Kernels

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Motivation

- Linear classifiers are great, but what if there exists no linear decision boundary?
- As it turns out, there is an elegant way to incorporate non-linearities into most linear classifiers.

Handcrafted Feature Expansion

We can make linear classifiers non-linear by applying basis function (feature transformations) on the input feature vectors. Formally, for a data vector $\mathbf{x} \in \mathbb{R}^d$, we apply the transformation $\mathbf{x} \rightarrow \phi(\mathbf{x})$ where $\phi(\mathbf{x}) \in \mathbb{R}^D$. Usually $D \gg d$ because we add dimensions that capture non-linear interactions among the original features.

Handcrafted Feature Expansion

Advantage

It is simple, and your problem stays convex and well behaved. (i.e. you can still use your original gradient descent code, just with the higher dimensional representation)

Disadvantage

$\phi(\mathbf{x})$ might be very high dimensional.

An Example of Handcrafted Feature Expansion

Consider the following example: $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{pmatrix}$, and define $\phi(\mathbf{x}) = \begin{pmatrix} 1 \\ x_1 \\ \vdots \\ x_d \\ x_1 x_2 \\ \vdots \\ x_{d-1} x_d \\ \vdots \\ x_1 x_2 \cdots x_d \end{pmatrix}$

Quiz

What is the dimensionality of $\phi(\mathbf{x})$?

This new representation, $\phi(\mathbf{x})$, is very expressive and allows for complicated non-linear decision boundaries - but the dimensionality is extremely high. This makes our algorithm unbearable (and quickly prohibitively) slow.

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The Kernel Trick

The kernel trick is a way to get around this dilemma by learning a function in the much higher dimensional space, without ever computing a single vector $\phi(\mathbf{x})$ or ever computing the full vector $\mathbf{w}$. It is a little magical.

Observation

It is based on the following observation:

Observation

If we use gradient descent with any one of our standard loss functions, the gradient is a linear combination of the input samples.

Revisiting Gradient Descent with Squared Loss

For example, let us take a look at the squared loss:

$$\ell(\mathbf{w}) = \sum_{i=1}^{n} (\mathbf{w}^\top \mathbf{x}_i - y_i)^2$$

The gradient descent rule, with step-size/learning-rate $s > 0$ (we denoted this as $\alpha > 0$ in our previous lectures), updates **w** over time,

$$w_{t+1} \leftarrow w_t - s(\frac{\partial \ell}{\partial \mathbf{w}}) \quad \text{where:} \quad \frac{\partial \ell}{\partial \mathbf{w}} = \sum_{i=1}^{n} \underbrace{2(\mathbf{w}^\top \mathbf{x}_i - y_i)}_{\gamma_i \ :\ \text{function of } \mathbf{x}_i, y_i} \mathbf{x}_i = \sum_{i=1}^{n} \gamma_i \mathbf{x}_i$$

We will now show that we can express **w** as a **linear combination of all input vectors**,

$$\mathbf{w} = \sum_{i=1}^{n} \alpha_i \mathbf{x}_i .$$

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Gradient Descent with Squared Loss

Since the loss is convex, the final solution is independent of the initialization, and we can initialize $\mathbf{w}^0$ to be whatever we want. For convenience, let us pick $\mathbf{w}_0 = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}$. For this initial choice of $\mathbf{w}_0$, the linear combination in $\mathbf{w} = \sum_{i=1}^{n} \alpha_i \mathbf{x}_i$ is trivially $\alpha_1 = \cdots = \alpha_n = 0$.

We now show that throughout the entire gradient descent optimization such coefficients $\alpha_1, \ldots, \alpha_n$ must always exist, as we can re-write the gradient updates entirely in terms of updating the α_i coefficients:

$$\begin{aligned}
\mathbf{w}_1 =& \mathbf{w}_0 - s\sum_{i=1}^{n} 2(\mathbf{w}_0^\top \mathbf{x}_i - y_i)\mathbf{x}_i = \sum_{i=1}^{n} \alpha_i^0 \mathbf{x}_i - s\sum_{i=1}^{n} \gamma_i^0 \mathbf{x}_i = \sum_{i=1}^{n} \alpha_i^1 \mathbf{x}_i && (\text{with } \alpha_i^1 = \alpha_i^0 - s\gamma_i^0)\\
\mathbf{w}_2 =& \mathbf{w}_1 - s\sum_{i=1}^{n} 2(\mathbf{w}_1^\top \mathbf{x}_i - y_i)\mathbf{x}_i = \sum_{i=1}^{n} \alpha_i^1 \mathbf{x}_i - s\sum_{i=1}^{n} \gamma_i^1 \mathbf{x}_i = \sum_{i=1}^{n} \alpha_i^2 \mathbf{x}_i && (\text{with } \alpha_i^2 = \alpha_i^1 \mathbf{x}_i - s\gamma_i^1)\\
\mathbf{w}_3 =& \mathbf{w}_2 - s\sum_{i=1}^{n} 2(\mathbf{w}_2^\top \mathbf{x}_i - y_i)\mathbf{x}_i = \sum_{i=1}^{n} \alpha_i^2 \mathbf{x}_i - s\sum_{i=1}^{n} \gamma_i^2 \mathbf{x}_i = \sum_{i=1}^{n} \alpha_i^3 \mathbf{x}_i && (\text{with } \alpha_i^3 = \alpha_i^2 - s\gamma_i^2)\\
\cdots & \qquad \cdots && \cdots\\
\mathbf{w}_t =& \mathbf{w}_{t-1} - s\sum_{i=1}^{n} 2(\mathbf{w}_{t-1}^\top \mathbf{x}_i - y_i)\mathbf{x}_i = \sum_{i=1}^{n} \alpha_i^{t-1} \mathbf{x}_i - s\sum_{i=1}^{n} \gamma_i^{t-1} \mathbf{x}_i = \sum_{i=1}^{n} \alpha_i^t \mathbf{x}_i && (\text{with } \alpha_i^t = \alpha_i^{t-1} - s\gamma_i^{t-1})
\end{aligned}$$

Formally, the argument is by induction. $\mathbf{w}$ is trivially a linear combination of our training vectors for $\mathbf{w}_0$ (base case). If we apply the inductive hypothesis for $\mathbf{w}_t$ it follows for $\mathbf{w}_{t+1}$. The update-rule for α_i^t is thus

$$\alpha_i^t = \alpha_i^{t-1} - s\gamma_i^{t-1}, \text{ and we have } \alpha_i^t = -s\sum_{r=0}^{t-1}\gamma_i^r.$$

Substitution of w

In other words, we can perform the entire gradient descent update rule without ever expressing **w** explicitly. We just keep track of the n coefficients $\alpha_1, \ldots, \alpha_n$. Now that **w** can be written as a linear combination of the training set, we can also express the inner-product of **w** with any input $\mathbf{x}_i$ purely in terms of inner-products between training inputs:

$$\mathbf{w}^\top \mathbf{x}_j = \sum_{i=1}^{n} \alpha_i \mathbf{x}_i^\top \mathbf{x}_j.$$

Substitution of $\mathbf{w}$

Consequently, we can also re-write the squared-loss from $\ell(\mathbf{w}) = \sum_{i=1}^{n}(\mathbf{w}^\top \mathbf{x}_i - y_i)^2$ entirely in terms of inner-product between training inputs:

$$\ell(\alpha) = \sum_{i=1}^{n}\left(\sum_{j=1}^{n}\alpha_j \mathbf{x}_j^\top \mathbf{x}_i - y_i\right)^2$$

Substitution of $\mathbf{w}$

During test-time we also only need these coefficients to make a prediction on a test-input x_t, and can write the entire classifier in terms of inner-products between the test point and training points:

$$h(\mathbf{x}_t) = \mathbf{w}^\top \mathbf{x}_t = \sum_{j=1}^{n} \alpha_j \mathbf{x}_j^\top \mathbf{x}_t.$$

Substitution of $\mathbf{w}$

Do you notice a theme?

The only information we ever need in order to learn a hyper-plane classifier with the squared-loss is **inner-products between all pairs of data vectors.**

Inner-Product Computation

Let's go back to the previous example, $\phi(\mathbf{x}) = \begin{pmatrix} 1 \\ x_1 \\ \vdots \\ x_d \\ x_1 x_2 \\ \vdots \\ x_{d-1} x_d \\ \vdots \\ x_1 x_2 \cdots x_d \end{pmatrix}$.

The inner product $\phi(\mathbf{x})^\top \phi(\mathbf{z})$ can be formulated as:

$$\phi(\mathbf{x})^\top \phi(\mathbf{z}) = 1 \cdot 1 + x_1 z_1 + x_2 z_2 + \cdots + x_1 x_2 z_1 z_2 + \cdots + x_1 \cdots x_d z_1 \cdots z_d = \prod_{k=1}^{d} (1 + x_k z_k).$$

The sum of 2^d terms becomes the product of d terms. We can compute the inner-product from the above formula in time $O(d)$ instead of $O(2^d)$!

We define the function

$$\underbrace{\mathsf{k}(\mathbf{x}_i, \mathbf{x}_j)}_{\text{this is called the } \textbf{kernel function}} = \phi(\mathbf{x}_i)^\top \phi(\mathbf{x}_j).$$

With a finite training set of n samples, inner products are often pre-computed and stored in a Kernel Matrix:

$$\mathsf{K}_{ij} = \phi(\mathbf{x}_i)^\top \phi(\mathbf{x}_j).$$

If we store the matrix K, we only need to do simple inner-product look-ups and low-dimensional computations throughout the gradient descent algorithm.
The final classifier becomes:

$$h(\mathbf{x}_t) = \sum_{j=1}^{n} \alpha_j \mathsf{k}(\mathbf{x}_j, \mathbf{x}_t).$$

From $O(2^d)$ to $O(n^2)$

During training in the new high dimensional space of $\phi(\mathbf{x})$ we want to compute γ_i through kernels, without ever computing any $\phi(\mathbf{x}_i)$ or even $\mathbf{w}$. We previously established that $\mathbf{w} = \sum_{j=1}^{n} \alpha_j \phi(\mathbf{x}_j)$, and $\gamma_i = 2(\mathbf{w}^\top \phi(\mathbf{x}_i) - y_i)$. It follows that $\gamma_i = 2(\sum_{j=1}^{n} \alpha_j K_{ij}) - y_i)$. The gradient update in iteration $t+1$ becomes $\alpha_i^{t+1} \leftarrow \alpha_i^t - 2s(\sum_{j=1}^{n} \alpha_j^t K_{ij}) - y_i)$. As we have n such updates to do, the amount of work per gradient update in the transformed space is $O(n^2)$ — far better than $O(2^d)$.

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Popular Kernel Functions

Below are some popular kernel functions:

- Linear: $\mathrm{K}(\mathbf{x}, \mathbf{z}) = \mathbf{x}^\top \mathbf{z}$.
  (The linear kernel is equivalent to just using a good old linear classifier - but it can be faster to use a kernel matrix if the dimensionality d of the data is high.)
- Polynomial: $\mathrm{K}(\mathbf{x}, \mathbf{z}) = (1 + \mathbf{x}^\top \mathbf{z})^d$.
- Radial Basis Function (RBF) (aka Gaussian Kernel): $\mathrm{K}(\mathbf{x}, \mathbf{z}) = e^{\frac{-\|\mathbf{x}-\mathbf{z}\|^2}{\sigma^2}}$.
  The RBF kernel is the most popular Kernel! It is a Universal approximator!! Its corresponding feature vector is infinite dimensional and cannot be computed. However, very effective low dimensional approximations exist (see this paper).
- Exponential Kernel: $\mathrm{K}(\mathbf{x}, \mathbf{z}) = e^{\frac{-\|\mathbf{x}-\mathbf{z}\|}{2\sigma^2}}$
- Laplacian Kernel: $\mathrm{K}(\mathbf{x}, \mathbf{z}) = e^{\frac{-|\mathbf{x}-\mathbf{z}|}{\sigma}}$
- Sigmoid Kernel: $\mathrm{K}(\mathbf{x}, \mathbf{z}) = \tanh(\mathbf{a}\mathbf{x}^\top + c)$

Q: Can any function $\mathrm{K}(\cdot,\cdot) \to \mathcal{R}$ be used as a kernel?
A: No, the matrix $\mathrm{K}(\mathbf{x}_i, \mathbf{x}_j)$ has to correspond to real inner-products after some transformation $\mathbf{x} \to \phi(\mathbf{x})$. This is the case if and only if K is positive semi-definite.

Definition of Positive Semi-definite

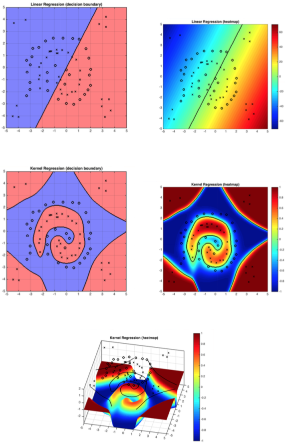
A matrix $A \in \mathbb{R}^{n \times n}$ is positive semi-definite iff $\forall \mathbf{q} \in \mathbb{R}^n, \mathbf{q}^\top A\mathbf{q} \geq 0$.

Kernel Functions

Remember $K_{ij} = \phi(\mathbf{x}_i)^\top \phi(\mathbf{x}_j)$. So $K = \Phi^\top \Phi$, where $\Phi = [\phi(\mathbf{x}_1), \ldots, \phi(\mathbf{x}_n)]$. It follows that K is p.s.d., because $\mathbf{q}^\top K \mathbf{q} = (\Phi^\top \mathbf{q})^2 \geq 0$. Inversely, if any matrix $\mathbf{A}$ is p.s.d., it can be decomposed as $A = \Phi^\top \Phi$ for some realization of Φ.

You can even define kernels over sets, strings, graphs and molecules.

Example: RBF Kernel



The demo shows how kernel function solves the problem linear classifiers can not solve. RBF works well with the decision boundary in this case.

The End