Nonlinear Learning with Kernels

Piyush Rai

Machine Learning (CS771A)

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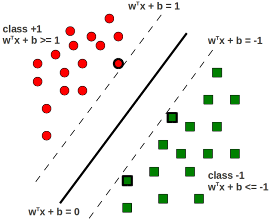
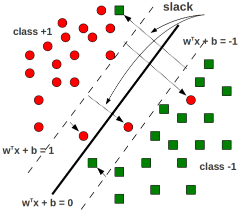
Recap

Support Vector Machines

- Looked at hard and soft-margin SVMs





- The dual objectives for hard-margin and soft-margin SVM

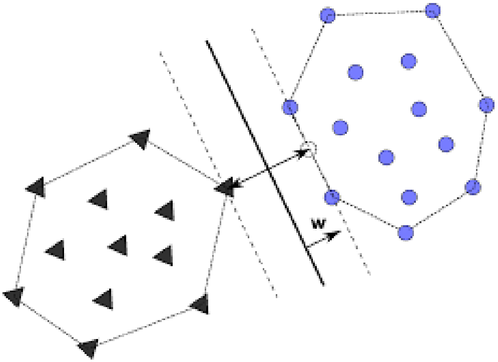
$$\text{Hard-Margin SVM:} \quad \max_{\boldsymbol{\alpha} \geq 0} \; \mathcal{L}_D(\alpha) = \boldsymbol{\alpha}^\top \mathbf{1} - \frac{1}{2}\boldsymbol{\alpha}^\top \mathbf{G}\boldsymbol{\alpha} \qquad \text{s.t.} \quad \sum_{n=1}^{N} \alpha_n y_n = 0$$

$$\text{Soft-Margin SVM:} \quad \max_{\boldsymbol{\alpha} \leq C} \; \mathcal{L}_D(\alpha) = \boldsymbol{\alpha}^\top \mathbf{1} - \frac{1}{2}\boldsymbol{\alpha}^\top \mathbf{G}\boldsymbol{\alpha} \qquad \text{s.t.} \quad \sum_{n=1}^{N} \alpha_n y_n = 0$$

where $\mathbf{G}$ is an $N \times N$ matrix with $G_{mn} = y_m y_n \boldsymbol{x}_m^\top \boldsymbol{x}_n$, and $\mathbf{1}$ is a vector of 1s

SVM Dual Formulation: A Geometric View

- Convex Hull Interpretation†: Solving the SVM dual is equivalent to finding the shortest line connecting the convex hulls of both classes (the SVM's hyperplane will be the perpendicular bisector of this line)



† See: "Duality and Geometry in SVM Classifiers" by Bennett and Bredensteiner

Loss Function Minimization View of SVM

- Recall, we want for each training example: $y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b) \geq 1 - \xi_n$

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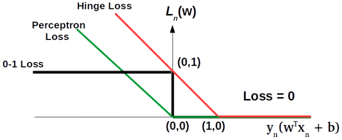
- This is called **"Hinge Loss"**. Can also learn SVMs by minimizing this loss via stochastic sub-gradient descent (can also add a regularizer on $\boldsymbol{w}$, e.g., ℓ_2)



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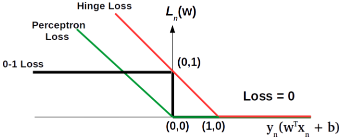

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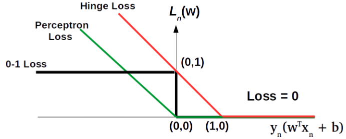

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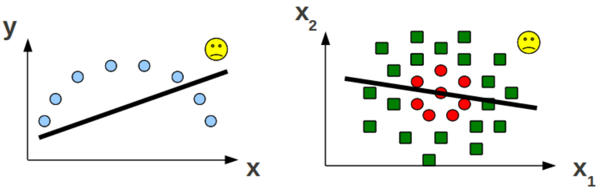
- Perceptron, SVM, Logistic Reg., all minimize convex approximations of the 0-1 loss (optimizing which is NP-hard; moreover it's non-convex/non-smooth)

Learning with Kernels

Linear Models

- Linear models (e.g., linear regression, linear SVM) are nice and interpretable but have limitations. Can't learn "difficult" nonlinear patterns.



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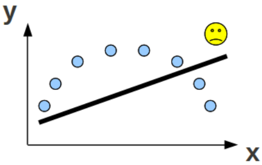
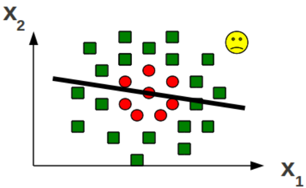




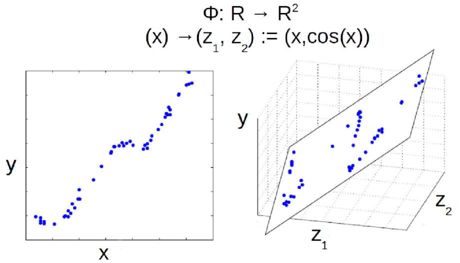
- Reason: Linear models rely on "linear" notions of similarity/distance

$$
\begin{aligned}
Sim(\boldsymbol{x}_n, \boldsymbol{x}_m) &= \boldsymbol{x}_n^\top \boldsymbol{x}_m \\
Dist(\boldsymbol{x}_n, \boldsymbol{x}_m) &= (\boldsymbol{x}_n - \boldsymbol{x}_m)^\top (\boldsymbol{x}_n - \boldsymbol{x}_m)
\end{aligned}
$$

.. which wouldn't work well if the patterns we want to learn are nonlinear

Kernels to the Rescue

- Kernels, using a **feature mapping** ϕ, map data to a new space where the original learning problem becomes "easy" (e.g., a linear model can be applied)



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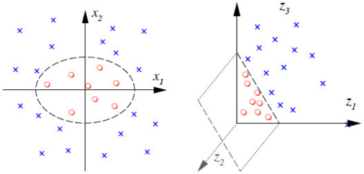

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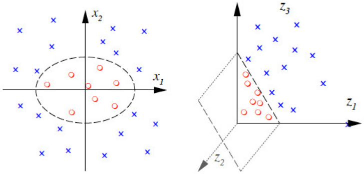

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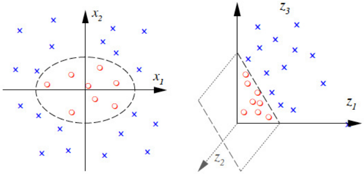

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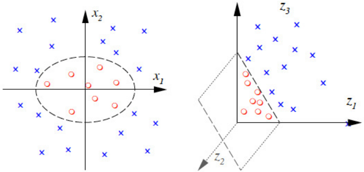

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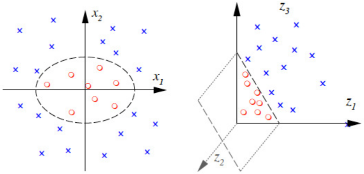

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  - Storing and using these mappings in later computations can be expensive (e.g., we may need to compute innner products in very high dimensional spaces)
- Kernels side-step these issues by defining an "implicit" feature map

Kernels as (Implicit) Feature Maps

- Consider two data points $\boldsymbol{x} = \{x_1, x_2\}$ and $\boldsymbol{z} = \{z_1, z_2\}$ (each in 2 dims)

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- We didn't need to pre-define/compute the mapping ϕ to compute $k(\boldsymbol{x}, \boldsymbol{z})$
- The function k is known as the kernel function
- Also, evaluating k is almost as fast as computing inner products

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  - No. The function k must satisfy **Mercer's Condition**

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  - The function k is p.s.d. if the following holds

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- Given N examples $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$, the (i, j)-th entry of $\mathbf{K}$ is defined as:

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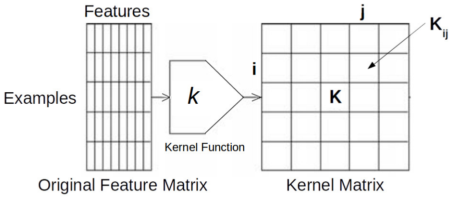

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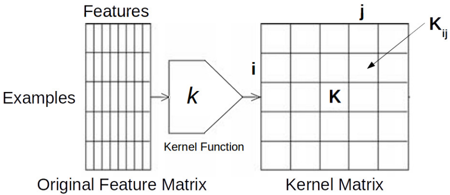

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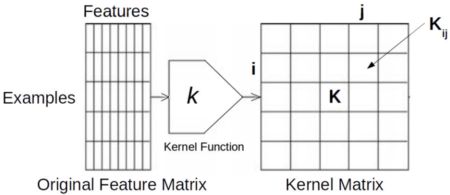

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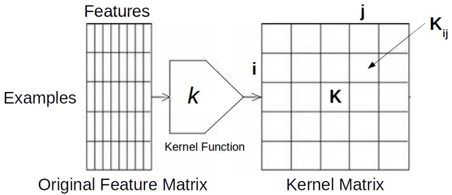

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  - Let's look at two examples: Kernelized SVM and Kernelized Ridge Regression

Example 1:
Kernel (Nonlinear) SVM

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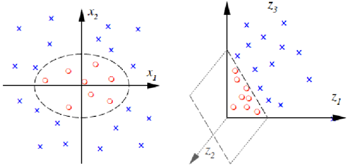

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Example 2:
Kernel (Nonlinear) Ridge Regression

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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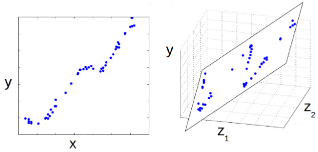

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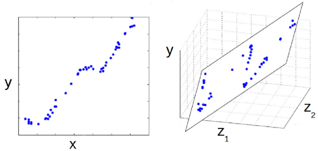

- Note: Just as in kernel SVM, prediction cost scales in N

The Representer Theorem

Theorem

Let $\mathcal{X}$ be some vector space and let $\phi()$ be a map from $\mathcal{X}$ to $\mathcal{F}$, a Reproducing Kernel Hilbert Space[†] *(RKHS) associated with kernel $k(.,.) : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$. Let f be some function defined in this RKHS, let $\ell(.,.)$ be a loss function, and let $R(.)$ be some non-decreasing function. Then the minimizer $\hat{f}$ of the loss function*

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Thus the solution (the minimizer of our regularized loss function) lies in the span of the inputs (mapped to $\mathcal{F}$). We already saw this in the case of SVM and kernel ridge regression. This property is however more generally applicable.

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  - 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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- Can think of this as a new feature vector (with N features) for inputs $\boldsymbol{x}_n$. Each feature represents the similarity of $\boldsymbol{x}_n$ with one of the inputs.

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

- For each input $\boldsymbol{x}_n$, we can define the following N dimensional vector

$$K(n,:) = [k(\boldsymbol{x}_n, \boldsymbol{x}_1) \; k(\boldsymbol{x}_n, \boldsymbol{x}_2) \; \ldots \; k(\boldsymbol{x}_n, \boldsymbol{x}_N)]$$

- Can think of this as a new feature vector (with N features) for inputs $\boldsymbol{x}_n$. Each feature represents the similarity of $\boldsymbol{x}_n$ with one of the inputs.

- Thus these new features are basically defined in terms of similarities of each input with a fixed set of basis points or "landmarks" $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N$

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- 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).

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- There is a huge literature on speeding up kernel methods
  - Approximating the kernel matrix using a set of kernel-derived new features
  - Identifying a small set of landmark points in the training data
  - .. and a lot more

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  - Trees (tree kernels): Comparing parse trees of phrases/sentences