Support Vector Machine (contd) and Kernel Methods

CS771: Introduction to Machine Learning

Announcements

- Mid-sem grading almost finished. Hope to release marks by tomorrow if not today
- Quiz 1 and Quiz 2 marks already released
 - We will clear remaining regrading requests in 1-2 days
- Will have 2 make-up lectures (dates announced later)



Plan for today

- Solving the SVM optimization problem efficiency using co-ordinate ascent
- SVM for multi-class classification
- SVM for regression
- Kernel methods for learning nonlinear models



A Co-ordinate Ascent Algorithm for SVM

■ Recall the dual objective of soft-margin SVM (assuming no bias b)

$$\underset{\mathbf{0} \leq \alpha \leq C}{\operatorname{argmax}} \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m,n=1}^{N} \alpha_m \alpha_n y_m y_n \mathbf{x}_m^{\mathsf{T}} \mathbf{x}_n$$

Note that $\mathbf{w} = \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n$.

Focusing on just one of the components of $\mathbf{\alpha}$ (say α_n), the objective becomes

- The above is a simple quadratic maximization of a concave function: Global maxima
- lacktriangle If constraint violated, project $lpha_n$ in $[0,\mathcal{C}]$: If $lpha_n<0$, set it to 0, if $lpha_n>\mathcal{C}$, set it to \mathcal{C}
- lacktriangle Can cycle through each coordinate $lpha_n$ in a random or cyclic fashion

Multi-class SVM

ullet Multiclass SVMs (assuming K > 2 classes) use K wt vectors $oldsymbol{W} = [oldsymbol{w}_1, oldsymbol{w}_2, ..., oldsymbol{w}_K]$

Prediction at test time: $\hat{y}_* = \operatorname{argmax}_{k \in \{1,2,...,K\}} \boldsymbol{w}_k^{\mathsf{T}} \boldsymbol{x}_*$

■ Like binary SVM, can formulate a maximum-margin problem (without or with slacks)

$$\hat{\mathbf{W}} = \arg\min_{\mathbf{W}} \sum_{k=1}^{K} \frac{||\mathbf{w}_k||^2}{2} \qquad \hat{\mathbf{W}} = \arg\min_{\mathbf{W}} \sum_{k=1}^{K} \frac{||\mathbf{w}_k||^2}{2} + C \sum_{n=1}^{N} \xi_n$$
s.t.
$$\mathbf{w}_{y_n}^{\top} \mathbf{x}_n \ge \mathbf{w}_k^{\top} \mathbf{x}_n + 1 \quad \forall k \ne y_n \qquad \text{s.t.} \quad \mathbf{w}_{y_n}^{\top} \mathbf{x}_n \ge \mathbf{w}_k^{\top} \mathbf{x}_n + 1 - \xi_n \quad \forall k \ne y_n$$

Score on correct class

Score on an incorrect class $k \neq y_n$

■ The version with slack corresponds to minimizing a multi-class hinge loss

$$\mathcal{L}(\mathbf{W}) = \sum_{n=1}^{N} \max \left\{ 0, 1 + \max_{k \neq y_n} \mathbf{w}_k^{\mathsf{T}} \mathbf{x}_n - \mathbf{w}_{y_n}^{\mathsf{T}} \mathbf{x}_n \right\} + \frac{\lambda}{2} \sum_{k=1}^{K} ||\mathbf{w}_k||^2$$

Loss=0 if score on correct class is at least 1 more than score on next-best_scoring class

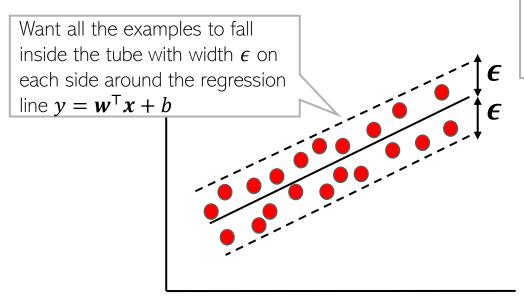
Crammer-Singer Multi-class SVM



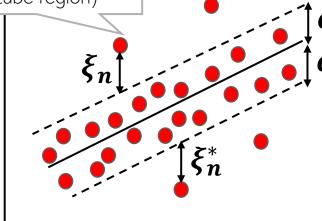
Support Vector Regression (SVR)

No loss if the prediction is within ϵ of the true output

■ SVR is a variant of SVM for regression problems. Uses ϵ -insensitive loss



Also allow some slacks (some points may fall outside the tube region)



SVR is more robust than linear regression in the presence of outliers (regression line/curve is not affected much by such points)

> SVR can also be made nonlinear using kernels

Minimize
$$\frac{\|\boldsymbol{w}\|^2}{2}$$
Subject to $y_n - \boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_n - b \leq \epsilon$
 $\boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_n + b - y_n \leq \epsilon$

Minimize
$$\frac{\|\boldsymbol{w}\|^2}{2} + C \sum_{n=1}^{N} (\xi_n + \xi_n^*)$$
 Subject to
$$y_n - \boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_n - b \leq \epsilon + \xi_n$$

$$\boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_n + b - y_n \leq \epsilon + \xi_n^*$$

$$\xi_n, \xi_n^* \geq 0$$
 CS771: Intro to

Nonlinear Models using Kernels



Linear Models for Nonlinear Problems?

Consider the following one-dimensional inputs from two classes

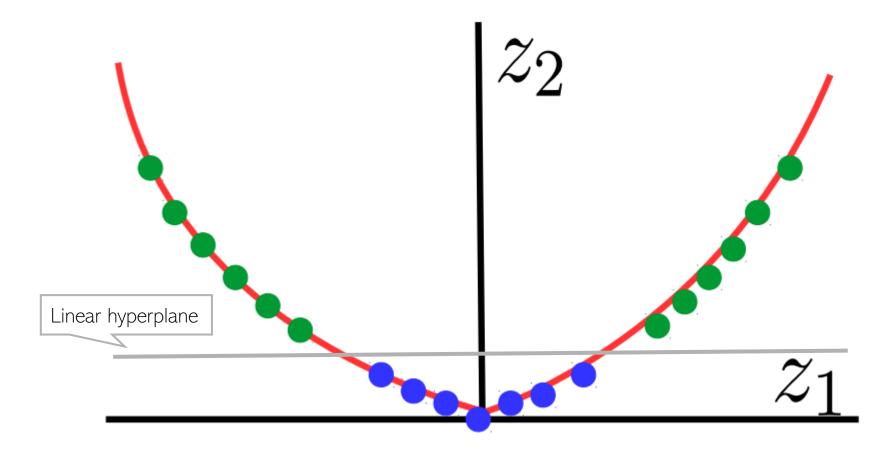


Can't separate using a linear hyperplane



Linear Models for Nonlinear Problems?

• Consider mapping each x to two-dimensions as $x \to z = [z_1, z_2] = [x, x^2]$



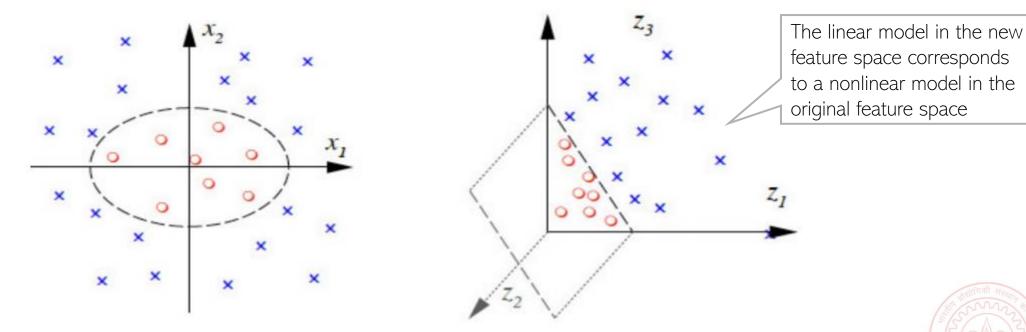
Classes are now linearly separable in the two-dimensional space



Linear Models for Nonlinear Problems

lacktrians Can assume a feature mapping ϕ that maps/transforms the inputs to a "nice" space

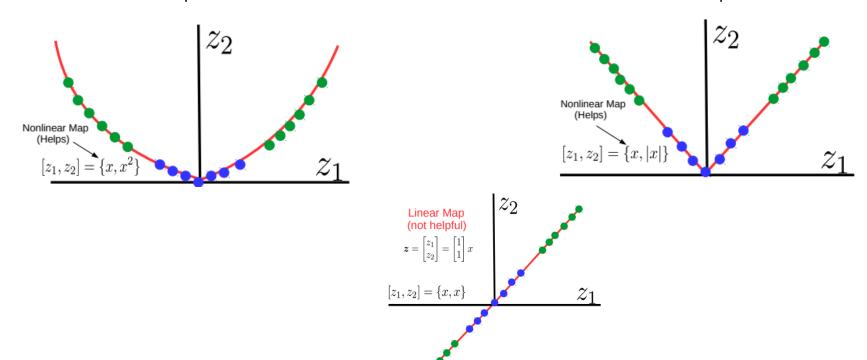
$$\phi: \mathbb{R}^2 \to \mathbb{R}^3$$
 $(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt{2}) \times (x_1, x_2, x_2^2)$



.. and then happily apply a linear model in the new space!

Not Every Mapping is Helpful

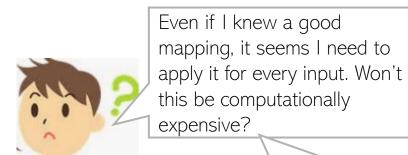
- Not every higher-dim mapping helps in learning nonlinear patterns
- Must be a <u>nonlinear</u> mapping
- For the nonlin classfn problem we saw earlier, consider some possible mappings





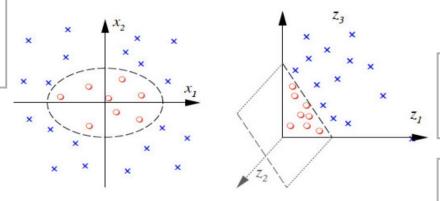
How to get these "good" (nonlinear) mappings?

- Learn good mappings from data itself (e.g., deep learning or distance metric learning)
- Use pre-defined "good" mappings (e.g., defined by kernel functions today's topic)



Also, the number of features will increase? Will it not slow down the learning algorithm?

 $\phi: \mathbb{R}^2 \to \mathbb{R}^3$ $(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt(2)x_1x_2, x_2^2)$



Thankfully, using kernels, you don't need to compute these mappings explicitly



The kernel will define an "implicit" feature mapping

Important: The idea can be applied to any ML algo in which training and test stage only require computing distances/similarities b/w inputs

In a high-dim space implicitly defined by an underlying mapping ϕ associated this this kernel function k(.,.)

ullet Kernel: A function k(.,.) that gives dot product similarity b/w two inputs, say $oldsymbol{x}_n$ and $oldsymbol{x}_m$

Important: As we will see, computing k(.,.) does not require computing the mapping ϕ

$$k(\boldsymbol{x}_n, \boldsymbol{x}_m) = \phi(\boldsymbol{x}_n)^{\mathsf{T}} \phi(\boldsymbol{x}_m)$$

Some Pre-defined Kernel Functions

■ Linear kernel: $k(x, z) = x^{T}z$

Several other kernels proposed for non-vector data, such as trees, strings, etc

Remember that kernels are a notion of similarity between pairs of inputs



■ Quadratic Kernel: $k(x,z) = (x^Tz)^2$ or $k(x,z) = (1 + x^Tz)^2$

Kernels can have a pre-defined form or can be learned from data (a bit advanced for this course)

- Polynomial Kernel (of degree d): $k(x,z) = (x^Tz)^d$ or $k(x,z) = (1+x^Tz)^d$
- Radial Basis Function (RBF) or "Gaussian" Kernel: $k(x,z) = \exp[-\gamma ||x z||^2]$
 - Gaussian kernel gives a similarity score between 0 and 1
 - > 0 is a hyperparameter (called the kernel bandwidth parameter)

Controls how the distance between two inputs should be converted into a similarity

- The RBF kernel corresponds to an infinite dim. feature space \mathcal{F} (i.e., you can't actually write down or store the map $\phi(x)$ explicitly but we don't need to do that anyway \odot)
- Also called "stationary kernel": only depends on the distance between x and z (translating both by the same amount won't change the value of k(x,z))
- Which kernel to use or its hyperparams (e.g.,d, γ) values can be set via cross-val.

Kernels as (Implicit) Feature Maps

- lacktriangle Consider two inputs (in the same two-dim feature space): $oldsymbol{x}=[x_1,x_2],oldsymbol{z}=[z_1,z_2]$
- lacktriangle Suppose we have a function k(.,.) which takes two inputs $m{x}$ and $m{z}$ and computes

Called the "kernel function"
$$k(x,z) = (x^{\mathsf{T}}z)^2$$
 Can think of this as a notion of similarity b/w x and z $= (x_1z_1 + x_2z_2)^2$

This is not a dot/inner product similarity but similarity using a more general function of \boldsymbol{x} and \boldsymbol{z} (square of dot product)

Thus kernel function $k(x, z) = (x^T z)^2$ implicitly defined a feature mapping ϕ such that for $x = [x_1, x_2]$, $\phi(x) = \left(x_1^2, \sqrt{2}x_1x_2, x_2^2\right)$

=
$$(x_1^2, \sqrt{2}x_1x_2, x_2^2)^{\mathsf{T}}(z_1^2, \sqrt{2}z_1z_2, z_2^2)$$

$$= \phi(\mathbf{x})^{\mathsf{T}}\phi(\mathbf{z})$$

Dot product similarity in the new feature space defined by the mapping ϕ

Remember that a kernel does two things: Maps the data implicitly into a new feature space (feature transformation) and computes pairwise similarity between any two inputs under the new feature representation



■ Also didn't have to compute $\phi(x)^{\mathsf{T}}\phi(z)$. Defin $k(x,z)=(x^{\mathsf{T}}z)^2$ gives that

 $= x_1^2 z_1^2 + x_2^2 z_2^2 + 2x_1 x_2 z_1 z_2$

RBF Kernel = Infinite Dimensional Mapping

- We saw that the RBF/Gaussian kernel is defined as $k(x,z) = \exp[-\gamma ||x z||^2]$
- Using this kernel corresponds to mapping data to infinite dimensional space

$$k(x,z) = \exp[-(x-z)^2] \qquad \text{(assuming } \gamma = 1 \text{ and } x \text{ and } z \text{ to be scalars)}$$

$$= \exp(-x^2) \exp(-z^2) \exp(2xz)$$

$$= \exp(-x^2) \exp(-z^2) \sum_{0=1}^{\infty} \frac{2^k x^k z^k}{k!}$$

$$= \phi(x)^{\mathsf{T}} \phi(z)$$
Thus an infinite-dim vector (ignoring the

constants coming from the 2^k and k! terms

- $\blacksquare \text{ Here } \phi(x) = [\exp(-x^2)x^0, \exp(-x^2)x^1, \exp(-x^2)x^2, \exp(-x^2)x^3, ..., \exp(-x^2)x^\infty]$
- But again, note that we never need to compute $\phi(x)$ to compute k(x,z)
 - k(x,z) is easily computable from its definition itself $(\exp[-(x-z)^2]$ in this case)

Kernel Function: Some Other Aspects

- Not every function of the form $k(x,z) = \phi(x)^{\mathsf{T}}\phi(z)$ is a kernel function
- *k* must satisfy Mercer's Condition
 - k must define a dot product for some Hilbert Space
 - \blacksquare Above is true if k is symmetric and positive semi-definite (p.s.d.) function (though there are

exceptions; there are also "indefinite" kernels)

For all "square integrable" functions f (such functions satisfy $\int f(x)^2 dx < \infty$

$$k(\mathbf{x}, \mathbf{z}) = k(\mathbf{z}, \mathbf{x})$$

$$\iint f(\mathbf{x})k(\mathbf{x},\mathbf{z})f(\mathbf{z})d\mathbf{x}d\mathbf{z} \geq 0$$

Loosely speaking a PSD <u>function</u> here means that if we evaluate this function for N inputs (N^2 pairs) then the $N \times N$ matrix will be PSD (also called a kernel matrix)

Can easily verify that the Mercer's Condition holds for these

- Let k_1 , k_2 be two kernel functions then the following are as well
 - $k(x,z) = k_1(x,z) + k_2(x,z)$: simple sum
 - $k(x,z) = \alpha k_1(x,z)$: scalar product with $\alpha > 0$
 - $k(x,z) = k_1(x,z)k_2(x,z)$: direct product of two kernels

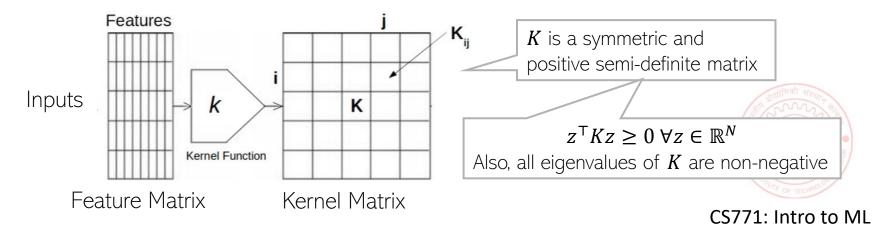
Can also combine these rules and the resulting function will also be a kernel function

Kernel Matrix

- Kernel based ML algos work with kernel matrices rather than feature vectors
- lacktriangle Given N inputs, the kernel function k can be used to construct a Kernel Matrix k
- The kernel matrix K is of size $N \times N$ with each entry defined as

$$K_{ij}=k(\pmb{x}_i,\pmb{x}_j)=\phi(\pmb{x}_i)^{\sf T}\;\phi(\pmb{x}_j)$$
 Note again that we don't need to compute ϕ and this dot product explicitly

 $lacksquare K_{ij}$: Similarity between the i^{th} and j^{th} inputs in the kernel induced feature space ϕ



Using Kernels in ML algorithms



Using Kernels

- Kernels can turn many linear models into nonlinear models
- lacktriangle Recall that $k(m{x},m{z})$ represents a dot product in some high-dim feature space ${\mathcal F}$
- Important: Any ML model/algo in which, during training and test, inputs only appear as dot product (pairwise similarity) can be "kernelized
- Just replace each term of the form $\boldsymbol{x}_i^{\mathsf{T}}\boldsymbol{x}_j$ by $\phi(\boldsymbol{x}_i)^{\mathsf{T}}\phi(\boldsymbol{x}_j) = k(\boldsymbol{x}_i,\boldsymbol{x}_j) = K_{ij}$
- Most ML models/algos can be kernelized
- Will look at an example: Kernelized SVM
 - Perhaps the most popular/natural example of kernelization



A Side-note: Kernelizing a Euclidean Distance

- Not just dot products but Eucliean distance can be kernelized too
- Many algorithms, e.g., LwP, KNN, etc. use Euclidean distances, e.g.,

$$d(a,b) = \|a - b\|^2 = \|a\|^2 + \|b\|^2 - 2a^{\mathsf{T}}b = a^{\mathsf{T}}a + b^{\mathsf{T}}b - 2a^{\mathsf{T}}b$$

ullet This can be kernelized as well by replacing the above norms and inner products by their kernelized versions, assuming a kernel k with feature map ϕ

$$d(\phi(a), \phi(b)) = \|\phi(a) - \phi(b)\|^{2}$$

$$= \phi(a)^{\mathsf{T}} \phi(a) + \phi(b)^{\mathsf{T}} \phi(b) - 2\phi(a)^{\mathsf{T}} \phi(b)$$

$$= k(a, a) + k(b, b) - 2k(a, b)$$



Nonlinear SVM using Kernels



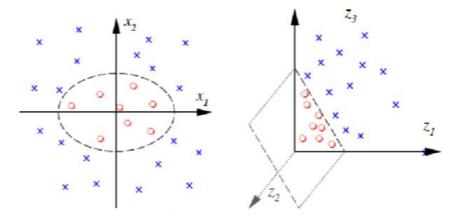
Kernelized SVM Training

■ Recall the soft-margin linear SVM objective (with no bias term)

Inputs only appear as dot products ©

$$\underset{\mathbf{0} \leq \boldsymbol{\alpha} \leq \boldsymbol{C}}{\operatorname{argmax}} \quad \boldsymbol{\alpha}^{\mathsf{T}} \mathbf{1} - \frac{1}{2} \boldsymbol{\alpha}^{\mathsf{T}} \mathbf{G} \boldsymbol{\alpha} = g_{ij} + g_{ij} \mathbf{1} \mathbf{1}$$

- lacktriangle To kernelize, we can simply replace $G_{ij}=y_iy_j\; m{x}_i^{\mathsf{T}} m{x}_j$ by $y_iy_jK_{ij}$
 - lacktriangle .. where $K_{ij} = kig(x_i, x_jig) = \phi(x_i)^{ op}\phi(x_j)$ for a suitable kernel function k
- The problem can now be solved just like the linear SVM case
- lacktriangle The new SVM learns a linear separator in kernel-induced feature space ${\mathcal F}$
 - ullet This corresponds to a non-linear separator in the original feature space ${\mathcal X}$





Kernelized SVM Prediction

- SVM weight vector for the kernelized case will be $\mathbf{w} = \sum_{n=1}^N \alpha_n y_n \phi(\mathbf{x}_n)$
- Imp: We can't store w unless the feature mapping $\phi(x_n)$ is finite dimensional
 - In practice, we store the α_n 's and the training data for test time (just like KNN)
 - In fact, need to store only training examples for which α_n is nonzero (i.e., the support vectors)
- lacktriangle Prediction for a new test input $oldsymbol{x}_*$ (assuming hyperplane's bias b=0) will be

$$y_* = \operatorname{sign}(\mathbf{w}^{\mathsf{T}} \phi(\mathbf{x}_*)) = \operatorname{sign}\left(\sum_{n=1}^{N} \alpha_n y_n \phi(\mathbf{x}_n)^{\mathsf{T}} \phi(\mathbf{x}_*)\right) = \operatorname{sign}\left(\sum_{n=1}^{N} \alpha_n y_n k(\mathbf{x}_n, \mathbf{x}_*)\right)$$

- Note that the prediction cost also scales linearly with N (actually in the number of support vectors, i.e., training inputs for which α_n is nonzero)
- Also note that, for unkernelized (i.e., linear) SVM, $w = \sum_{n=1}^{N} \alpha_n y_n x_n$ can be computed and stored as a $D \times 1$ vector and we can compute $w^T x_*$ in O(D) time

Kernel extensions of other ML models



Kernel extensions of other ML models

- Most of the models what have studied can be kernelized
 - Kernel based linear/ridge regression
 - Kernel based LwP
 - Kernel based nearest neighbors
 - Kernel logistic regression
 - Kernel Perceptron

But the extra price has to be paid in terms of storage cost and slower predictions

Kernel extension makes these approaches more powerful (nonlinear patterns can be learned)



- Some of these extensions are simple to obtain, some not so (but possible)
- Imp: In these models, just like kernel SVM, the model parameters (e.g., the weight vector) can't be stored as a finite-dim vector (unless ϕ is finite dim)
 - Thus the training inputs need to be stored at test time as well
- Also, just like kernel SVM, all of these will in general be slower at test time

Speeding-up Kernel Methods



Speeding-up Kernel Methods

Kernels assume that

$$k(\boldsymbol{x}_n, \boldsymbol{x}_m) = \phi(\boldsymbol{x}_n)^{\mathsf{T}} \phi(\boldsymbol{x}_m)$$

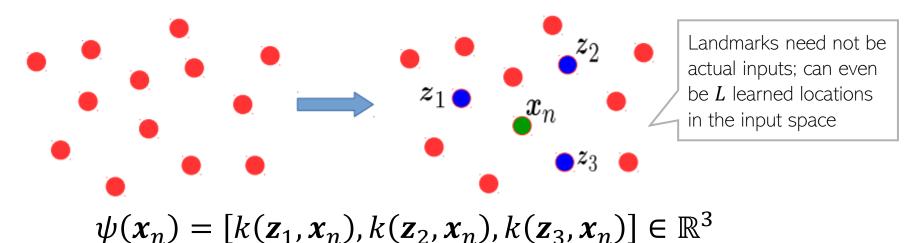
lacktriangle Suppose for this kernel, we can get an L-dim feature vector $\psi(x)$ such that

$$k(\mathbf{x}_n, \mathbf{x}_m) \approx \boldsymbol{\psi}(\mathbf{x}_n)^{\mathsf{T}} \boldsymbol{\psi}(\mathbf{x}_m)$$

- Using features $\psi(x)$, we can learn a <u>linear model</u> with weights $w \in \mathbb{R}^L$
- This model will be a good approximation to the kernelized model
- Training will be faster because no need to store and work with kernel matrices
- lacktriangle Prediction at test time will also be faster we just need to compute $m{w}^{\mathsf{T}}\psi(m{x}_*)$
- Many ways to get such features $\psi(x)$ for standard kernels

Extracting Features using Kernels: Landmarks

 \blacksquare Suppose we choose a small set of L "landmark" inputs z_1, z_2, \ldots, z_L in the training data



lacktriangle For each input $oldsymbol{x}_n$, using a kernel k, define an L-dimensional feature vector as follows

$$\psi(\mathbf{x}_n) = [k(\mathbf{z}_1, \mathbf{x}_n), k(\mathbf{z}_2, \mathbf{x}_n), \dots, k(\mathbf{z}_L, \mathbf{x}_n)] \in \mathbb{R}^L$$

- lacktriangle Can now apply a linear model on ψ representation (L-dimensional now) of the inputs
- lacktriangle This will be fast both at training as well as test time if L is small
- No need to kernelize the linear model while still reaping the benefits of kernels ©

Extracting Feat. using Kernels: Random Features

Many kernel functions* can be written as

$$k(\boldsymbol{x}_n, \boldsymbol{x}_m) = \phi(\boldsymbol{x}_n)^{\top} \phi(\boldsymbol{x}_m) = \mathbb{E}_{\boldsymbol{w} \sim p(\boldsymbol{w})} [t_{\boldsymbol{w}}(\boldsymbol{x}_n) t_{\boldsymbol{w}}(\boldsymbol{x}_m)]$$

- .. where $t_{w}(.)$ is a function with params $w \in \mathbb{R}^{D}$ with w drawn from some distr. p(w)
- Example: For the RBF kernel, $t_w(.)$ is cosine func. and p(w) is zero mean Gaussian $k(x_n, x_m) = \mathbb{E}_{w \sim p(w)}[\cos(w^\top x_n)\cos(w^\top x_m)]$
- Given $w_1, w_2, ..., w_L$ from p(w), using Monte-Carlo approx. of above expectation

$$k(\mathbf{x}_n, \mathbf{x}_m) \approx \frac{1}{L} \sum_{\ell=1}^{L} \cos(\mathbf{w}_{\ell}^{\top} \mathbf{x}_n) \cos(\mathbf{w}_{\ell}^{\top} \mathbf{x}_m) = \psi(\mathbf{x}_n)^{\top} \psi(\mathbf{x}_m)$$

- .. where $\psi(\mathbf{x}_n) = \frac{1}{\sqrt{L}}[\cos(\mathbf{w}_1^{\top}\mathbf{x}_n), \dots, \cos(\mathbf{w}_L^{\top}\mathbf{x}_n)]$ is an L-dim vector
- \blacksquare Can apply a linear model on this L-dim rep. of the inputs (no need to kernelize)

Learning with Kernels: Some Aspects

- Storage/computational efficiency can be a bottleneck when using kernels
- lacktriangle During training, need to compute and store the $N \times N$ kernel matrix K in memory
- Need to store training data (or at least support vectors in case of SVMs) at test time
- Test time can be slow: O(N) cost to compute a quantity like $\sum_{n=1}^{N} \alpha_n k(x_n, x_*)$
- Approaches like landmark and random features can be used to speed up
- Choice of the right kernel is also very important
- Some kernels (e.g., RBF) work well for many problems but hyperparameters of the kernel function may need to be tuned via cross-validation

 Also, a lot of recent work on connections
- Quite a bit of research on learning the right kernel from data
 - Learning a combination of multiple kernels (Multiple Kernel Learning) learning
 - Bayesian kernel methods (e.g., Gaussian Processes) can learn the kernel hyperparameters from data(thus can be seen as learning the kernel)
 - Deep Learning can also be seen as learning the kernel from data (more on this later)

between kernel

methods and deep