UVA CS 4774: Machine Learning

Lecture 5: Linear Regression with Basis Functions Expansion

Dr. Yanjun Qi

University of Virginia
Department of Computer Science

Today : Multivariate (non-) Linear Regression with Basis Expansion

Data: X

↓

Task: y

↓

Representation: : x, f()

↓

Score Function: L()

↓

Search/Optimization : argmin()

↓

Models, Parameters

→

X: Tabular

↓

Regression: y continuous

↓

Y = Weighted linear sum of (X basis expansion)

↓

Sum of Squared Error (Least Squared)

↓

Normal Equation / GD / SGD

↓

Metrics, Implementation, Regression coefficients w, b

$$\hat{y} = \theta_0 + \sum_{j=1}^{m} \theta_j \varphi_j(x) = \varphi(x)^T \theta$$

Linear Regression with non-linear basis functions

- LR can deal with nonlinear relationships

$$\hat{y} = \theta^T \mathbf{x} \quad \Longrightarrow \quad \hat{y} = \theta_0 + \sum_{j=1}^{m} \theta_j \varphi_j(\mathbf{x}) = \theta^T \varphi(\mathbf{x})$$

$$\vec{\theta} = [\theta_0, \theta_1, \cdots, \theta_m]^T$$

$$\vec{\phi} = [1, \phi_1(x), \cdots, \phi_m(x)]^T$$

LR with non-linear basis functions

- Free to design basis functions (e.g., non-linear features:

Here $\varphi_j(x)$ are predefined basis functions (also $\varphi_0(x)=1$)

- E.g.: polynomial regression with degree up-to two (d=2) :

$$\varphi(x) := \left[1, x, x^2\right]^T$$

linear $\vec{x} : [1, x]^T$

Polynomial basis based Regression

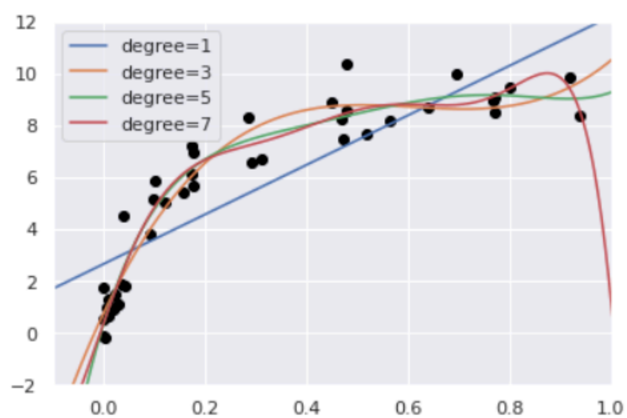
https://colab.research.google.com/github/jakevdp/PythonDataScienceHandbook/blob/master/notebooks/05.06-Linear-Regression.ipynb

My google-colab modified version: (I will cell-run it during class)
https://colab.research.google.com/drive/1gKEk0BuVORnpw_5jQ10wY1ZkA2mSXEAG?usp=sharing

```
%matplotlib inline
import matplotlib.pyplot as plt
import seaborn; seaborn.set()  # plot formatting

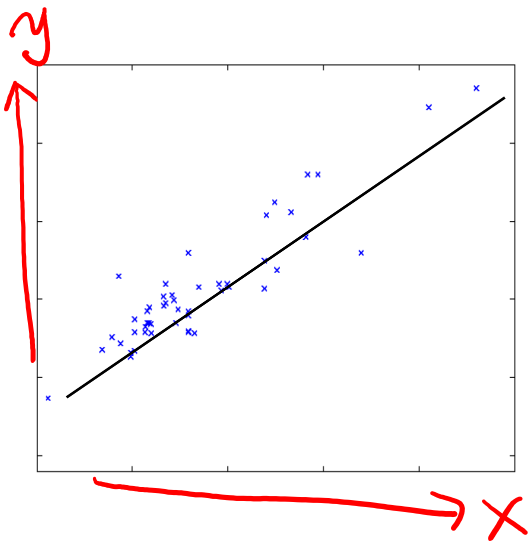
X_test = np.linspace(-0.1, 1.1, 500)[:, None]

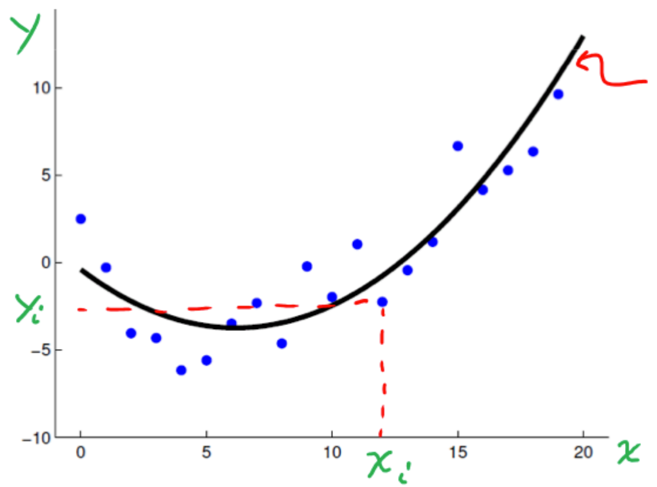
plt.scatter(X.ravel(), y, color='black')
axis = plt.axis()
for degree in [1, 3, 5, 7]:
    y_test = PolynomialRegression(degree).fit(X, y).predict(X_test)
    plt.plot(X_test.ravel(), y_test, label='degree={0}'.format(degree))
plt.xlim(-0.1, 1.0)
plt.ylim(-2, 12)
plt.legend(loc='best');
```



e.g. (1) polynomial regression

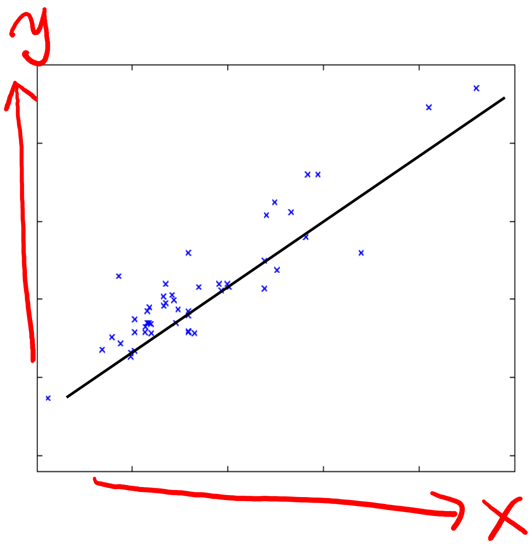
$$\hat{y} = \theta^T \mathbf{x} \quad \Rightarrow \quad \hat{y} = \theta^T \varphi(\mathbf{x})$$





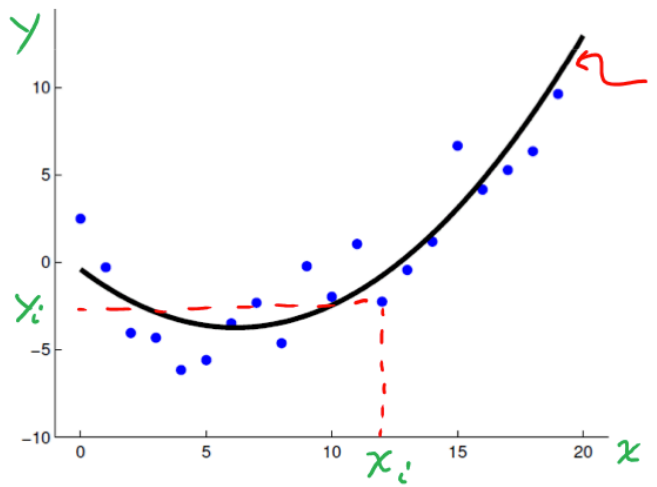
$= \theta_0 + x\theta_1 + x^2\theta_2$

$$\hat{y} = \theta^T \mathbf{x}$$



$$\theta^* = \left(X^T X\right)^{-1} X^T \vec{y}$$

$$\hat{y} = \theta^T \varphi(\mathbf{x})$$



$= \theta_0 + x\theta_1 + x^2\theta_2$

$$\theta^* = \left(\varphi^T \varphi\right)^{-1} \varphi^T \vec{y}$$

$$\varphi(x) := \left[1, x, x^2\right]^T$$

feature engineering

linear $\vec{x} : [1, x]^T$

$$\theta^* = \left(X^T X\right)^{-1} X^T \vec{y}$$

$$X_{n \times p} = \begin{bmatrix} 1 \\ 2 \\ \vdots \\ n \end{bmatrix} \quad (p+1)$$

$$\varphi(x) := \left[1, x, x^2\right]^T$$

$1 \quad 2 \quad \ldots \quad m$

$$\theta^* = \left(\varphi^T \varphi\right)^{-1} \varphi^T \vec{y}$$

$m \times n \quad n \times m \quad m \times n \quad n \times 1 \quad m \times 1$

$$\varphi(x) = \begin{bmatrix} 1 \\ 2 \\ 3 \\ \vdots \\ n \end{bmatrix}$$

$1 \quad \ldots \quad m$

$\Downarrow$

$\vec{\theta} \in R^m$

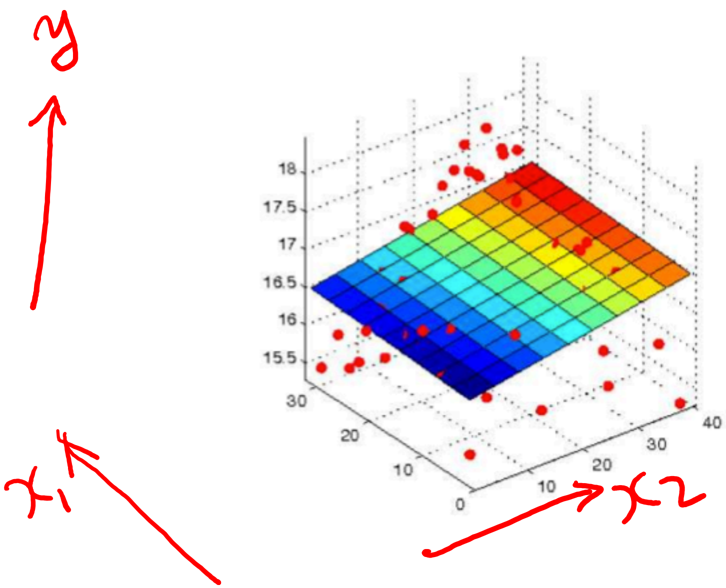
KEY: when the basis func are given, the problem of learning the parameters from data is still LR.

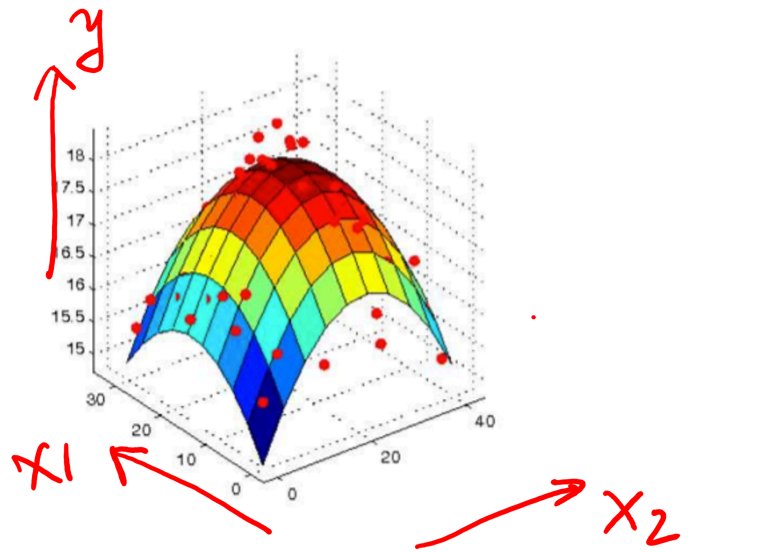
$$\hat{y} = \theta^T \mathbf{x}$$

$$\hat{y} = \theta^T \varphi(\mathbf{x})$$

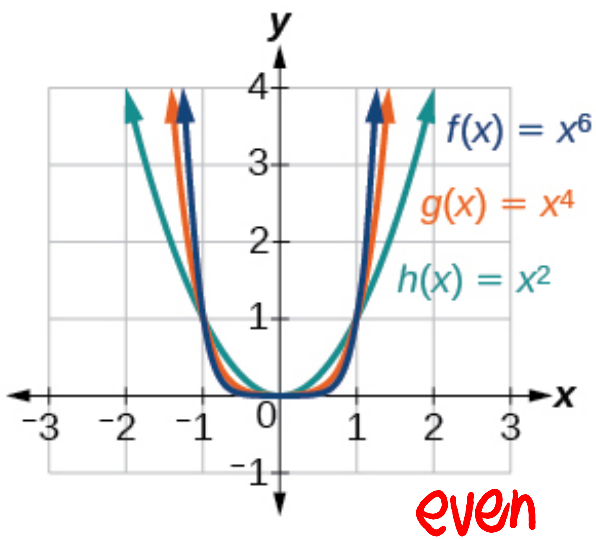
$$\boldsymbol{\phi}(\mathbf{x}) = [1, x_1, x_2]$$

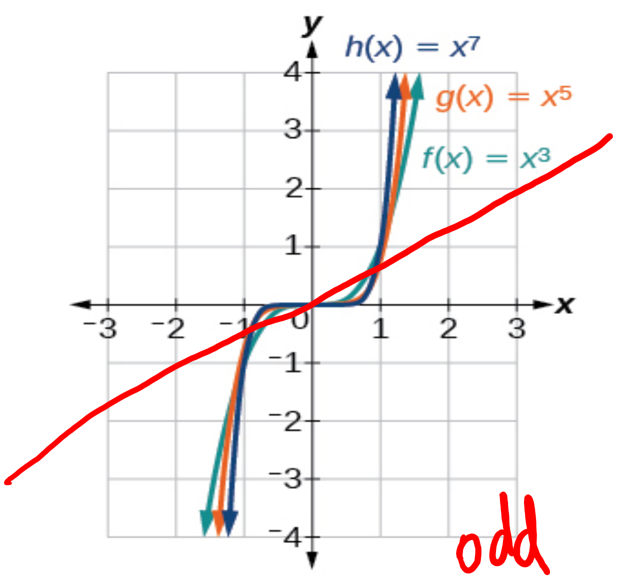
$$\boldsymbol{\phi}(\mathbf{x}) = [1, x_1, x_2, x_1^2, x_2^2]$$





$$\varphi_j(x) = x^{j-1}$$





My google-colab modified version: (I will cell-run it) https://colab.research.google.com/drive/1gKEk0BuVORnpw_5jQ10wY1ZkA2mSXEAG?usp=sharing

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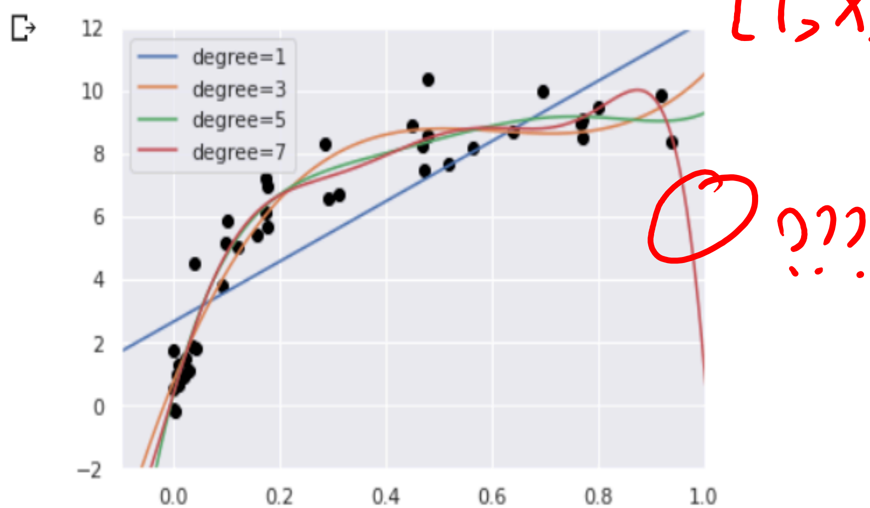
plt.xlim(-0.1, 1.0)
plt.ylim(-2, 12)
plt.legend(loc='best');
```

$[1, x, x^2, \ldots, x^7]$



UVA CS 4774: Machine Learning

Lecture 5: Linear Regression with Basis Functions Expansion

Module 2

Dr. Yanjun Qi

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$$\hat{y} = \theta^T \mathbf{x} \quad \Rightarrow \quad \hat{y} = \theta^T \varphi(\mathbf{x})$$

Many Possible Basis functions

Recap : Multivariate (non-) Linear Regression with Basis Expansion

Data: X

↓

Task: y

↓

Representation: :   x, f()

↓

Score Function: L()

↓

Search/Optimization : argmin()

↓

Models, Parameters

⇒

X: Tabular

↓

Regression: y continuous

↓

Y = Weighted linear sum of (X basis expansion)

$\hat{y} = \varphi(x)^T\theta$

↓

Sum of Squared Error (Least Squared)

↓

Normal Equation / GD / SGD

↓

Metrics, Implementation, Regression coefficients w, b

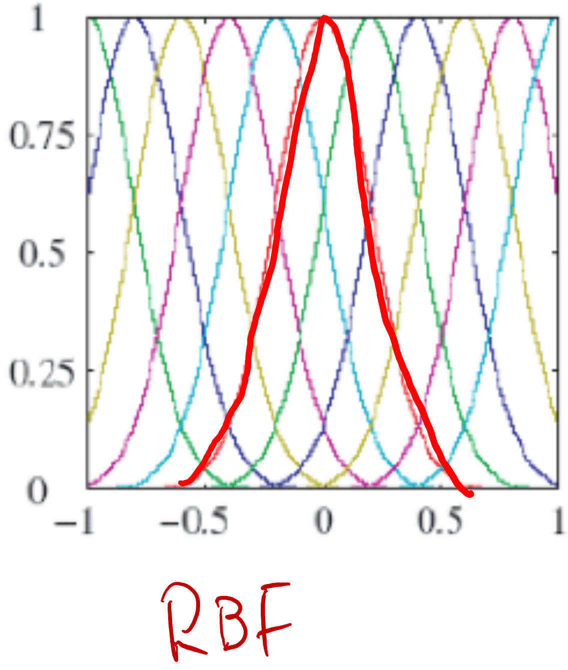
φ: Which and what type?

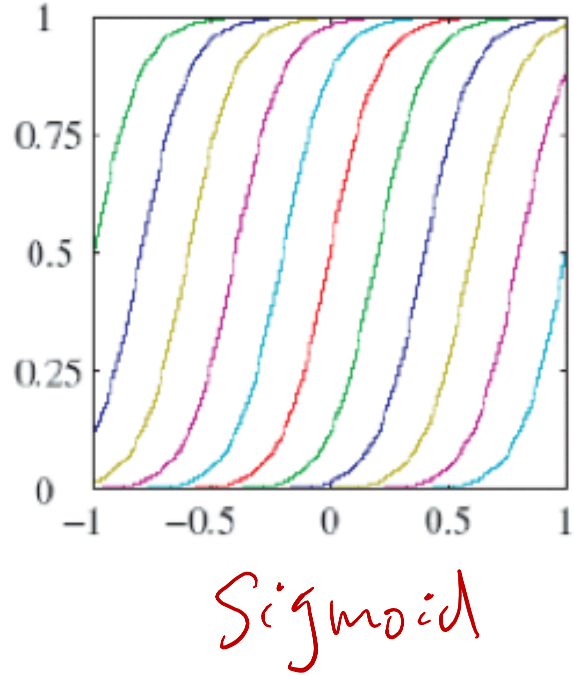
Many Possible Basis functions

- There are many basis functions, e.g.:
  - Polynomial $\varphi_j(x) = x^{j-1}$ $[1, x, x^2, x^3, \ldots, x^d]$
  - Radial basis functions $$\varphi_j(x) = \exp\left(-\frac{(x-\mu_j)^2}{2\lambda^2}\right)$$
  - Sigmoidal $$\phi_j(x) = \sigma\left(\frac{x-\mu_j}{s}\right)$$
  - Splines,
  - Fourier,
  - Wavelets, etc

$$\varphi_j(x) = \exp\left(-\frac{(x-\mu_j)^2}{2\lambda^2}\right)$$

$$\phi_j(x) = \sigma\left(\frac{x-\mu_j}{s}\right)$$





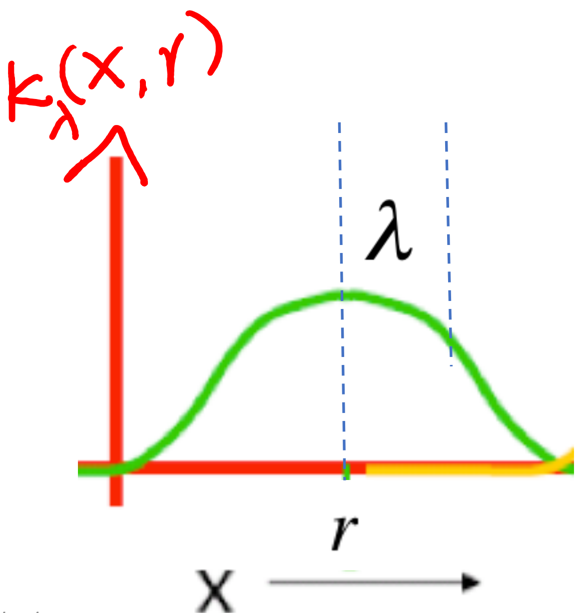
"bell"-Shaped

"S"-Shaped

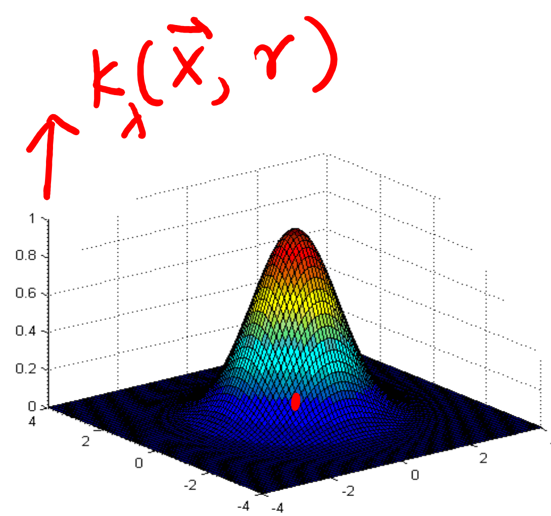
RBF = radial-basis function: a function which depends on the radial distance from a Centre point

Gaussian RBF → $$K_{\lambda}(x,r) = \exp\left(-\frac{(x-r)^2}{2\lambda^2}\right)$$

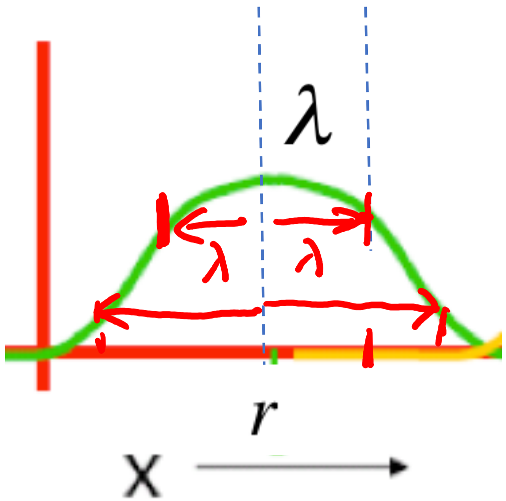
as distance from the center r increases, the output of the RBF decreases



1D case



2D case



$$K_\lambda(x,r) = \exp\left(-\frac{(x-r)^2}{2\lambda^2}\right)$$

X =	$K_\lambda(x,r) =$
r	1
$r+\lambda$	0.6065307
$r+2\lambda$	0.1353353
$r+3\lambda$	0.0001234098 ~0

θ

$x > r+3\lambda$

$x < r-3\lambda$

LR with radial-basis functions

- E.g.: LR with RBF regression:

$$\hat{y} = \theta_0 + \sum_{j=1}^{m} \theta_j \varphi_j(x) = \varphi(x)^T \theta$$

$$\varphi_j(x) := K_{\lambda_j}(x, r_j) = \exp\left(-\frac{(x - \mu_j)^2}{2\lambda_j^2}\right)$$

r_j, λ_j

hyperparameters of RBF basis functions
(the predefined Centers and Width)

LR with radial-basis functions

- E.g.: LR with RBF regression:

$$\hat{y} = \theta_0 + \sum_{j=1}^{m} \theta_j \varphi_j(x) = \varphi(x)^T \theta$$

$$\varphi_j(x) := K_{\lambda_j}(x, r_j) = \exp\left(-\frac{(x-\mu_j)^2}{2\lambda_j^2}\right)$$

$\varphi(x)$: E.g. with four predefined RBF kernels

$$= \left[1, K_{\lambda_1}(x, r_1), K_{\lambda 2}(x, r_2), K_{\lambda_3}(x, r_3), K_{\lambda_4}(x, r_4)\right]^T$$

e.g. (2) LR with radial-basis functions

- E.g.: LR with RBF regression:

$$\hat{y} = \theta_0 + \sum_{j=1}^{m} \theta_j \varphi_j(x) = \varphi(x)^T \theta$$

$$\varphi(x) := \left[1, K_{\lambda_1}(x, r_1), K_{\lambda 2}(x, r_2), K_{\lambda_3}(x, r_3), K_{\lambda 4}(x, r_4)\right]^T$$

bias weights

$$\vec{\theta} = [\theta_0, \theta_1, \theta_2, \theta_3, \theta_4]^T$$

r_1, λ_1; r_2, λ_2; λ_3, r_3; r_4, λ_4 } hyper para

$$\theta^* = \left(\varphi^T \varphi\right)^{-1} \varphi^T \vec{y}$$

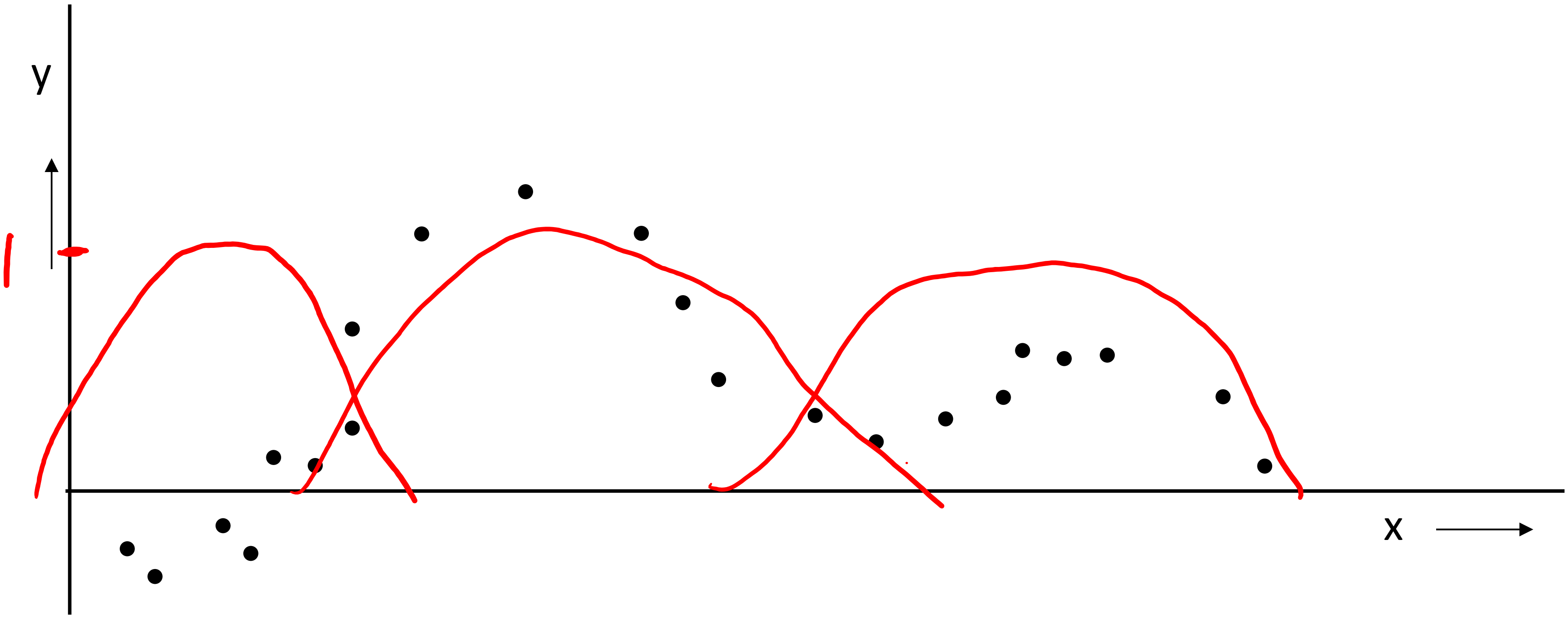
Users need to define the hyperparameters of RBF basis functions (the predefined Centers and Width)

$\varphi(x)$: E.g. with four predefined RBF kernels

$$= \left[1, K_{\lambda_1}(x, r_1), K_{\lambda 2}(x, r_2), K_{\lambda_3}(x, r_3), K_{\lambda_4}(x, r_4)\right]^T$$

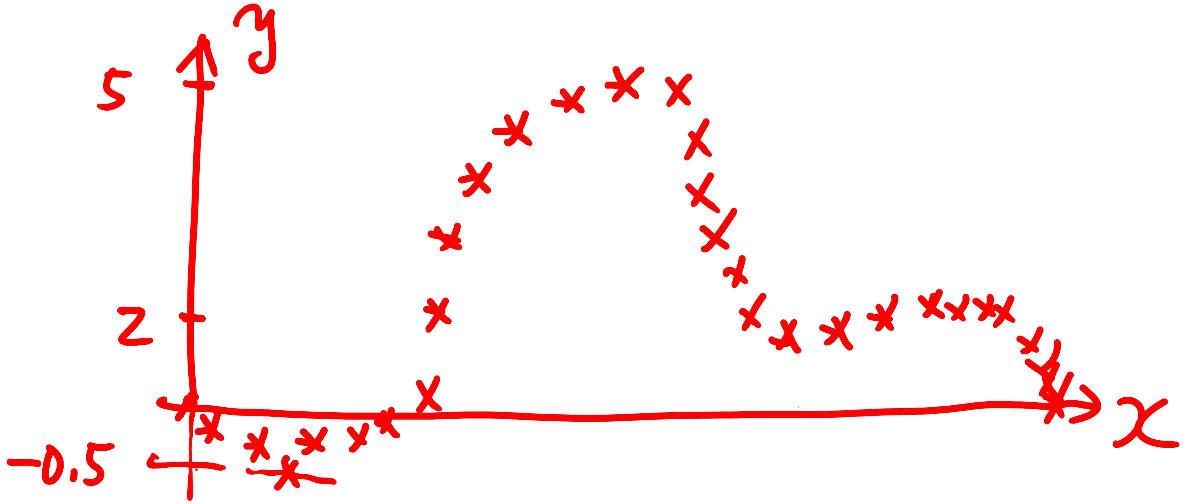
$$\theta^* = \left(\varphi^T \varphi\right)^{-1} \varphi^T \vec{y}$$

For example: I want to using 3 RBF basis functions to fit the following data points
(I need to assume 3 predefined centres and width)



Given Training Data's scatter plot:

$(x_i, y_i) \quad i = 1, \dots, n$



After my 3 RBF fit:

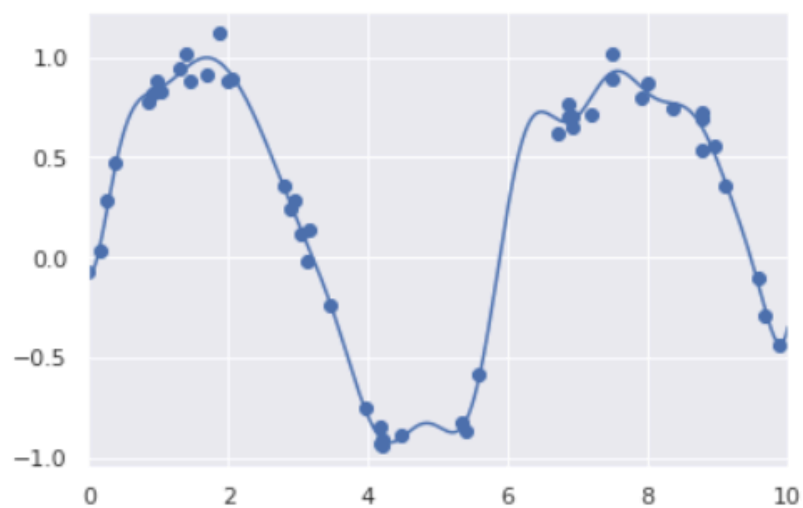
$$f(x) = \theta_0 - 0.5\, K_{\lambda_1}(x, r_1) + 5\, K_{\lambda_2}(x, r_2) + 2\, K_{\lambda_3}(x, r_3)$$

https://colab.research.google.com/drive/1BVcHUBYDO4AlwldcKmpmj5blAbf7lSJb?usp=sharing

Modified from:
https://jakevdp.github.io/PythonDataScienceHandbook/05.06-linear-regression.html

```
gauss_model = make_pipeline(GaussianFeatures(20),
                            LinearRegression())
gauss_model.fit(x[:, np.newaxis], y)
yfit = gauss_model.predict(xfit[:, np.newaxis])

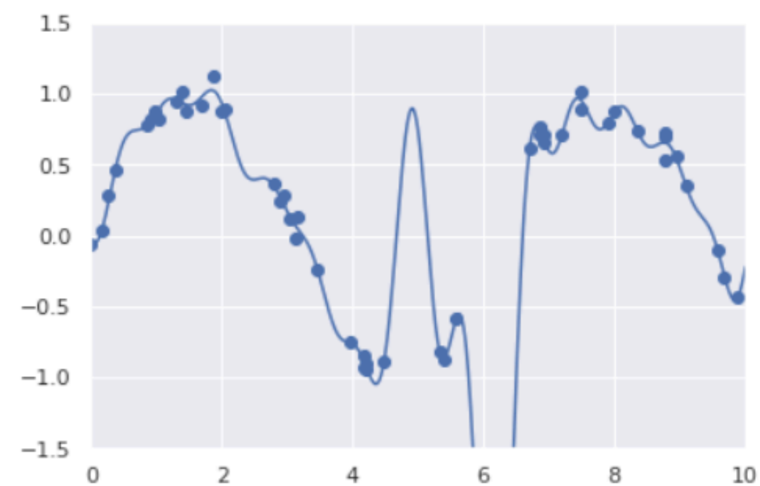
plt.scatter(x, y)
plt.plot(xfit, yfit)
plt.xlim(0, 10);
```



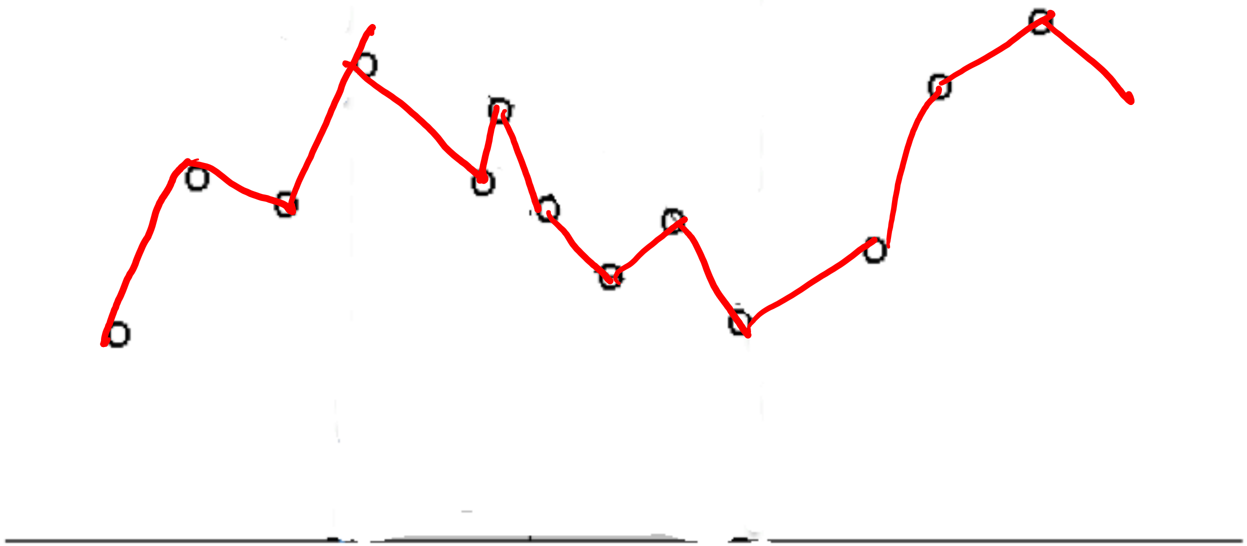

```
model = make_pipeline(GaussianFeatures(30),
                      LinearRegression())
model.fit(x[:, np.newaxis], y)

plt.scatter(x, y)
plt.plot(xfit, model.predict(xfit[:, np.newaxis]))

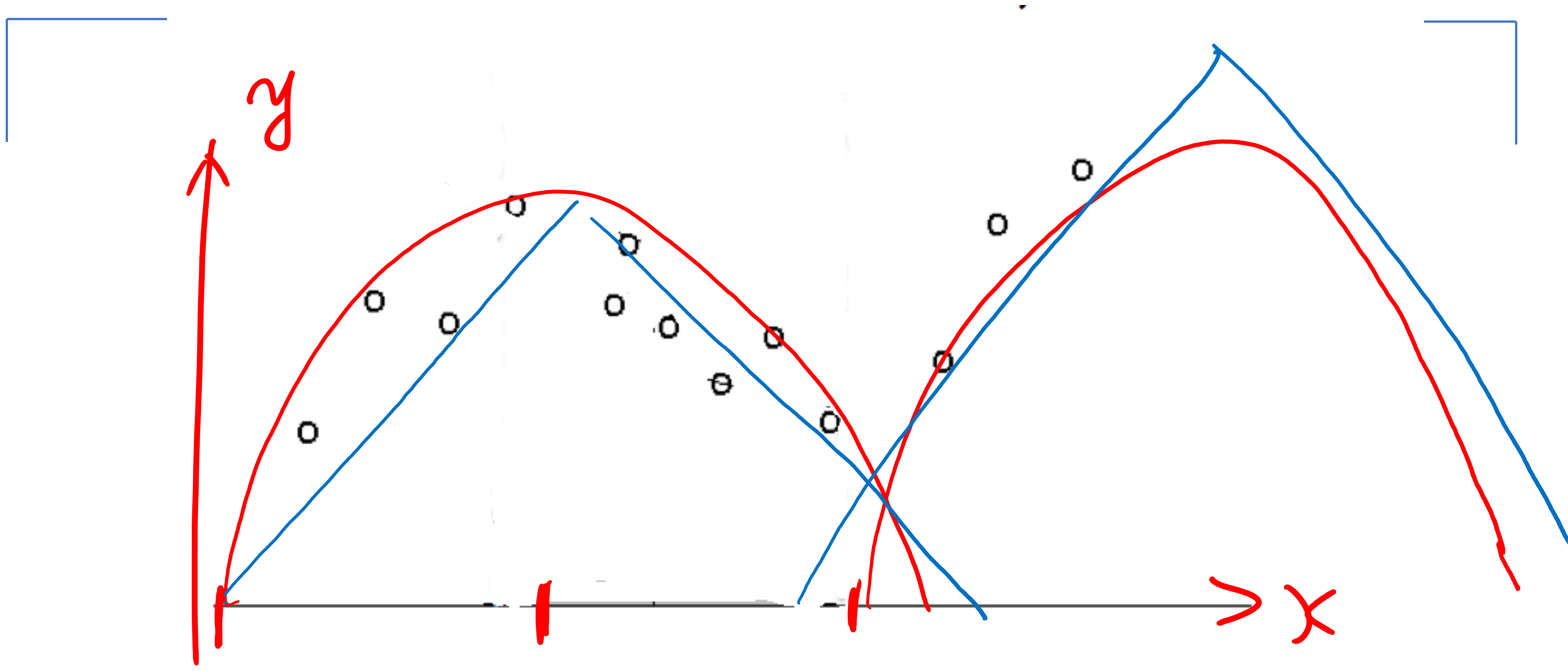
plt.xlim(0, 10)
plt.ylim(-1.5, 1.5);
```



Extra: even more possible Basis Function: RBF, or Piecewise Linear based?



e.g. Even more possible Basis Func?



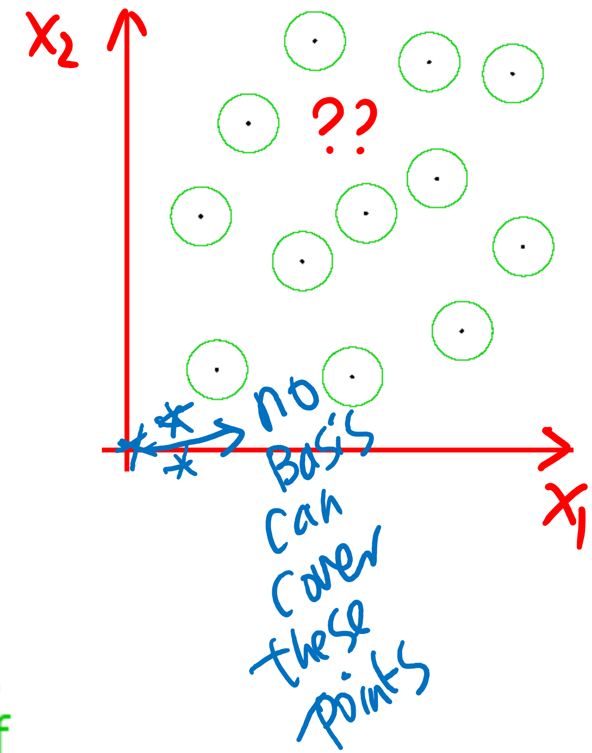
Thank You

Extra

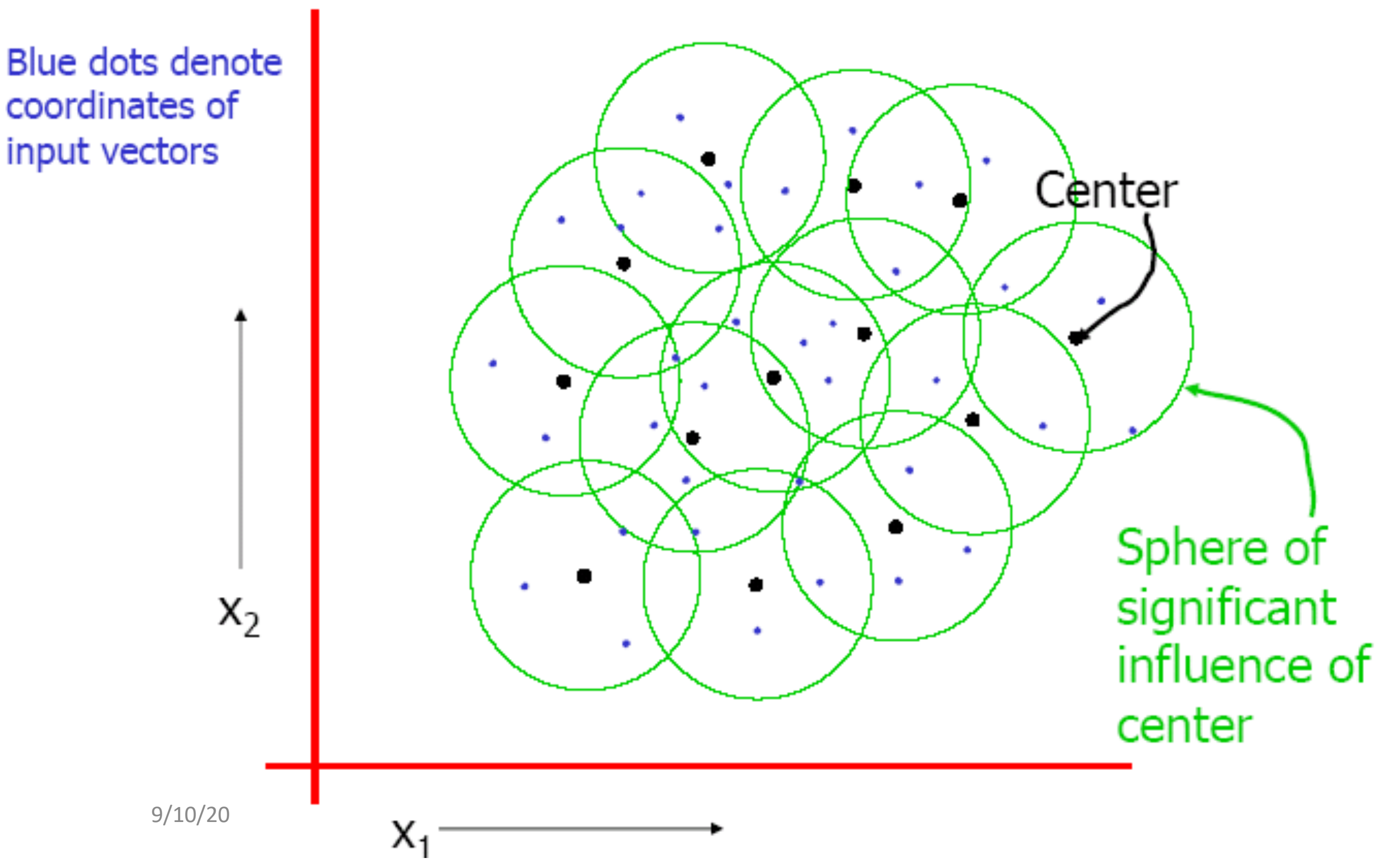
Extra: e.g. 2D Good and Bad RBF Basis

Contour view

- A Bad set of predefined 2D RBFs



- A good set of 2D predefined RBF basis



Extra: Nonparametric Regression Models

- K-Nearest Neighbor (KNN) and Locally weighted linear regression are **non-parametric** algorithms.

- The (unweighted) linear regression algorithm that we saw earlier is known as a **parametric** learning algorithm
  - because it has a fixed, finite number of parameters which are fit to the data;
  - Once we've fit the *theta* and stored them away, we no longer need to keep the training data around to make future predictions.
  - In contrast, to make predictions using KNN or locally weighted linear regression, we need to keep the entire training set around.

- The term "non-parametric" (roughly) refers to the fact that the amount of knowledge we need to keep, in order to represent the hypothesis grows with linearly the size of the training set.