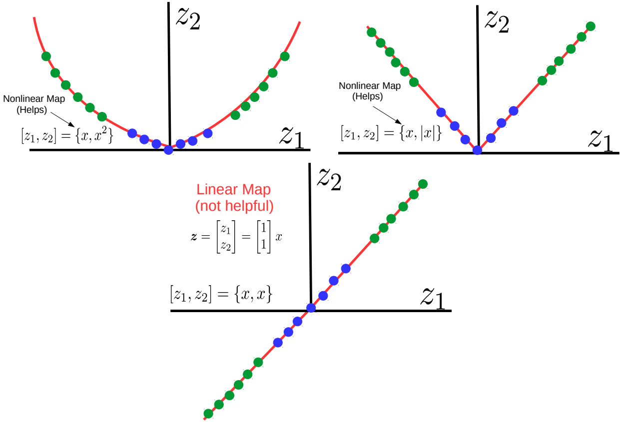


- .. and then happily apply a linear model in the new space!
- Linear in the new space but nonlinear in the original space!

Not Every Mapping is Helpful

- Not every mapping helps in learning nonlinear patterns. Must at least be nonlinear!
- For the nonlinear classification problem we saw earlier, consider some possible mappings



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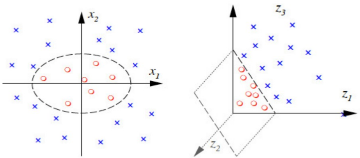

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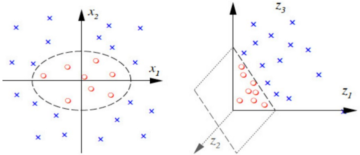

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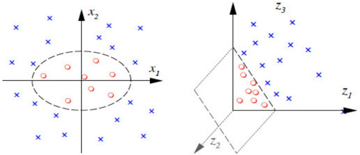

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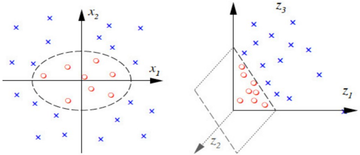

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  - A kernel defines an "implicit" mapping for the data

Kernels as (Implicit) Feature Maps

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- We didn't need to pre-define/compute the mapping ϕ to compute $k(\boldsymbol{x}, \boldsymbol{z})$
- We can simply use the definition of the kernel - $(\boldsymbol{x}^\top \boldsymbol{z})^2$ in this case
- Also, evaluating $k(\boldsymbol{x}, \boldsymbol{z}) = \phi(\boldsymbol{x})^\top \phi(\boldsymbol{z})$ is almost as fast as computing the inner product $\boldsymbol{x}^\top \boldsymbol{z}$

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  - This is the Mercer's Condition
- Let k_1, k_2 be two kernel functions then the following are as well:
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Kernel Functions

- For k to be a kernel function
  - k must define a dot product for some Hilbert Space $\mathcal{F}$
  - Above is true if k is symmetric and positive semi-definite (p.s.d.) function (though there are exceptions; there are also "indefinite" kernels).
  - The function k is p.s.d. if the following holds

$$\int\int f(\boldsymbol{x})k(\boldsymbol{x},\boldsymbol{z})f(\boldsymbol{z})d\boldsymbol{x}d\boldsymbol{z} \geq 0 \quad (\forall f \in L_2)$$

  .. for all functions f that are "square integrable", i.e., $\int f(\boldsymbol{x})^2 d\boldsymbol{x} < \infty$
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  - Kernels can also be constructed by composing these rules

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- Kernel hyperparameters (e.g., d, γ) need to be chosen via cross-validation

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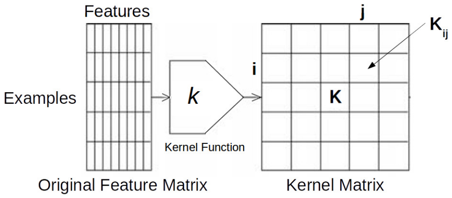

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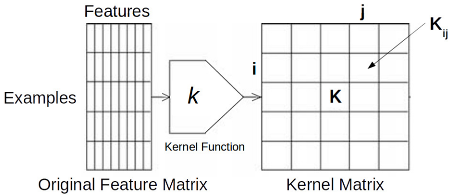

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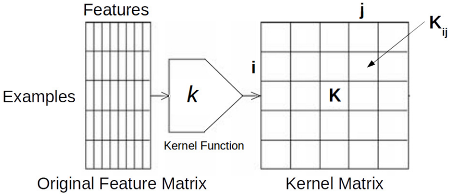

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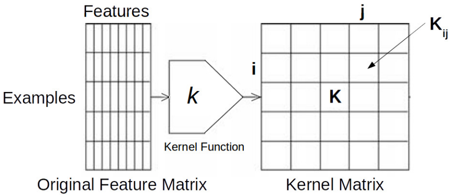

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  - Let's look at two examples: Kernelized SVM and Kernelized Ridge Regression

Example 1:
Kernel (Nonlinear) SVM

Kernelized SVM Training

- Recall the soft-margin SVM dual problem:

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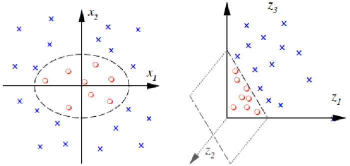

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Example 2:
Kernel (Nonlinear) Ridge Regression

Ridge Regression: Revisited

- Recall the ridge regression problem

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- Note: $\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n \boldsymbol{x}_n$ is known as "dual" form of ridge regression solution. However, so far it is still a linear model. But now it is easily kernelizable.

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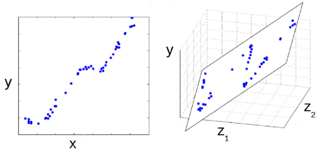

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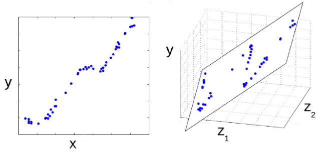

- Note: Just as in kernel SVM, prediction cost scales in N

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    .. various methods can be seen as learning adaptive basis functions, e.g., (Deep) Neural Networks, mixture of experts, Decision Trees, etc.
  - Kernel methods use a "fixed" set of basis functions or "landmarks". The basis functions are the training data points themselves; also see the next slide.

Kernels: Viewed as Defining Fixed Basis Functions

- Consider each row (or column) of the $N \times N$ kernel matrix (it's symmetric)

$$K = \begin{bmatrix} k(x_1,x_1) & k(x_1,x_2) & \cdots & k(x_1,x_n) \\ k(x_2,x_1) & k(x_2,x_2) & \cdots & k(x_2,x_n) \\ \vdots & \vdots & \ddots & \vdots \\ k(x_n,x_1) & k(x_n,x_2) & \cdots & k(x_n,x_n) \end{bmatrix}$$

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- Thus these new features are basically defined in terms of similarities of each input with a fixed set of basis points or "landmarks" $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N$
- In general, the set of basis points or landmarks can be any set of points (not necessarily the data points) and can even be learned (which is what Adaptive Basis Function methods basically do).

Learning with Kernels: Some Aspects (Contd.)

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Learning with Kernels: Some Aspects (Contd.)

- Storage/computational efficiency can be a bottleneck when using kernels
- Training phase usually requires computing and keeping the $N \times N$ kernel matrix $\mathbf{K}$ in memory
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Learning with Kernels: Some Aspects (Contd.)

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- There is a huge literature on speeding up kernel methods
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