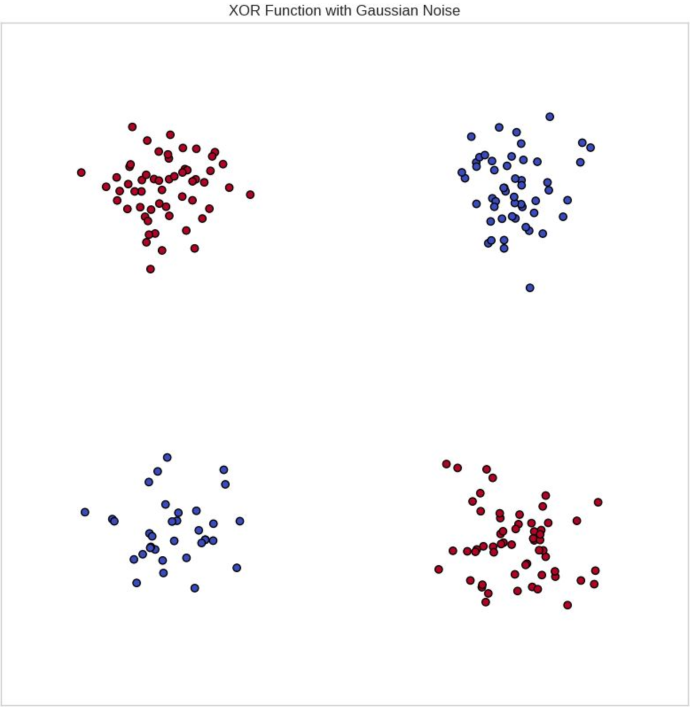
Approximating Kernels with Random Fourier Features

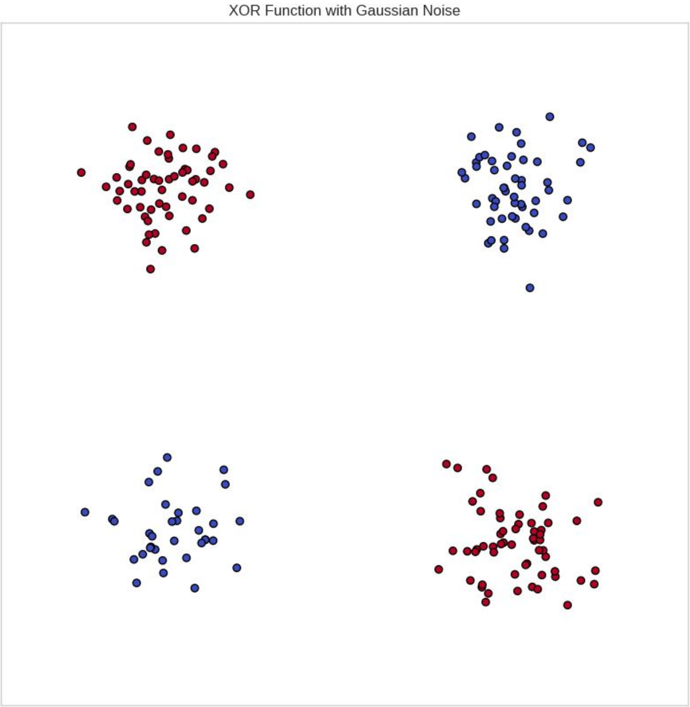
Mathis Rost
Tanja Zast

Motivation

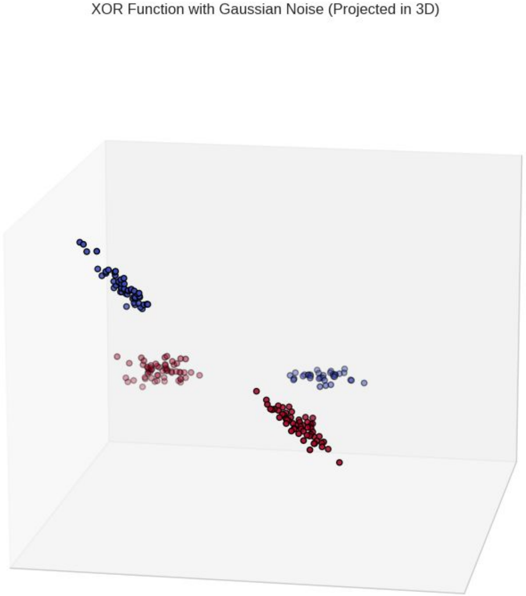


- Dataset is not linear seperable
- Project Data into a Featurespace where Data is linear sperable
- XOR function with noise

Motivation

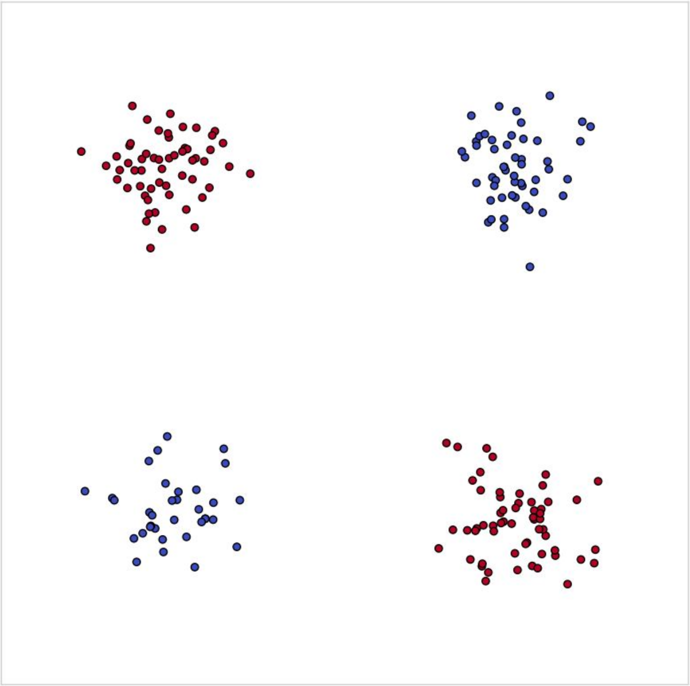


$$\phi(x_1, x_2) = (x_1, x_2, x_1 x_2) \in \mathbb{R}^3$$



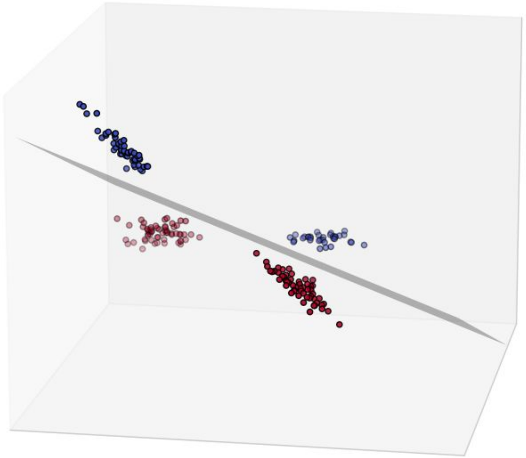
Motivation

XOR Function with Gaussian Noise

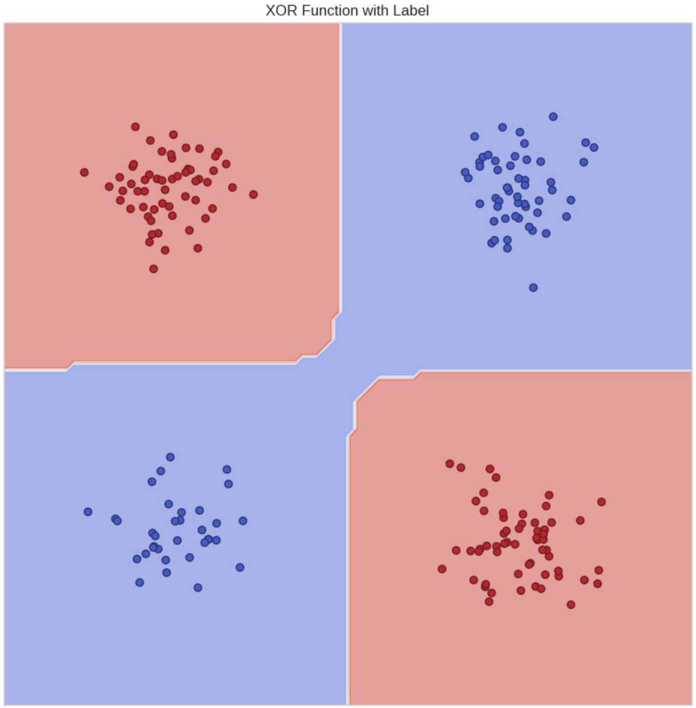


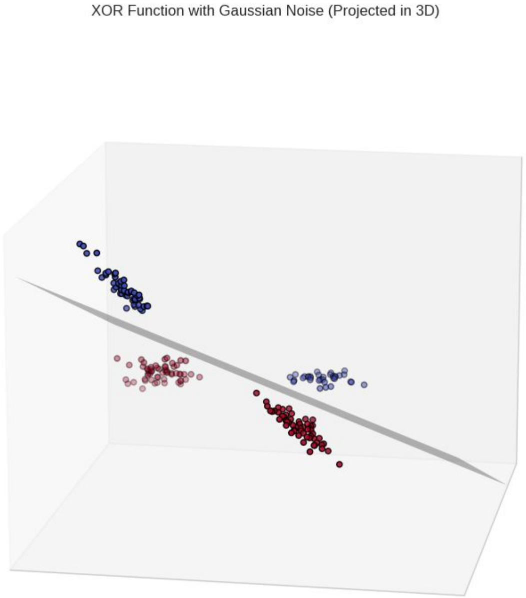
$$\phi(x_1, x_2) = (x_1, x_2, x_1 x_2) \in \mathbb{R}^3$$

XOR Function with Gaussian Noise (Projected in 3D)



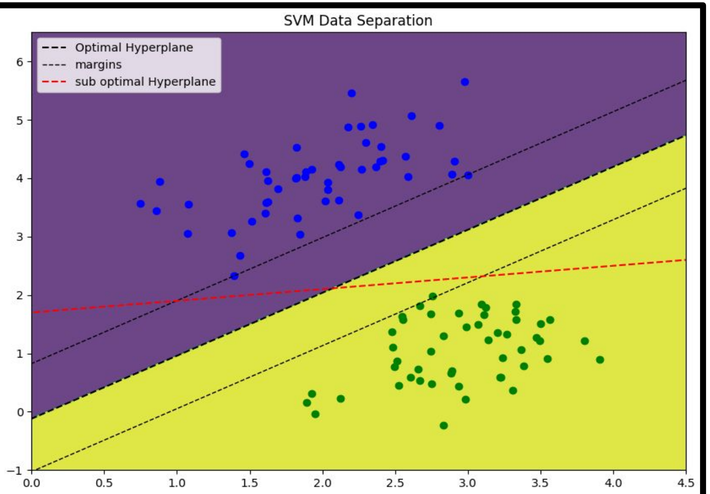
Motivation


XOR Function with Label


XOR Function with Gaussian Noise (Projected in 3D)

Kernel SVMs and the Kernel Trick

- Hyperplane can be represented with a vector $w \in \mathcal{H}$
- $\text{sign}(w^T x_i + b) = y_i$
- Support Vector Machines (SVM) calculate the best possible Hyperplane.
- SVMs can be kernelized with $\phi : X \to \mathcal{H}$
- Resulting Hyperplane: $w^T \phi(z) + b = \langle w, \phi(z) \rangle_{\mathcal{H}} + b$



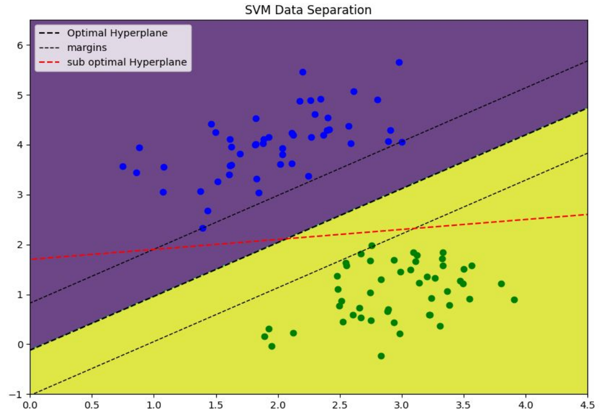
Kernel SVMs and the Kernel Trick

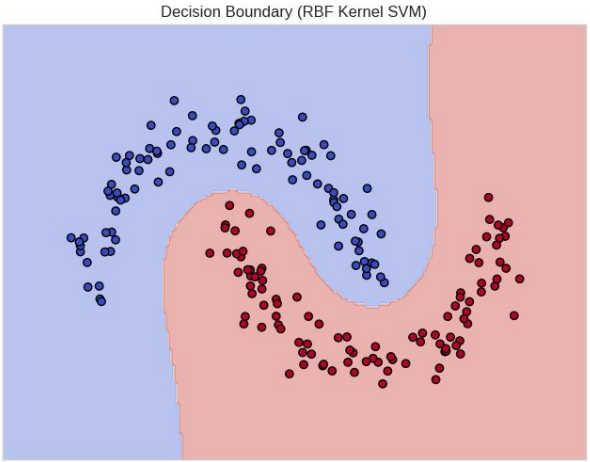
- Formula for Hyperplane in data-space

$$w^T z + b = \sum_{(x,y)} y \alpha_x x^T z + b$$

- Formula for hyperplane in feature-space

$$w^T \phi(z) + b = \langle w, \phi(z) \rangle_{\mathcal{H}} + b = \sum_{x,y} \alpha_x y \phi(x) \phi(z) = \sum_{x,y} \alpha_x y k(z, x) + b$$





Definition of a kernel

Definition 2. *Let X be our data set. A function $k : X \times X \to \mathbb{R}$ is called kernel if there exists an Hilbertspace $\mathcal{H}$ and a map $\phi : X \to \mathcal{H}$ such that $\forall x, y \in X$,*

$$k(x, y) = \langle \phi(x), \phi(y) \rangle_{\mathcal{H}} \tag{3.3}$$

Kernel Machines and the Kernel Trick

Mercer's Theorem

Mercer's Theorem: A symmetric function k can be expresses as an inner Product, i.e.

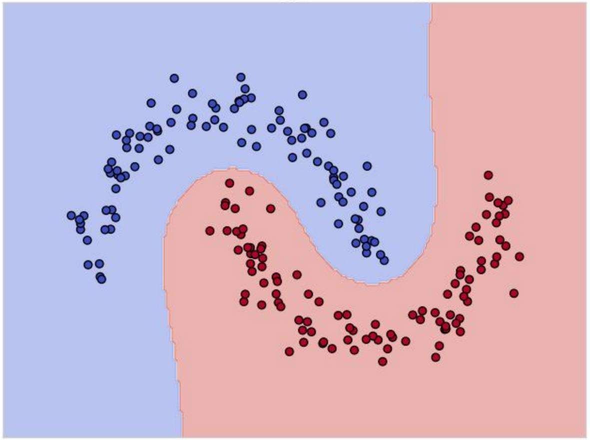
$$k(x, y) = \langle \phi(x), \phi(y) \rangle \tag{3.6}$$

for some $\phi : X \to \mathcal{H}$ if and only if k is positive semi definite

Kernel Matrix

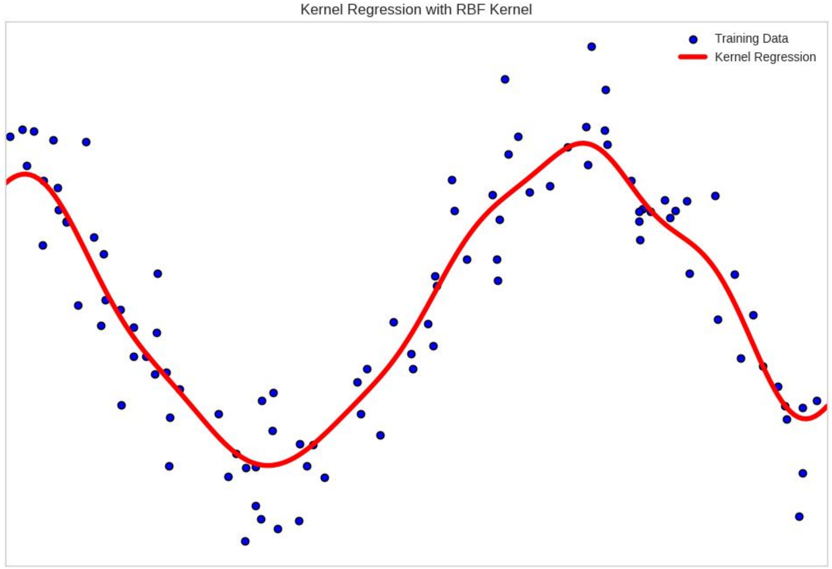
$$K = \begin{pmatrix} k(x_1, x_1) & \cdots & k(x_1, x_n) \\ \vdots & \ddots & \vdots \\ k(x_n, x_1) & \cdots & k(x_n, x_n) \end{pmatrix}$$

- We don't need to calculate the mapping $\phi : X \to \mathcal{H}$
- We can calculate decision boundaries with Help of the kernel Matrix
- this saves a lot of time for large dimensional features spaces
- Feature Space could also be infinity



Kernel Machines and the Kernel Trick

- Regression can also be kernelized
- Linear regression is implicit calculated in feature space
- This also works with the kernel trick



- optimal regression line in data-space
- $\hat{w} = (X^T X)^{-1} X^T y$
- optimal regression in feature-space
- $\hat{w} = (\Phi^T \Phi)^{-1} \Phi^T y$ with $\Phi = \phi(X)$
- can be calculated with kernel matrix
- $y = w^T \phi(z) = y(\Phi^T \Phi)^{-1} \Phi^T \phi(z) = (\Phi^T \Phi)^{-1} \sum_{x \in X} k(x, z)$

Kernel Machines and the Kernel Trick

- **Problem with kernel Machines:**
  - kernel Methods do not scale very well with large amount of data
  - For regression the inverse of the kernel matrix has to be computed
  - Kernel matrix will be very large. This can be a Problem for the RAM.
- **Solution**
  - Approximate kernel function
  - We need a map $z : X \to \mathbb{K}^M$, also called random feature

$$\boxed{k(x,y) = \langle \phi(x), \phi(y) \rangle \approx z(x)^T z(y) = \langle z(x), z(y) \rangle}$$

Random Fourer Features (RFFs)

- Translations-invariant kernel: $\forall x, y, z \in X \; k(x, y) = k(x - z, y - z).$
- RBF-kernel is translations-invariant

$$\boxed{k(x,y) = \exp\left(-\frac{\|x-y\|^2}{2\sigma^2}\right)}$$

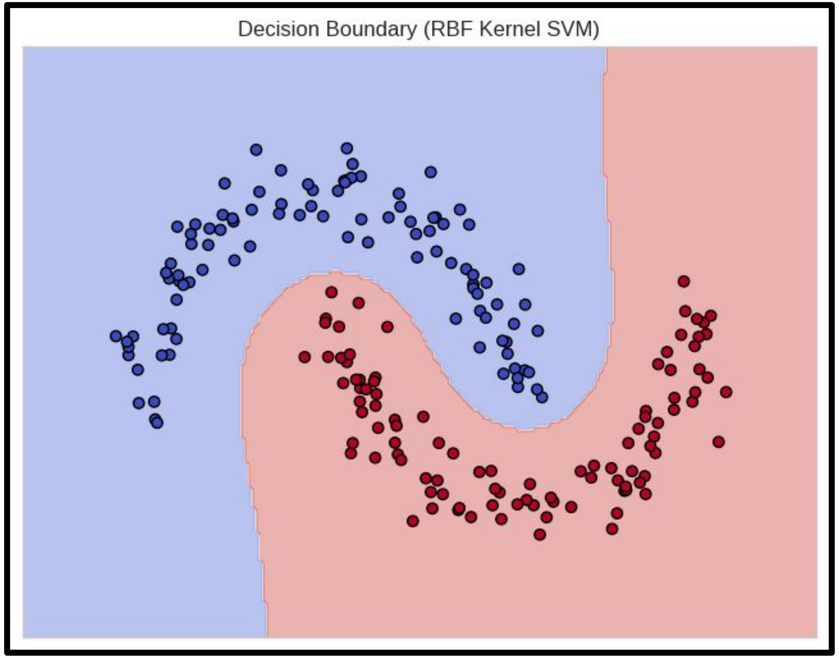
- We can approximate RBF-kernel with $z : x \to \exp\left(iw^T x\right)$, and $w \sim \mathcal{N}(0, I_d)$
- Using multiple Features for better approximation

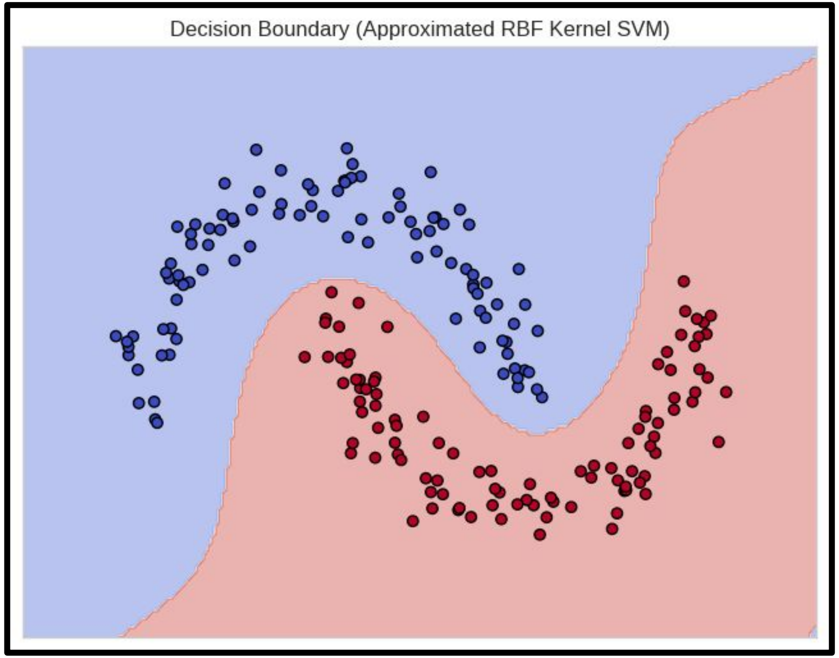
$$\boxed{\langle z(x), z(y) \rangle = \frac{1}{R} \sum_r z_{w_r}(x), z_{w_r}(y)^*}$$

Definition 3. *We call the map $z : \mathbb{R}^d \to \mathbb{K}^R$ a random fourier feature if it approximates a translations-invariant positive definite kernel k, i.e.*

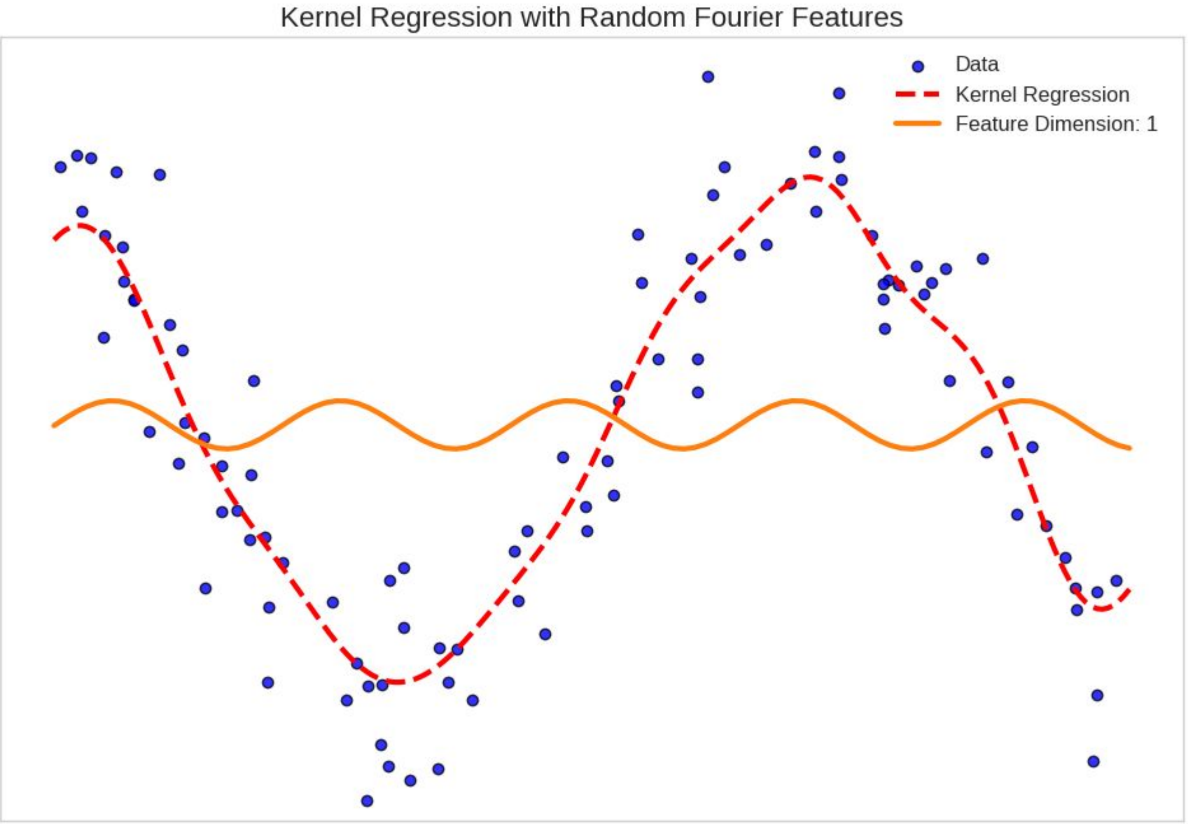
$$\mathbb{E}\left[\langle z(x), z(y) \rangle\right] = k(x - y) = k(x, y) \tag{4.9}$$

Random Fourer Features (RFFs)

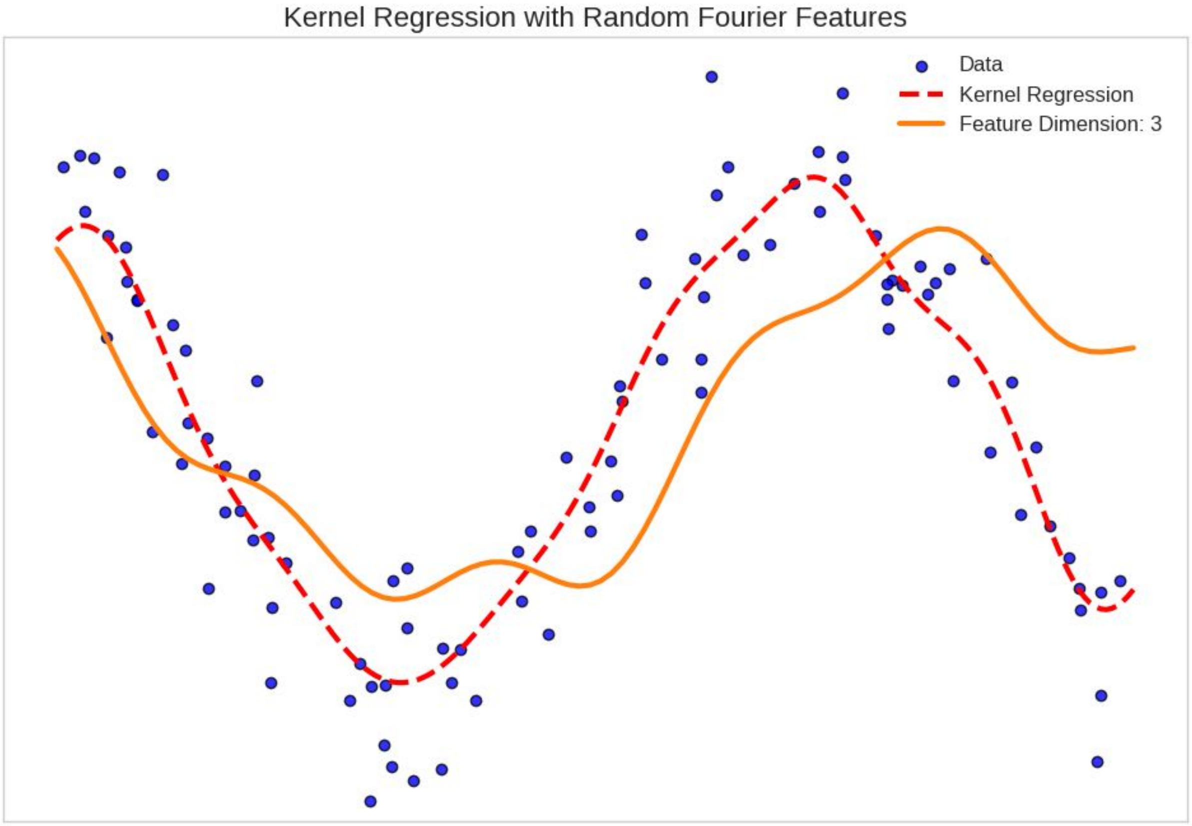




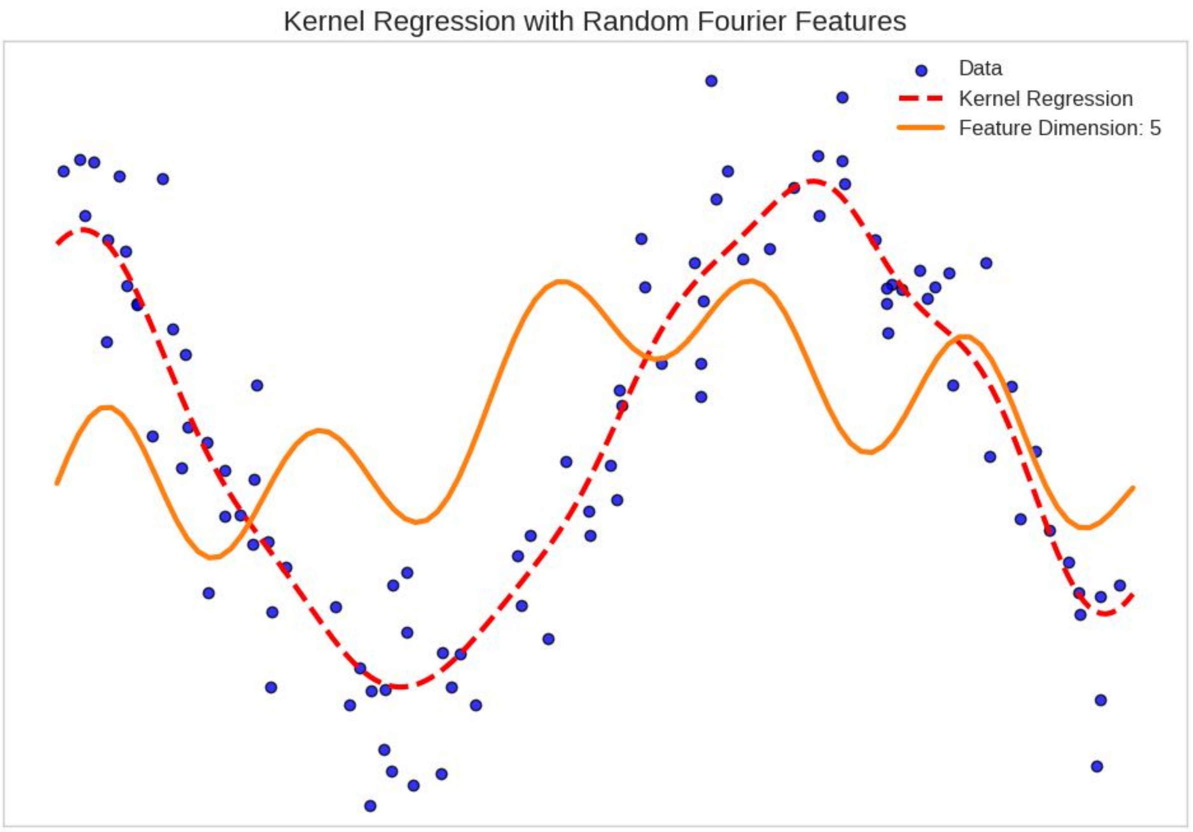
Approximating Kernel with RFFs



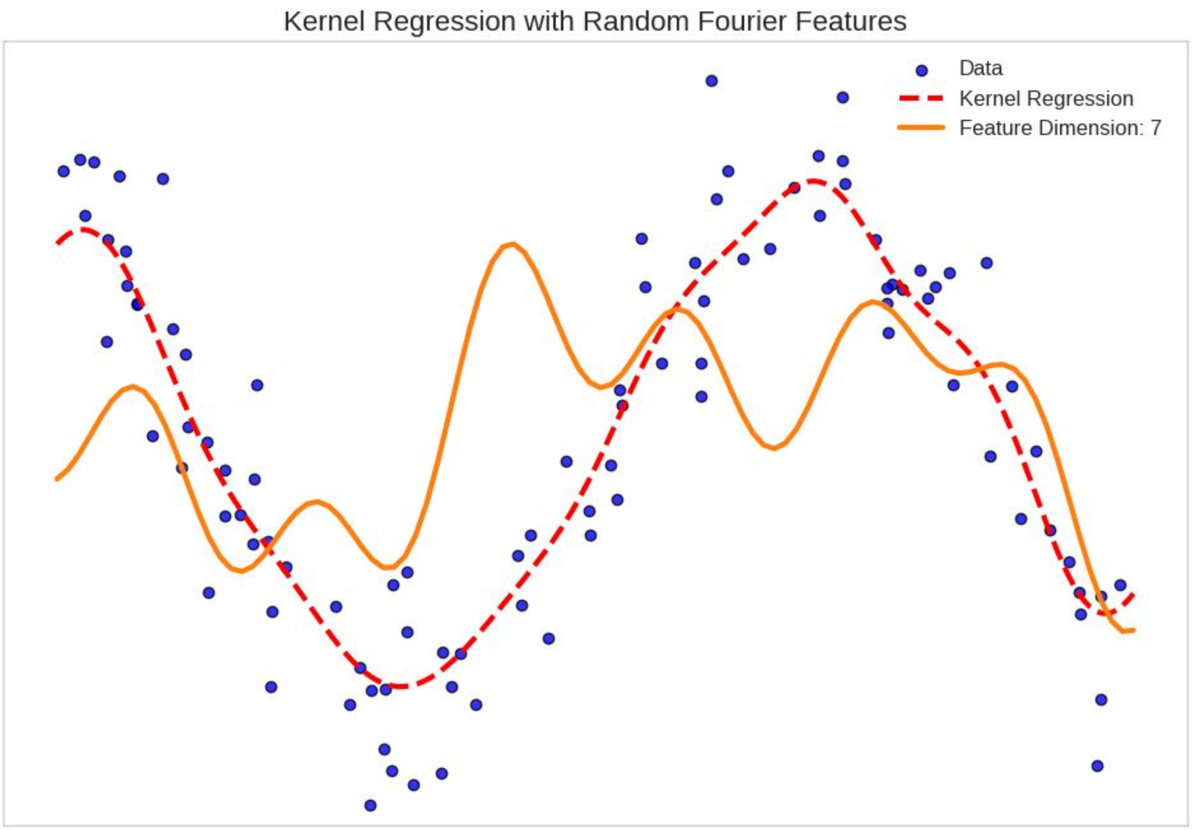
Approximating Kernel with RFFs



Approximating Kernel with RFFs



Approximating Kernel with RFFs



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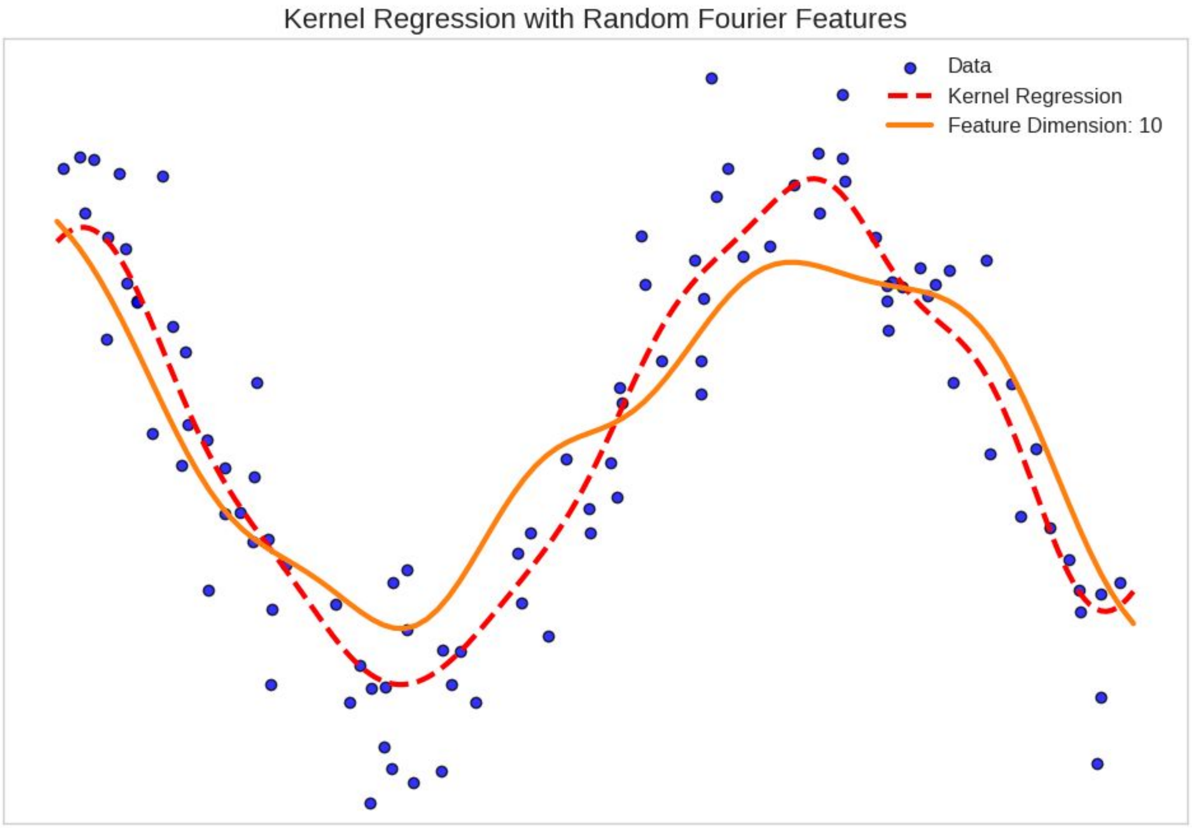
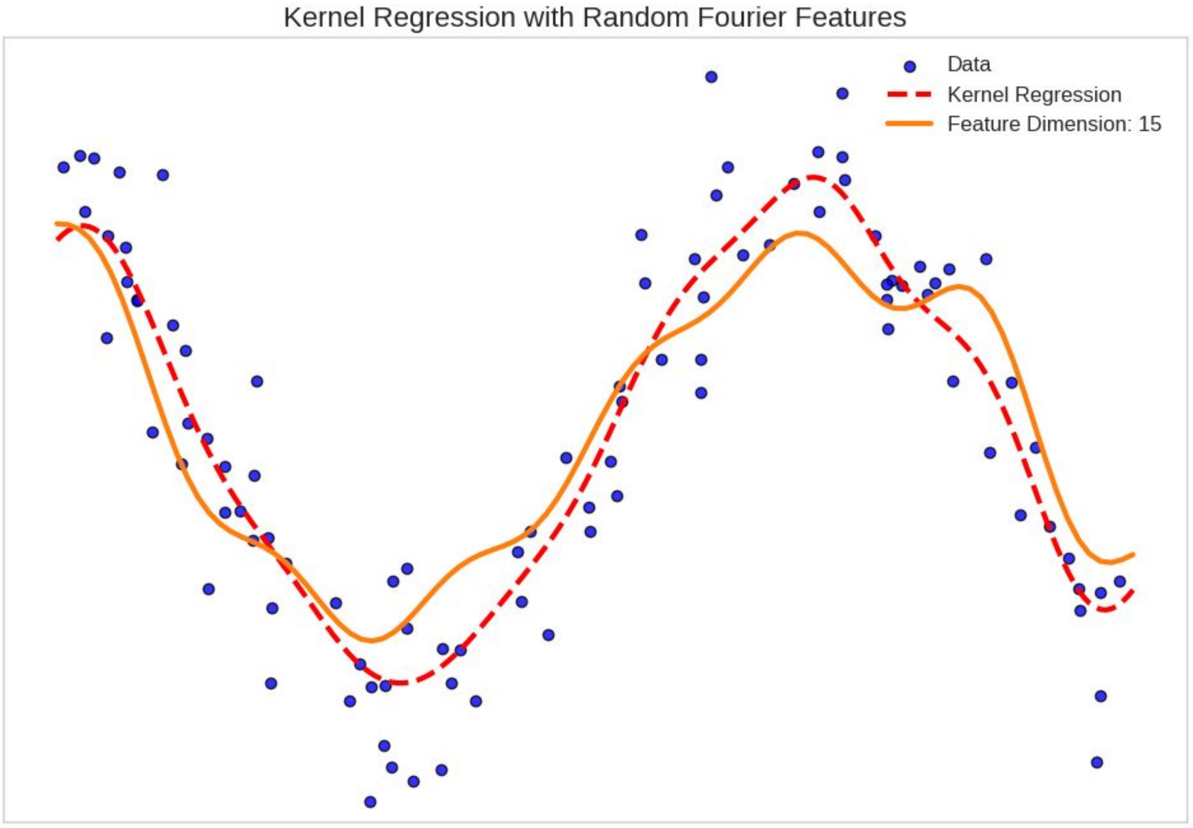
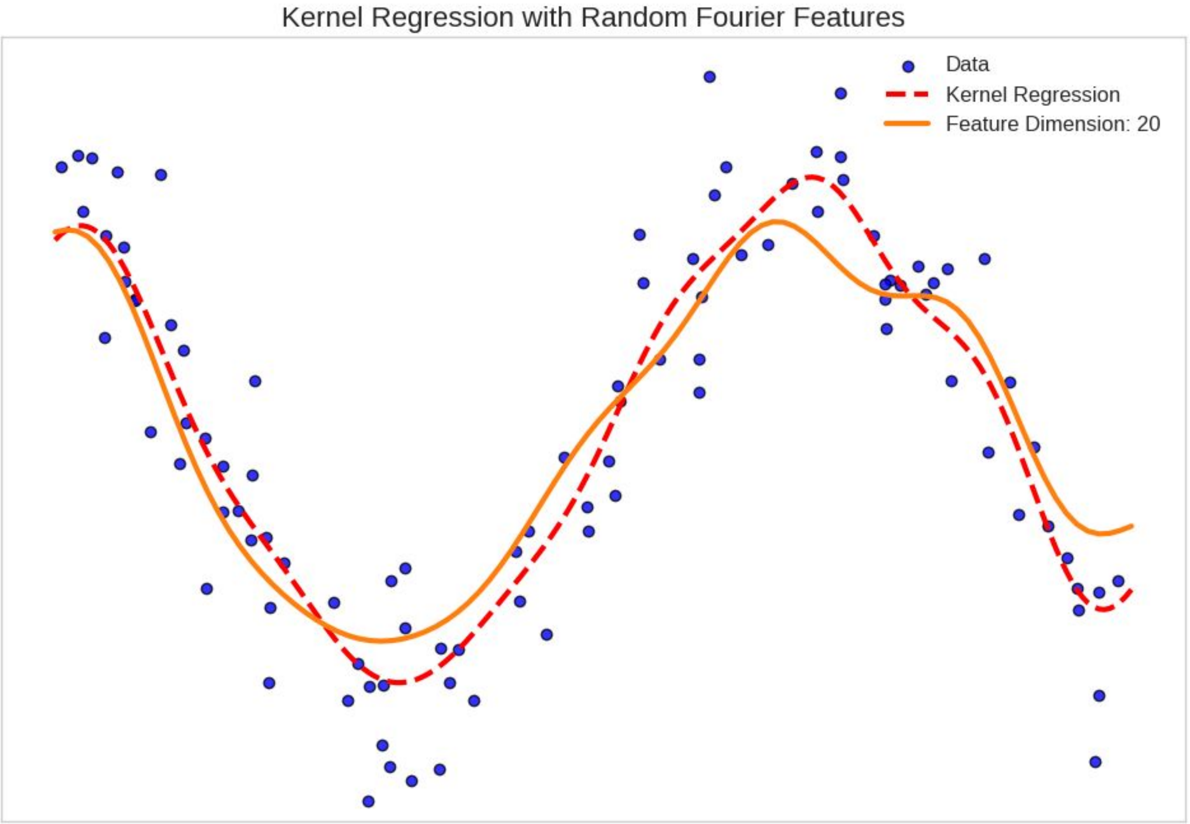


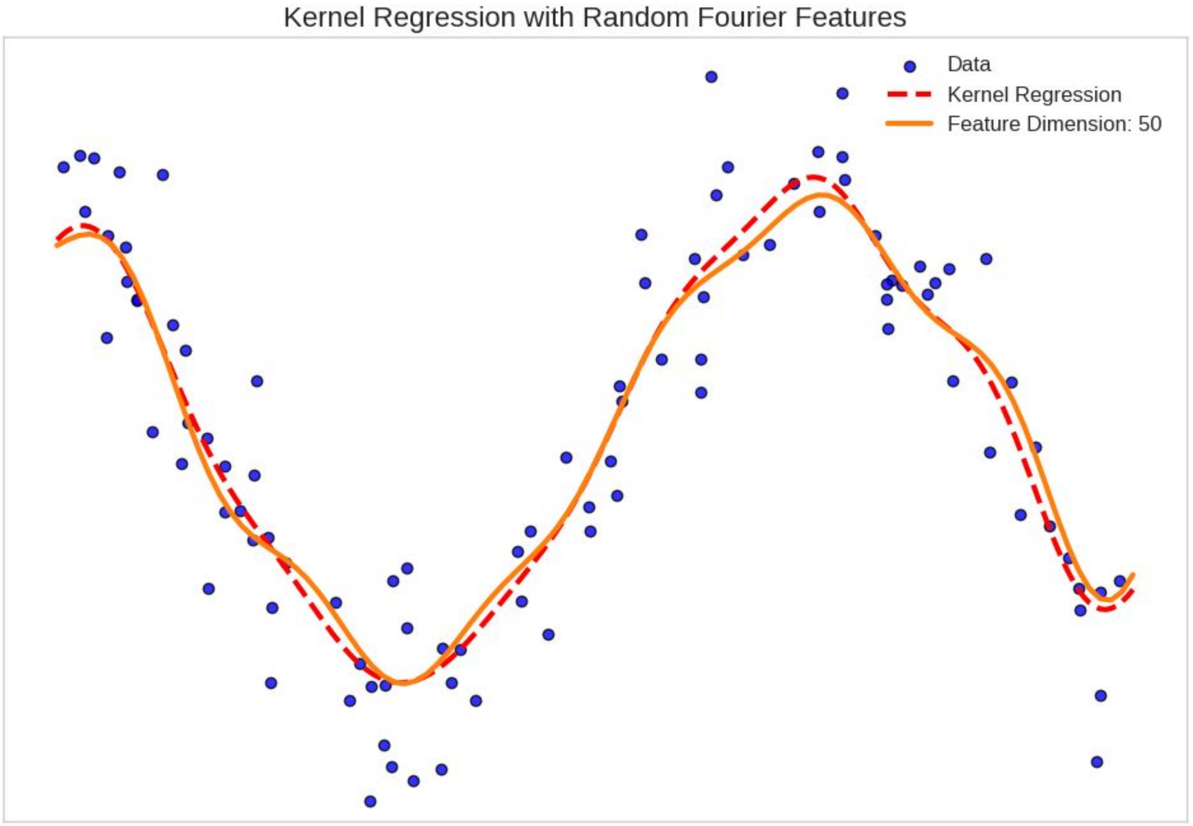
Approximating Kernel with RFFs



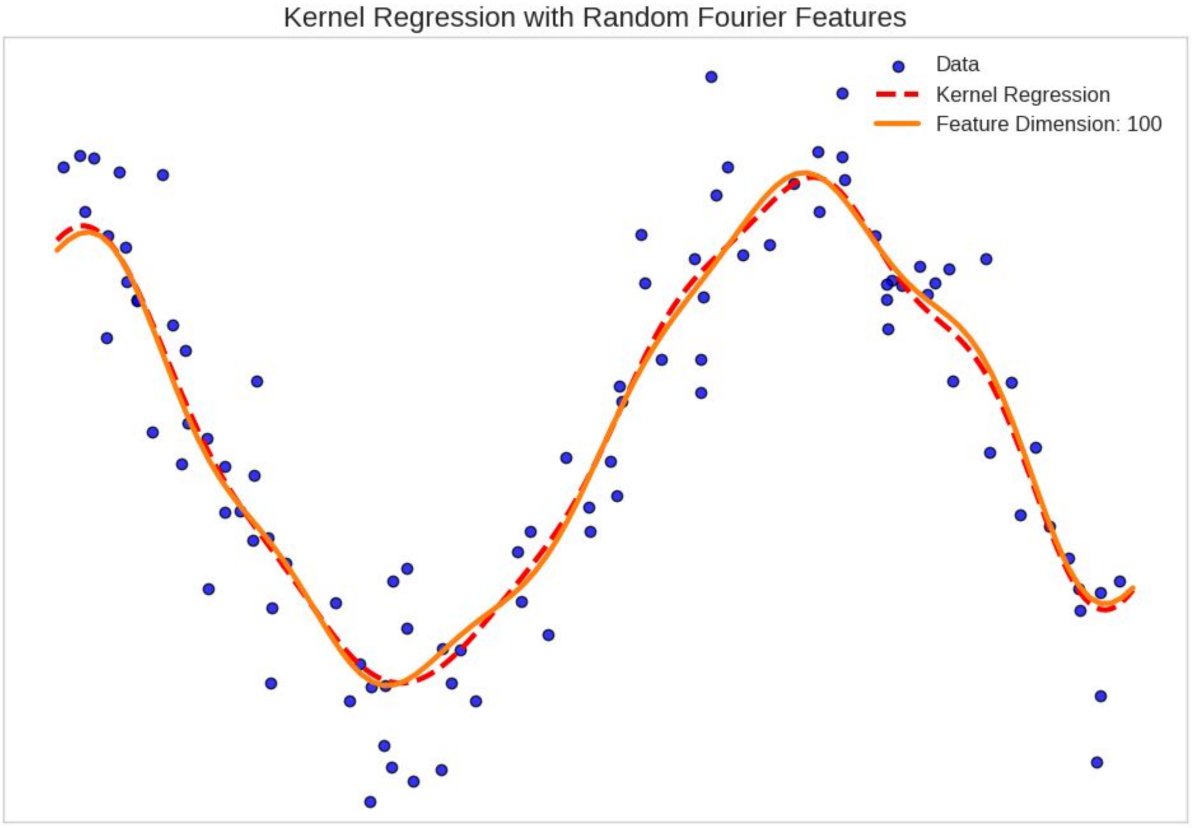
Approximating Kernel with RFFs



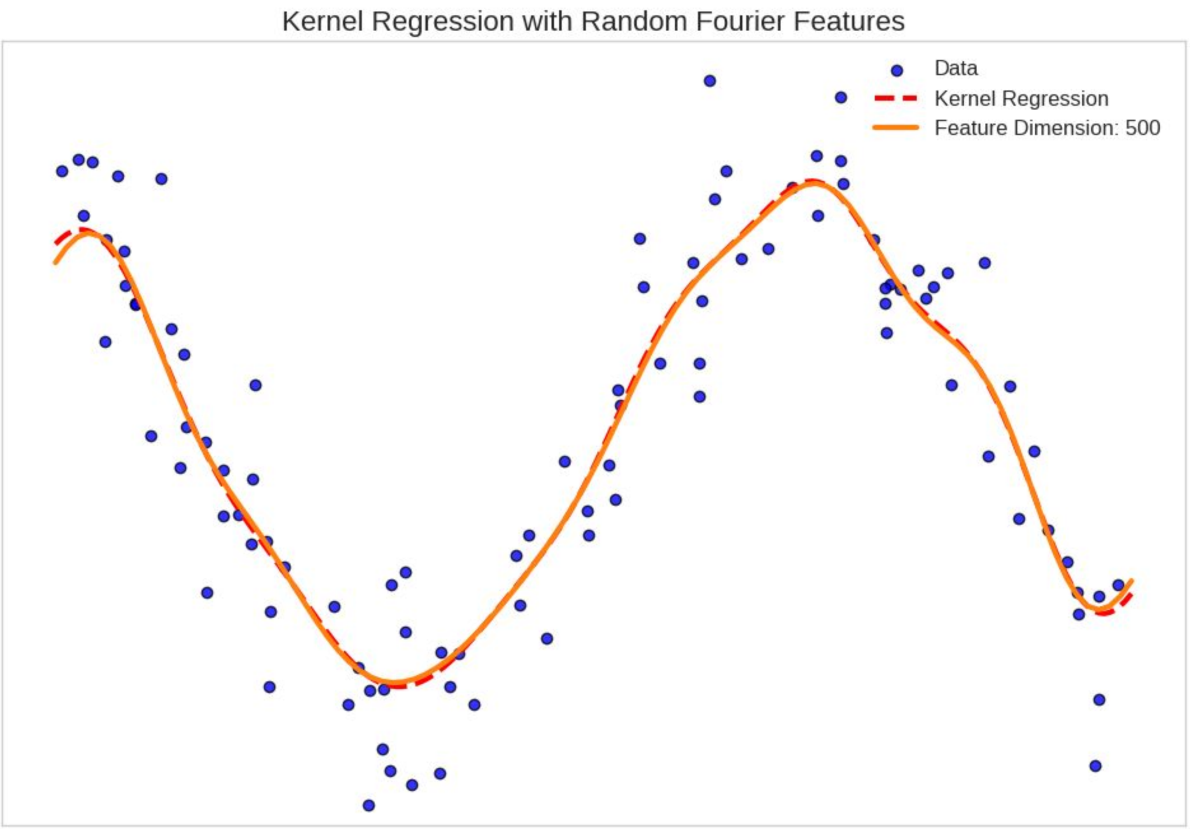
Approximating Kernel with RFFs



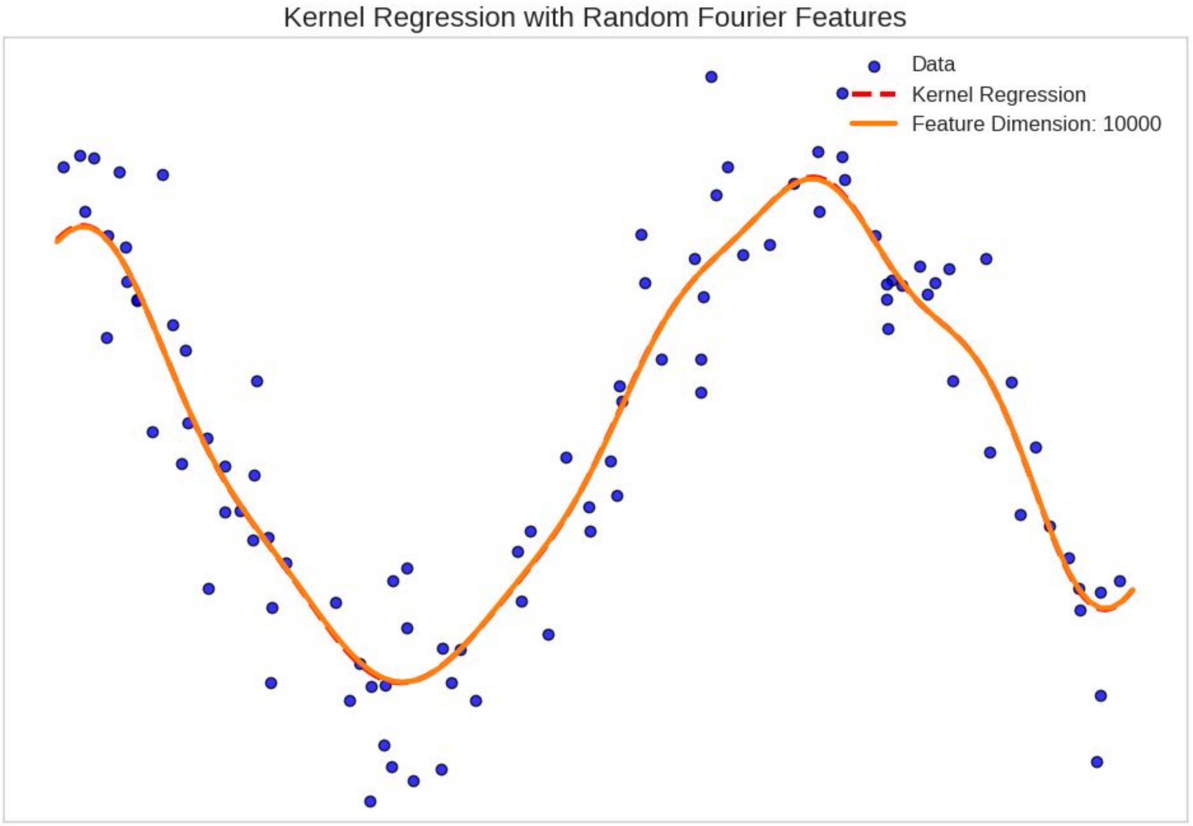
Approximating Kernel with RFFs



Approximating Kernel with RFFs

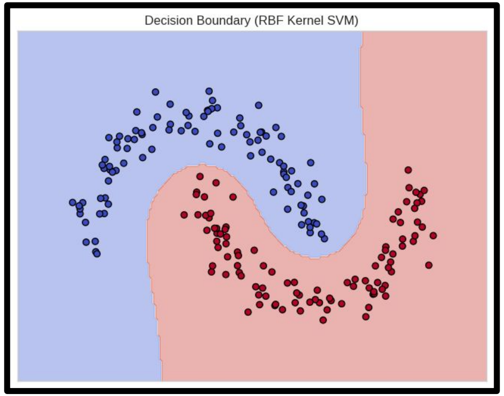


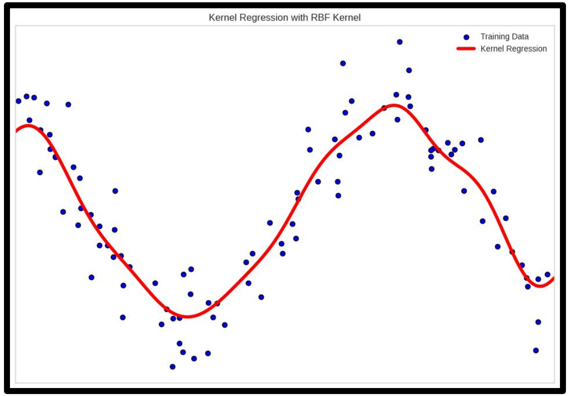
Approximating Kernel with RFFs



Experiments

- Regression with Random Fourier Features approximation
- Classification with Random Fourier Features approximation
- Ensemble Learning with Random Fourier Features





Model Architecture and Hyperparameter

- 2 datasets for regression and 2 datasets for classification
- Using Maxpool Operation for RAM saving and better results
- Using regularization term $\lambda = 1$
- Variance for RBF-kernel $\sigma = 2$

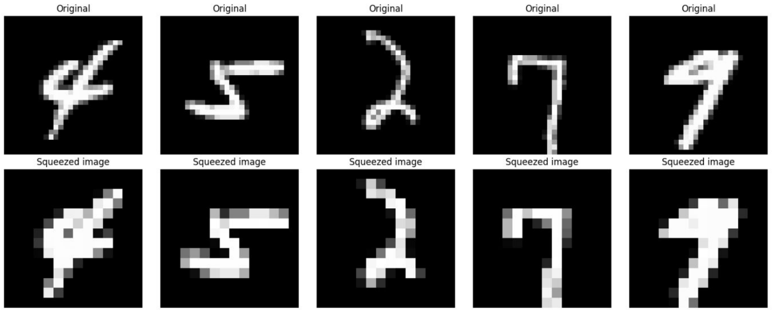
Dataset	#Entries	#Features
Avocado	18 200	8
Wine	1 143	11

Table 5.1.: Dataset Avocado and Wine Quality for Regression

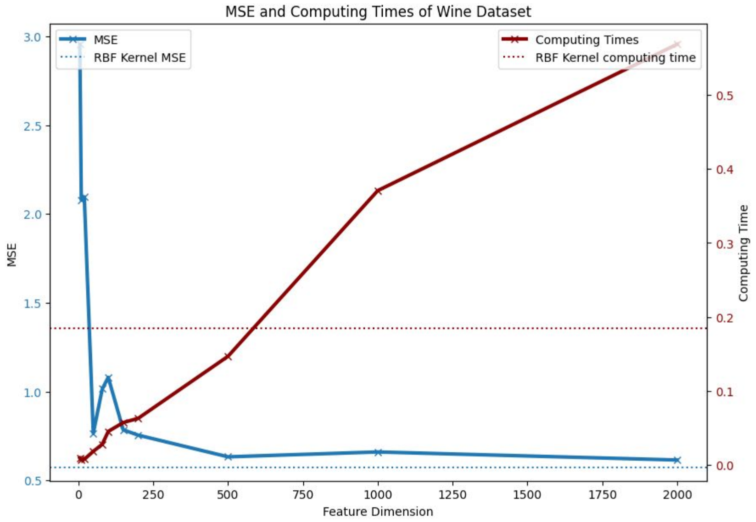
Dataset	#Entries	#Classes
MNIST	70 000	10
Fashion-MNIST	70 000	10

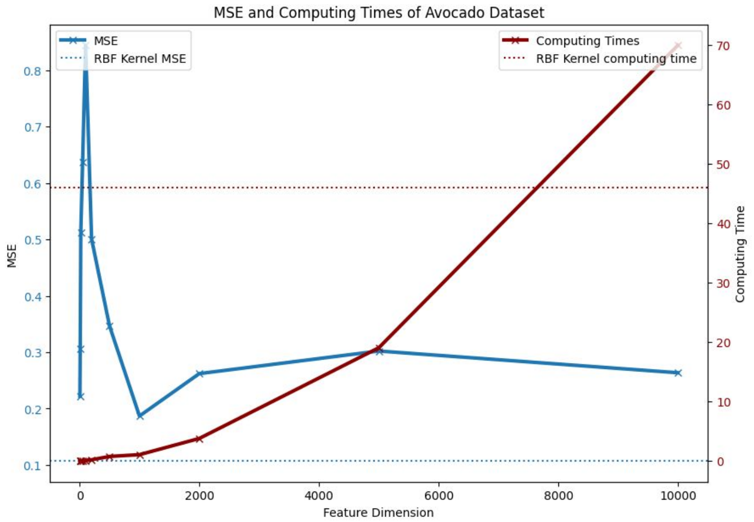
Table 5.2.: Dataset MNIST and Fashion-MNIST for Classification

$$\mathcal{L}(X) = \sum_{x,y \in X \times Y} (w^T \phi(x) - y)^2 + \frac{\lambda}{2} \|w\|^2$$

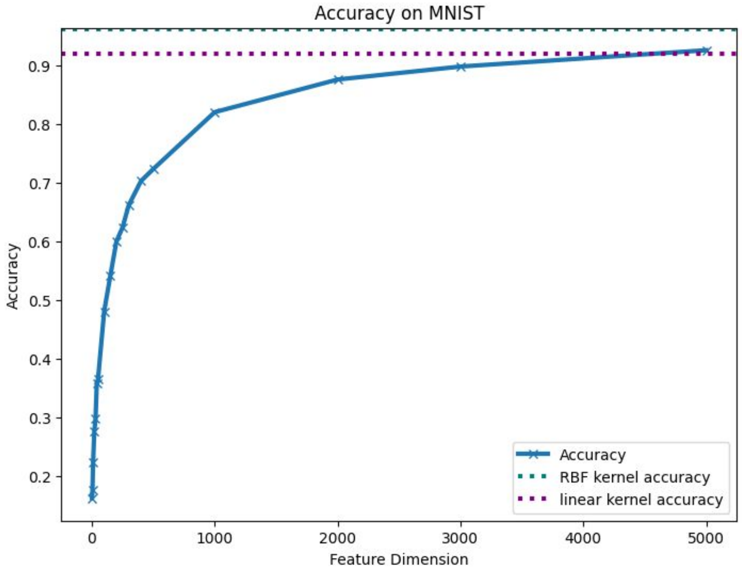


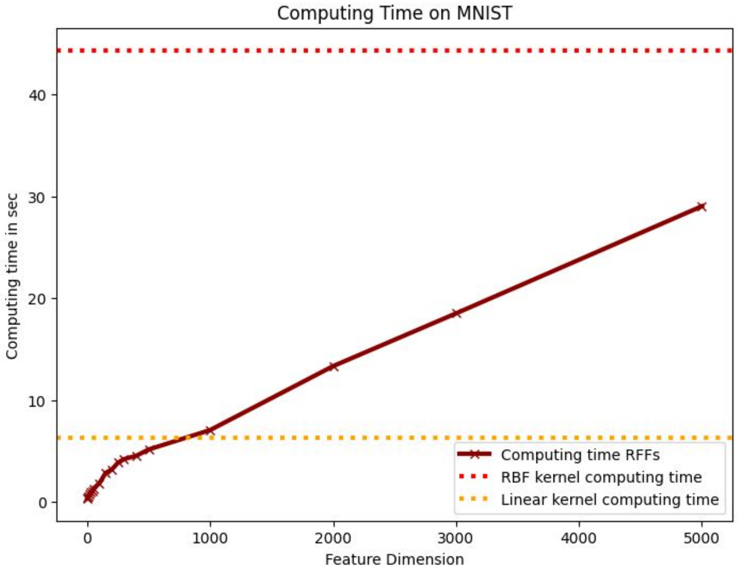
Approximating Kernel Regression



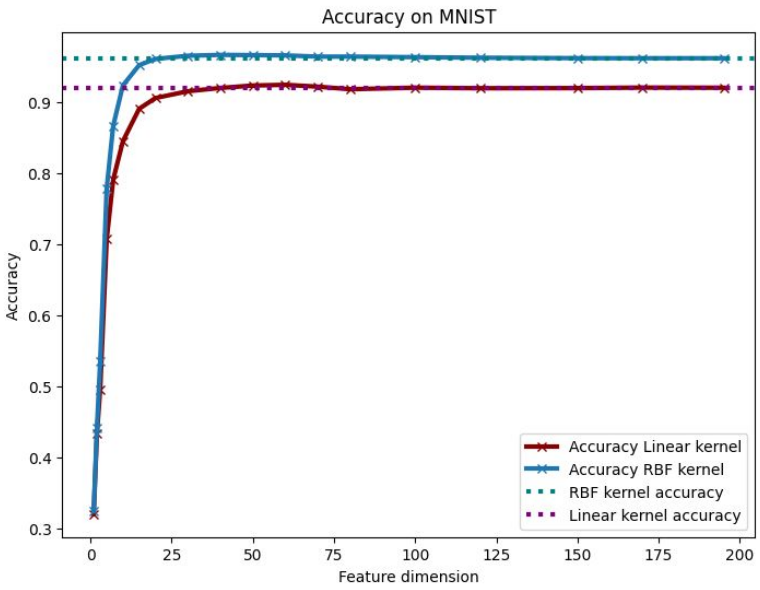


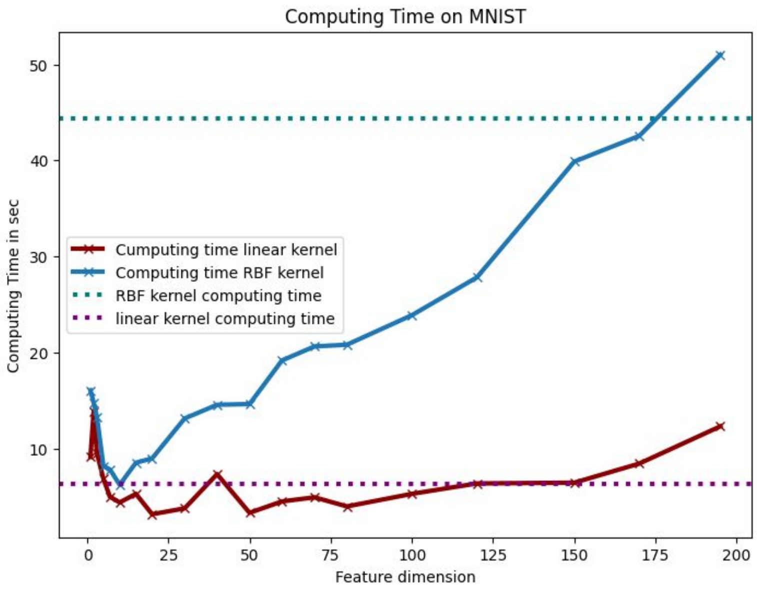
Approximating Kernel Support Vector Machine





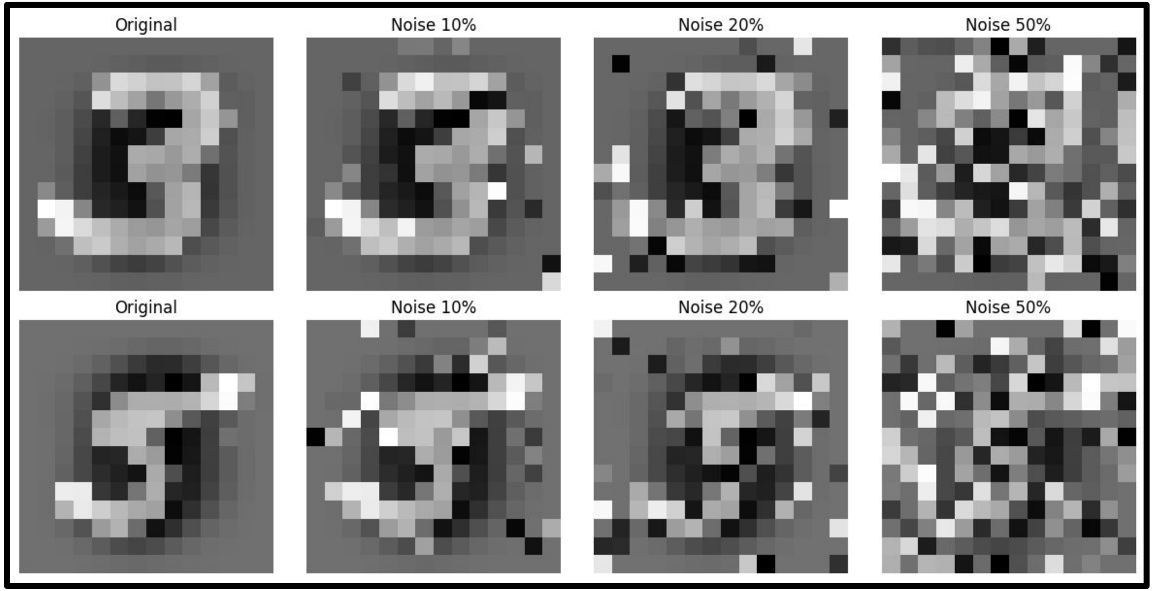
Comparing to PCA



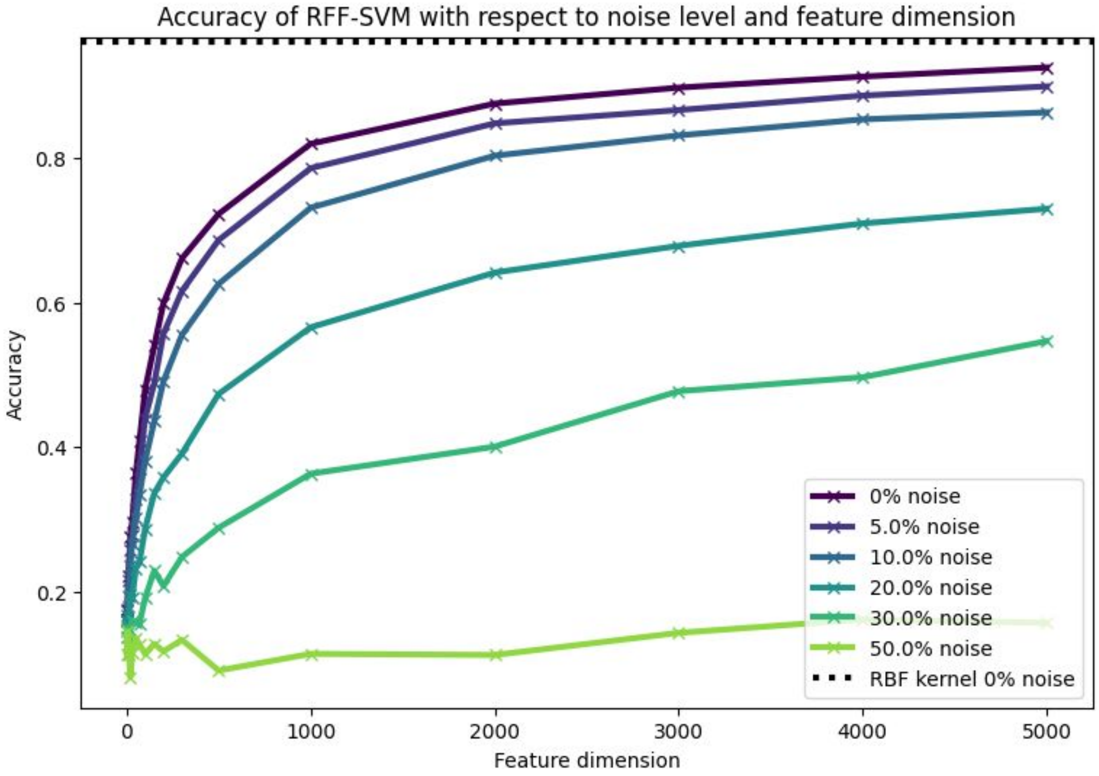


Noisy Data

- evaluating impact of noise
- *p*: prob. of each pixel to be uniform random
- testing for $p = 0$, $p = 0.05$, $p = 0.1$, $p = 0.2$, $p = 0.3$ and $p = 0.5$



Noisy Data

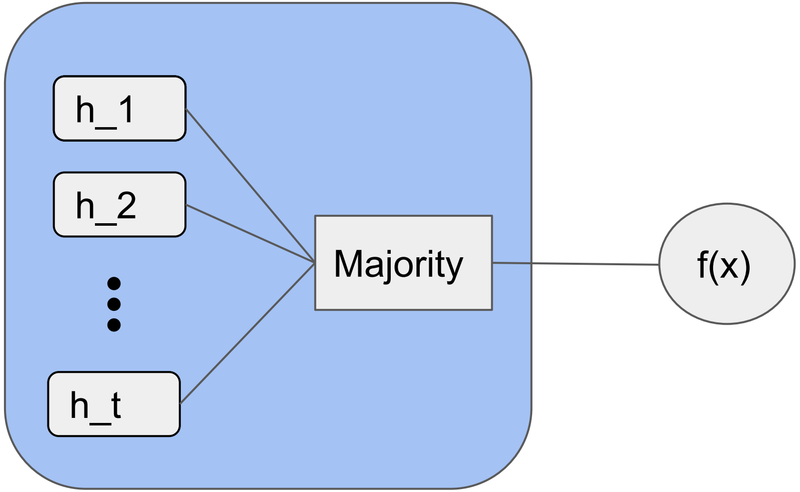


Accuracy of RFF-SVM with respect to noise level and feature dimension
Accuracy
0.2
0.4
0.6
0.8
Feature dimension
0
1000
2000
3000
4000
5000
0% noise
5.0% noise
10.0% noise
20.0% noise
30.0% noise
50.0% noise
RBF kernel 0% noise

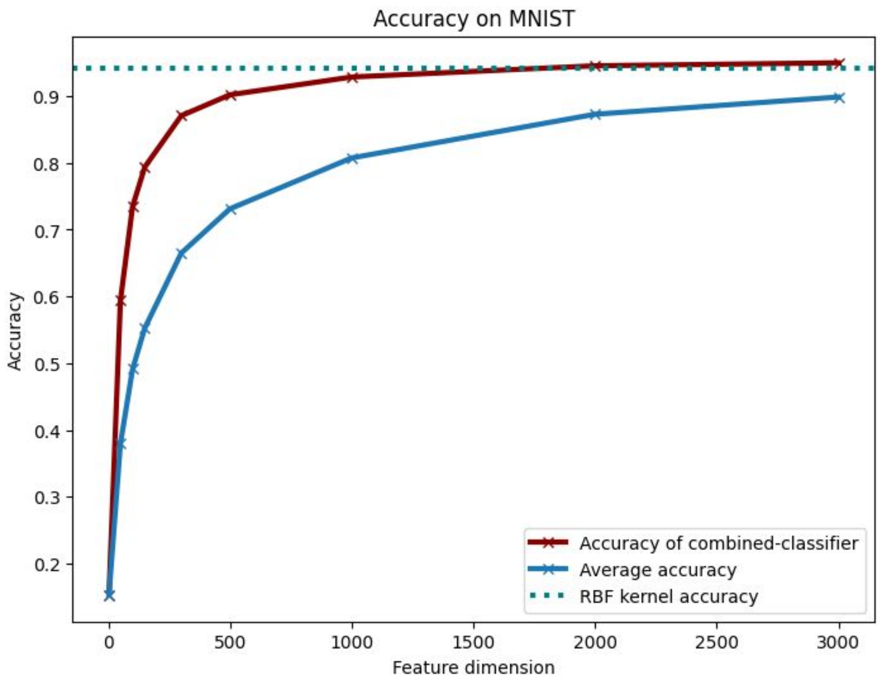
Ensemble Learning

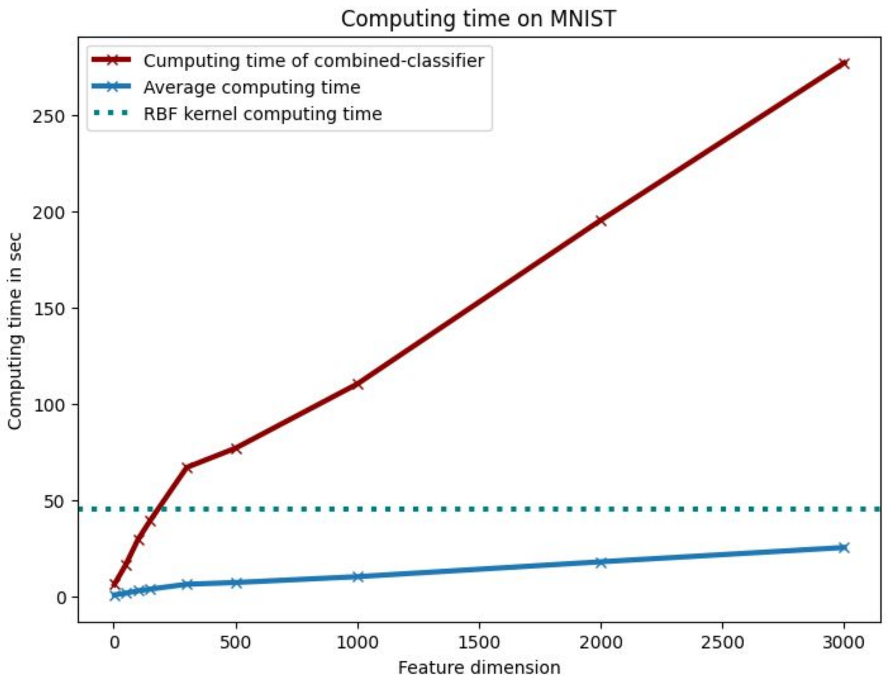
- RFF approximation can be used for ensemble learning
  - Classifiers are “random”
  - Classifiers will produce different Predictions
- Using majority Voting for Combined Classifier

$$\boxed{V(x) = \max_{y \in Y}(h_1(x), h_2(x), \cdots, h_t(x))}$$

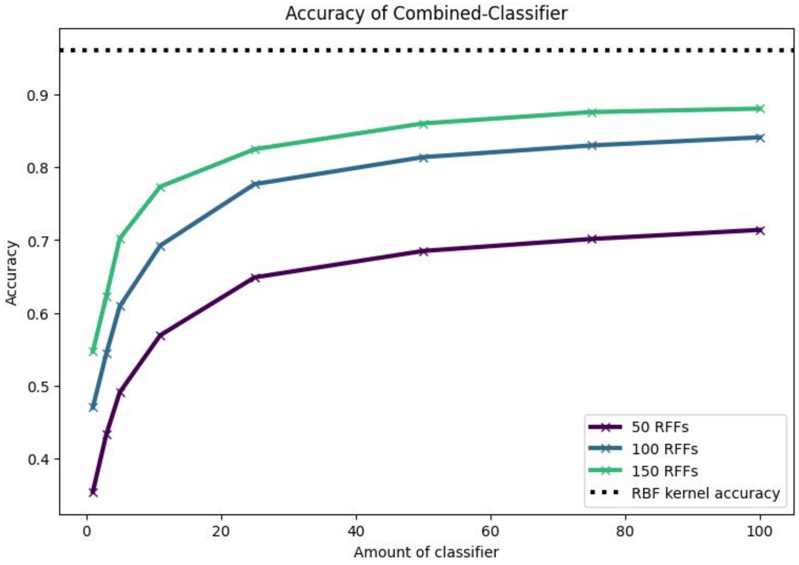


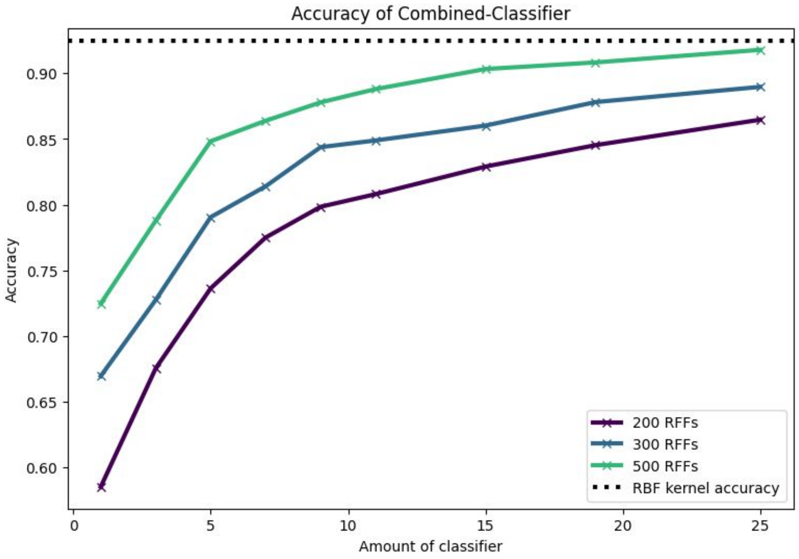
Ensemble Learning





Ensemble Learning





Conclusion and Discussion

- Always a trade-off between time and performance
- Still good performance with way less computing time
  - For regression and Classification

- Kernel approximation with RFFs is well suited for ensemble-learning
- Should be compared with other ensemble methods in future work.

Danke für ihre Aufmerksamkeit

Backup

Boncher's theorem: A continuous and translations-invariant kernel $k(x,y) = k(x-y)$ is positive definite if and only if $k(\Delta)$ is the Fourier transform of a non-negative measure $p(w)$ i.e.

$$k(\Delta) = \int p(w)\exp(iw\Delta)dw$$

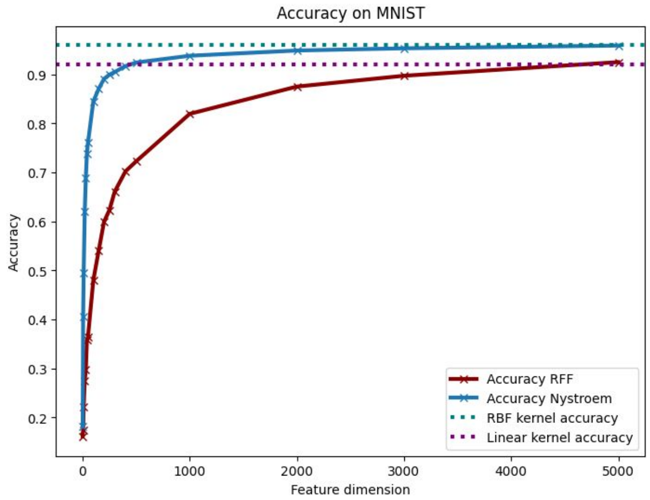
Translations-invariant means that $\forall x, y, z \in X \; k(x,y) = k(x-z, y-z)$. This means that the kernel-function does only depend on the distance between x and y.

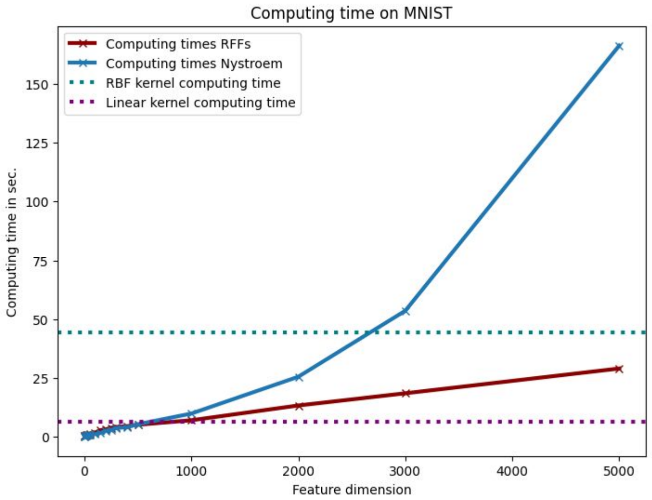
$$\langle z(x), z(y) \rangle = \frac{1}{R}\sum_r z_{w_r}(x), z_{w_r}(y)^* \tag{4.7}$$

It's also possible to show the convergence in probability of the inner product of our approximated features towards the true kernel function, if R is large enough i,e

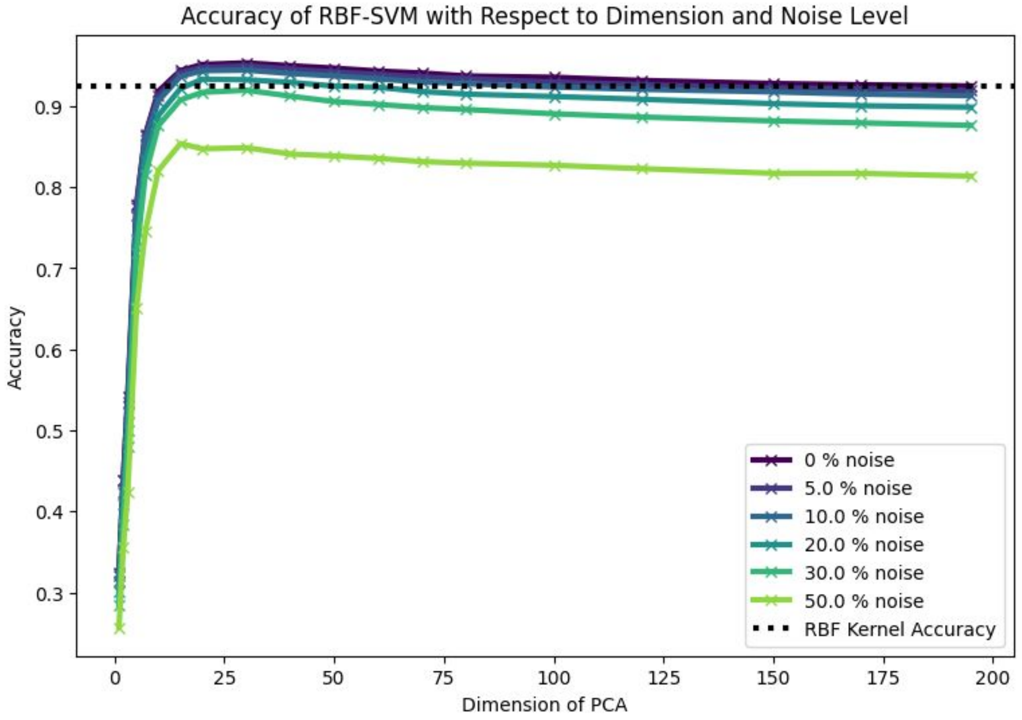
$$\mathbb{P}\left[\sup_{x,y\in X} |\langle z(x), z(y)\rangle - k(x,y)| \geq \epsilon\right] \xrightarrow{R\to\infty} 0 \tag{4.8}$$

Backup


Accuracy on MNIST
Accuracy
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
0
1000
2000
3000
4000
5000
Feature dimension
Accuracy RFF
Accuracy Nystroem
RBF kernel accuracy
Linear kernel accuracy

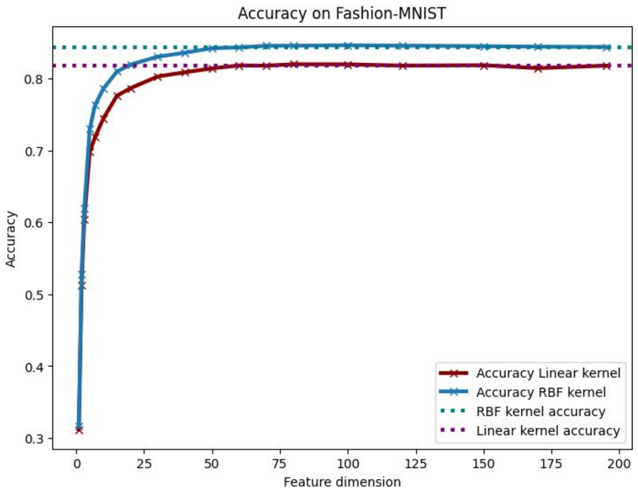

Computing time on MNIST
Computing time in sec.
0
25
50
75
100
125
150
0
1000
2000
3000
4000
5000
Feature dimension
Computing times RFFs
Computing times Nystroem
RBF kernel computing time
Linear kernel computing time

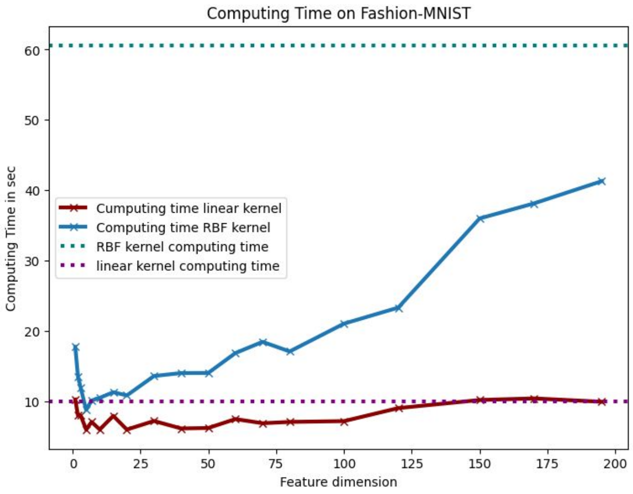
Backup



Accuracy of RBF-SVM with Respect to Dimension and Noise Level
Accuracy
0.3
0.4
0.5
0.6
0.7
0.8
0.9
0
25
50
75
100
125
150
175
200
Dimension of PCA
0 % noise
5.0 % noise
10.0 % noise
20.0 % noise
30.0 % noise
50.0 % noise
RBF Kernel Accuracy

Backup


Accuracy on Fashion-MNIST
Accuracy
Feature dimension
0.3
0.4
0.5
0.6
0.7
0.8
0
25
50
75
100
125
150
175
200
Accuracy Linear kernel
Accuracy RBF kernel
RBF kernel accuracy
Linear kernel accuracy


Computing Time on Fashion-MNIST
Computing Time in sec
Feature dimension
10
20
30
40
50
60
0
25
50
75
100
125
150
175
200
Computing time linear kernel
Computing time RBF kernel
RBF kernel computing time
linear kernel computing time