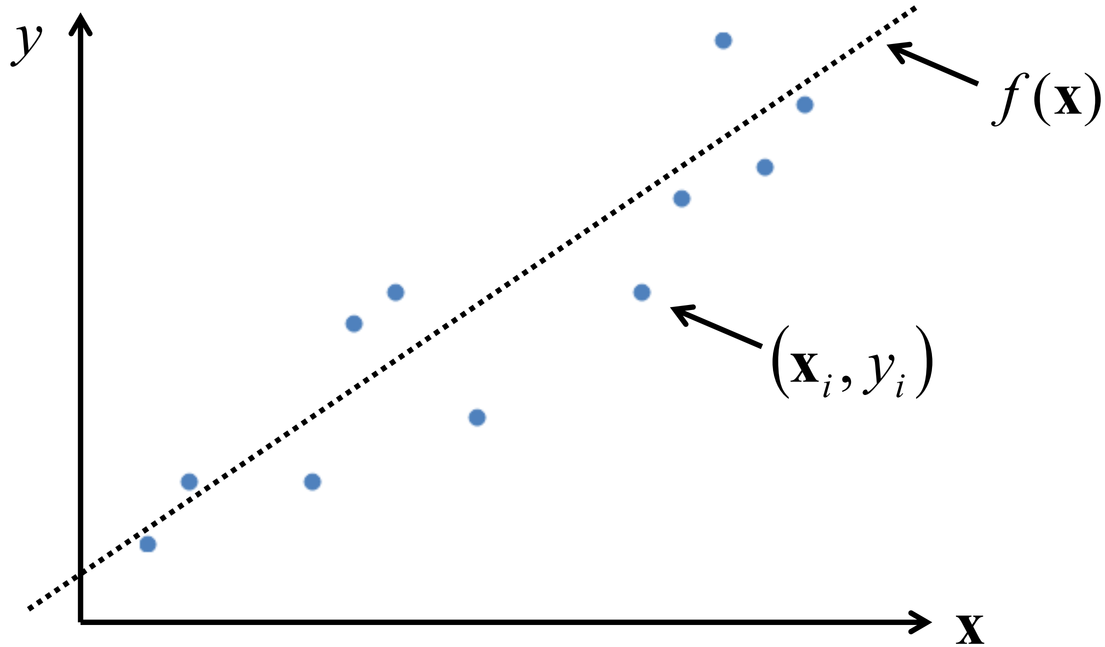
Linear Regression &
Additive Linear Model

Introduction

- **Find the line which best fits the data**
  - We want to find a line which generalizes the given data

$(x_{11}, x_{12}, \ldots, x_{1d}, y_1)$
$(x_{21}, x_{22}, \ldots, x_{2d}, y_2)$
…
$(x_{i1}, x_{i2}, \ldots, x_{id}, y_i)$
…
$(x_{n1}, x_{n2}, \ldots, x_{nd}, y_n)$



$$f(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_d x_d = w_0 + \sum_{j=1}^{d} w_j x_j$$

Introduction

- **We have *n* sample data**

$$D = \{D_1, D_2, \cdots, D_n\} \text{ where } D_i = (\mathbf{x}_i, y_i)$$

$\mathbf{x}_i = (x_{i1}, x_{i2}, \cdots, x_{id})$ is an input in d dimensional space

y_i is the output for $\mathbf{x}_i$

Find $\mathbf{w} = (w_0, w_1, \cdots, w_d)$ which minimizes $E(\mathbf{w})$

$$E(\mathbf{w}) = \sum_{i=1}^{n} (f(\mathbf{x_i}) - y_i)^2$$

$$f(\mathbf{x}_i) = w_0 + w_1 x_{i1} + w_2 x_{i2} + \cdots + w_d x_{id} = w_0 + \sum_{j=1}^{d} w_j x_{ij}$$

Introduction

- **In Other Words**
  - So, our problem can be stated as follows:

$$\text{Find } \mathbf{w} = (w_0, w_1, \cdots, w_d) \text{ which minimizes } E(\mathbf{w}) \text{ where}$$

$$E(\mathbf{w}) = \sum_{i=1}^{n} \left(f(\mathbf{x}_i) - y_i \right)^2$$

$$f(\mathbf{x}_i) = w_0 + w_1 x_{i1} + w_2 x_{i2} + \cdots + w_d x_{id} = w_0 + \sum_{j=1}^{d} w_j x_{ij}$$

$$D = \{D_1, D_2, \cdots, D_n\} \text{ where } D_i = (\mathbf{x}_i, y_i)$$

$$\mathbf{x}_i = (x_{i1}, x_{i2}, \cdots, x_{id}) \text{ is an input in } d \text{ dimensional space}$$

$$y_i \text{ is the output for } \mathbf{x}_i$$

Introduction

- **In Other Words**
  - So, our problem can be stated as follows:

$$\text{Find } \mathbf{w} = (w_0, w_1, \cdots, w_d) \text{ which minimizes } E(\mathbf{w}) \text{ where}$$

$$E(\mathbf{w}) = \sum_{i=1}^{n} \left(f(\mathbf{x}_i) - y_i \right)^2$$

$$f(\mathbf{x}_i) = w_0 x_{i0} + w_1 x_{i1} + w_2 x_{i2} + \cdots + w_d x_{id} = \sum_{j=0}^{d} w_i x_{ij}$$

$$D = \{D_1, D_2, \cdots, D_n\} \text{ where } D_i = (\mathbf{x}_i, y_i)$$

$$\mathbf{x}_i = (x_{i0}, x_{i1}, x_{i2}, \cdots, x_{id}) \text{ where } x_{i0} = 1 \text{ for } i = 1, \cdots, d$$

Introduction

- **How to solve this?**

Find $\mathbf{w} = (w_0, w_1, \cdots, w_d)$ which minimizes $E(\mathbf{w})$ where

$$E(\mathbf{w}) = \sum_{i=1}^{n} \left(f(\mathbf{x}_i) - y_i \right)^2$$

$$f(\mathbf{x}_i) = w_0 x_{i0} + w_1 x_{i1} + w_2 x_{i2} + \cdots + w_d x_{id} = \sum_{j=0}^{d} w_i x_{ij}$$

$$D = \{D_1, D_2, \cdots, D_n\} \text{ where } D_i = (\mathbf{x}_i, y_i)$$

$$\mathbf{x}_i = (x_{i0}, x_{i1}, x_{i2}, \cdots, x_{id}) \text{ where } x_{i0} = 1 \text{ for } i = 1, \cdots, d$$

x and y are given values
E is a quadratic function of w's

- There are various ways to solve
- Here, the SIMPLEST one will be presented

Solution

- **Quadratic Function Optimization**
  - At the point which minimizes $E(\mathbf{w}) = \sum_{i=1}^{n} \left(f(\mathbf{x}_i) - y_i\right)^2$

$$\frac{\partial}{\partial w_j} E(w_0, w_1, \cdots, w_d) = 0 \ \text{ for } j = 0, \cdots, d$$

  - That is

$$\frac{\partial}{\partial w_j} E(\mathbf{w}) = \sum_{\mathrm{i}=1}^{\mathrm{n}} \left(\frac{\partial}{\partial w_j} \left(f(\mathbf{x}_i) - y_i\right)^2 \right) = \sum_{i=1}^{n} 2x_{ij} \left(f(\mathbf{x}_\mathbf{i}) - y_i\right) = 0 \quad j \geq 0$$

$$f(\mathbf{x}_i) = w_0 x_{i0} + w_1 x_{i1} + w_2 x_{i2} + \cdots + w_d x_{id} = \sum_{j=0}^{d} w_i x_{ij}$$

Solution

- **Quadratic Function Optimization**

$$E(\mathbf{w}) = \sum_{i=1}^{n} \left(f(\mathbf{x}_i) - y_i \right)^2$$

$$\left.\begin{aligned}
\frac{\partial}{\partial w_0} E(\mathbf{w}) &= \sum_{i=1}^{n} x_{i0} \left(f(\mathbf{x_i}) - y_i \right) = 0 \\
\frac{\partial}{\partial w_1} E(\mathbf{w}) &= \sum_{i=1}^{n} x_{i1} \left(f(\mathbf{x_i}) - y_i \right) = 0 \\
\frac{\partial}{\partial w_d} E(\mathbf{w}) &= \sum_{i=1}^{n} x_{id} \left(f(\mathbf{x_i}) - y_i \right) = 0
\end{aligned}\right\}$$

There are *d* variables *d* equations.
If we solve the equation system,
we can obtain

$$\mathbf{w} = \left(w_0, w_1, \cdots, w_d \right)$$

$$f(\mathbf{x}_i) = w_0 x_{i0} + w_1 x_{i1} + w_2 x_{i2} + \cdots + w_d x_{id} = \sum_{j=0}^{d} w_i x_{ij}$$

Solution

- **Quadratic Function Optimization**

$$\sum_{i=1}^{n} x_{i0}(f(\mathbf{x_i}) - y_i) = 0 \quad \longrightarrow \quad \sum_{i=1}^{n} x_{i0}(w_0 x_{i0} + w_1 x_{i1} + \cdots + w_d x_{id} - y_i) = 0$$

$$\sum_{i=1}^{n} x_{i1}(f(\mathbf{x_i}) - y_i) = 0 \quad \longrightarrow \quad \sum_{i=1}^{n} x_{i1}(w_0 x_{i0} + w_1 x_{i1} + \cdots + w_d x_{id} - y_i) = 0$$

$$\cdots \qquad\qquad \cdots$$

$$\sum_{i=1}^{n} x_{id}(f(\mathbf{x_i}) - y_i) = 0 \quad \longrightarrow \quad \sum_{i=1}^{n} x_{id}(w_0 x_{i0} + w_1 x_{i1} + \cdots + w_d x_{id} - y_i) = 0$$

$$\Rightarrow$$

$$w_0 \sum_{i=1}^{n} x_{i0}x_{i0} + w_1 \sum_{i=1}^{n} x_{i0}x_{i1} + w_2 \sum_{i=1}^{n} x_{i0}x_{i2} + \cdots + w_d \sum_{i=1}^{n} x_{i0}x_{id} = \sum_{i=1}^{n} x_{i0}y_i$$

$$w_0 \sum_{i=1}^{n} x_{i1}x_{i0} + w_1 \sum_{i=1}^{n} x_{i1}x_{i1} + w_2 \sum_{i=1}^{n} x_{i1}x_{i2} + \cdots + w_d \sum_{i=1}^{n} x_{i1}x_{id} = \sum_{i=1}^{n} x_{i1}y_i$$

$$\cdots$$

$$w_0 \sum_{i=1}^{n} x_{id}x_{i0} + w_1 \sum_{i=1}^{n} x_{id}x_{i1} + w_d \sum_{i=1}^{n} x_{id}x_{i2} + \cdots + w_d \sum_{i=1}^{n} x_{id}x_{id} = \sum_{i=1}^{n} x_{id}y_i$$

Solution

- **Quadratic Function Optimization**

$$\mathbf{A}\mathbf{w} = \mathbf{b}$$

$$\mathbf{A} = \begin{pmatrix} \sum_{i=1}^{n} x_{i0}x_{i0}, \sum_{i=1}^{n} x_{i0}x_{i1}, \cdots, \sum_{i=1}^{n} x_{i0}x_{id} \\ \sum_{i=1}^{n} x_{i1}x_{i0}, \sum_{i=1}^{n} x_{i1}x_{i1}, \cdots, \sum_{i=1}^{n} x_{i1}x_{id} \\ \cdots \\ \sum_{i=1}^{n} x_{id}x_{i0}, \sum_{i=1}^{n} x_{id}x_{i1}, \cdots, \sum_{i=1}^{n} x_{id}x_{id} \end{pmatrix} \qquad \mathbf{w} = \begin{pmatrix} w_0 \\ w_1 \\ \cdots \\ w_d \end{pmatrix} \qquad \mathbf{b} = \begin{pmatrix} \sum_{i=1}^{n} x_{i0}y_i \\ \sum_{i=1}^{n} x_{i1}y_i \\ \cdots \\ \sum_{i=1}^{n} x_{id}y_i \end{pmatrix}$$

Solution

- **Quadratic Function Optimization**
  - Using given data, let's define **X** and **Y**

$$(x_{11}, x_{12}, \dots, x_{1d}, y_1)$$
$$(x_{21}, x_{22}, \dots, x_{2d}, y_2)$$
$$\dots$$
$$(x_{n1}, x_{n2}, \dots, x_{nd}, y_n)$$

$$\mathbf{X} = \begin{pmatrix} x_{10}, x_{11}, x_{12}, \cdots, x_{1d} \\ x_{20}, x_{21}, x_{22}, \cdots, x_{2d} \\ \cdots \\ x_{n0}, x_{n1}, x_{n2}, \cdots, x_{nd} \end{pmatrix} \qquad \mathbf{Y} = \begin{pmatrix} y_1 \\ y_2 \\ \cdots \\ y_n \end{pmatrix}$$

  - Then,

$$\mathbf{A} = \begin{pmatrix} \sum_{i=1}^{n} x_{i0}x_{i0}, \sum_{i=1}^{n} x_{i0}x_{i1}, \cdots, \sum_{i=1}^{n} x_{i0}x_{id} \\ \sum_{i=1}^{n} x_{i1}x_{i0}, \sum_{i=1}^{n} x_{i1}x_{i1}, \cdots, \sum_{i=1}^{n} x_{i1}x_{id} \\ \cdots \\ \sum_{i=1}^{n} x_{id}x_{i0}, \sum_{i=1}^{n} x_{id}x_{i1}, \cdots, \sum_{i=1}^{n} x_{id}x_{id} \end{pmatrix} = \mathbf{X}^T\mathbf{X} \qquad \mathbf{b} = \begin{pmatrix} \sum_{i=1}^{n} x_{i0}y_i \\ \sum_{i=1}^{n} x_{i1}y_i \\ \cdots \\ \sum_{i=1}^{n} x_{id}y_i \end{pmatrix} = \mathbf{X}^T\mathbf{Y}$$

Solution

- **Quadratic Function Optimization**

$$\mathbf{w} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\left(\mathbf{X}^T\mathbf{Y}\right)$$

$$f(\mathbf{x}_i) = w_0 x_{i0} + w_1 x_{i1} + w_2 x_{i2} + \cdots + w_d x_{id} = \sum_{j=0}^{d} w_i x_{ij}$$

$$(x_{11}, x_{12}, \dots, x_{1d}, y_1)$$
$$(x_{21}, x_{22}, \dots, x_{2d}, y_2)$$
$$\dots$$
$$(x_{n1}, x_{n2}, \dots, x_{nd}, y_n)$$

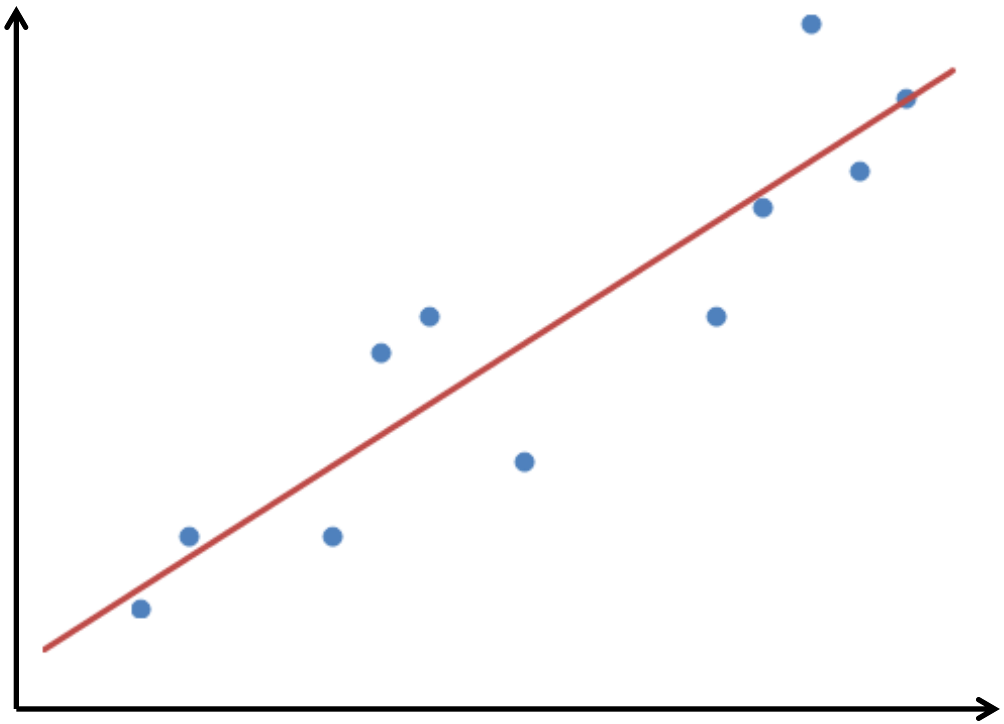
$$\mathbf{X} = \begin{pmatrix} 1, x_{11}, x_{12}, \cdots, x_{1d} \\ 1, x_{21}, x_{22}, \cdots, x_{2d} \\ \cdots \\ 1, x_{n1}, x_{n2}, \cdots, x_{nd} \end{pmatrix} \qquad \mathbf{Y} = \begin{pmatrix} y_1 \\ y_2 \\ \cdots \\ y_n \end{pmatrix}$$

Solution

- **Example**

(2, 2)
(3, 4)
(6, 4)
(7, 9)
(8, 10)
(10, 6)
(14, 10)
(15, 13)
(16, 18)
(17, 14)
(18, 16)

Y=0.840708+0.834071x



Solution

- **Example**

(2, 2)
(3, 4)
(6, 4)
(7, 9)
(8, 10)
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(18, 16)

$$\mathbf{X} = \begin{pmatrix} 1,2 \\ 1,3 \\ 1,6 \\ 1,7 \\ 1,8 \\ 1,10 \\ 1,14 \\ 1,15 \\ 1,16 \\ 1,17 \\ 1,18 \end{pmatrix} \quad \mathbf{Y} = \begin{pmatrix} 2 \\ 4 \\ 4 \\ 9 \\ 10 \\ 6 \\ 10 \\ 13 \\ 18 \\ 14 \\ 16 \end{pmatrix}$$

$$\mathbf{A} = \mathbf{X}^T\mathbf{X} = \begin{pmatrix} 11, 116 \\ 116, 1552 \end{pmatrix}$$

$$\mathbf{b} = \mathbf{X}^T\mathbf{Y} = \begin{pmatrix} 106 \\ 1392 \end{pmatrix}$$

$$\mathbf{w} = (A)^{-1}(b) = \begin{pmatrix} 0.840708 \\ 0.834071 \end{pmatrix}$$

Additive Linear Model

- **Generalized Version of Linear Regression**
  - Linear Regression

$$f(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_d x_d = w_0 + \sum_{j=1}^{d} w_j x_j$$

    - Find *w*'s so that *f(x)* best fits given data

  - Generalized Linear Regression
    - Instead of single variables, let's use pre-determined functions of **x**, *h(x)*'s

$$f(\mathbf{x}) = w_0 + w_1 h_1(\mathbf{x}) + w_2 h_2(\mathbf{x}) + \cdots + w_d h_d(\mathbf{x}) = w_0 + \sum_{j=1}^{d} w_j h_j(\mathbf{x})$$

    - Find *w*'s so that *f(x)* best fits given data

For example, $f(x) = w_0 + w_1 \sin(\pi x) + w_2 e^x$

Additive Linear Model

- **Example**
  - Find the 3rd order Polynomial which best fits the data

(2, 2)
(3, 4)
(6, 4)
(7, 9)
(8, 10)
(10, 6)
(14, 10)
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(16, 18)
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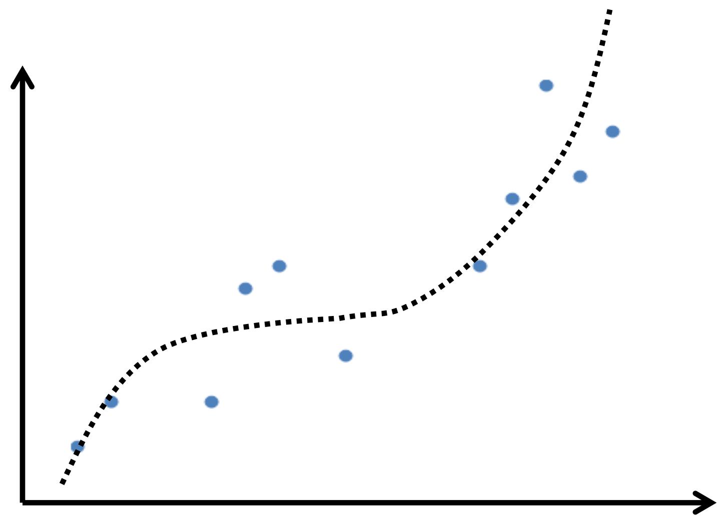
(18, 16)



Use this model $f(x) = w_0 + w_1 h_1(x) + w_2 h_2(x) + w_3 h_3(x)$

where, $h_1(x) = x,\ h_2(x) = x^2,\ h_3(x) = x^3$

Additive Linear Model

- **Example**
  - You think that the given data are periodic

(2, 2)
(3, 4)
(6, 4)
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(10, 6)
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(17, 14)
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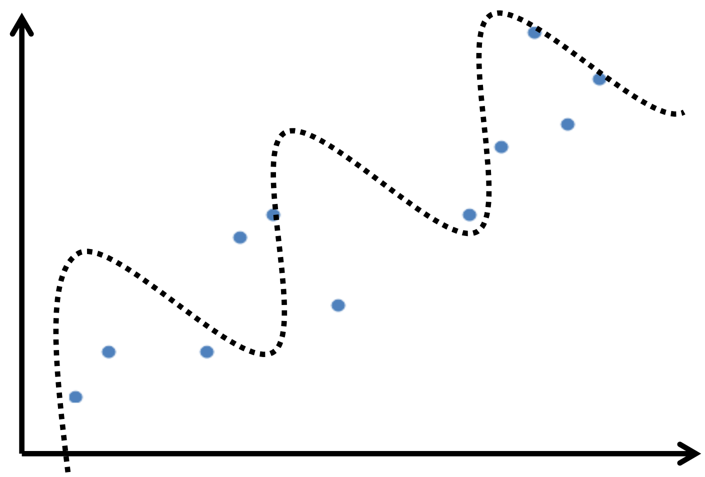

You may use $f(x) = w_0 + w_1 h_1(x) + w_2 h_2(x)$

where, $h_1(x) = x$, $h_2(x) = \sin(ax)$

Additive Linear Model

- **How to solve this???**

Find $\mathbf{w} = \left(w_0, w_1, \cdots, w_k\right)$ which minimizes $E\left(\mathbf{w}\right)$ where

$$E\left(\mathbf{w}\right) = \sum_{i=1}^{n} \left(f\left(\mathbf{x}_i\right) - y_i\right)^2$$

$$f\left(\mathbf{x}_i\right) = w_0 h_0\left(\mathbf{x}_i\right) + w_1 h_1\left(\mathbf{x}_i\right) + \cdots + w_k h_k\left(\mathbf{x}_i\right) \quad \text{where } h_0\left(\mathbf{x}_i\right) = 1$$

$$D = \left\{D_1, D_2, \cdots, D_n\right\}$$

$$D_i = \left(\mathbf{x}_i, y_i\right)$$

$$\mathbf{x}_i = \left(x_{i1}, x_{i2}, \cdots, x_{id}\right)$$

Additive Linear Model

- **How to solve this**
  - Solution

$$\mathbf{w} = \left(\mathbf{H}^T\mathbf{H}\right)^{-1}\left(\mathbf{H}^T\mathbf{Y}\right)$$

  - Where

$$\mathbf{H} = \begin{pmatrix} h_0(\mathbf{x}_1), h_1(\mathbf{x}_1), \cdots, h_k(\mathbf{x}_1) \\ h_0(\mathbf{x}_2), h_1(\mathbf{x}_2), \cdots, h_k(\mathbf{x}_2) \\ \cdots \\ h_0(\mathbf{x}_n), h_1(\mathbf{x}_n), \cdots, h_k(\mathbf{x}_n) \end{pmatrix} \qquad \mathbf{Y} = \begin{pmatrix} y_1 \\ y_2 \\ \cdots \\ y_n \end{pmatrix}$$

Additive Linear Model

- **Example**
  - Find the 3rd order Polynomial which best fits the data

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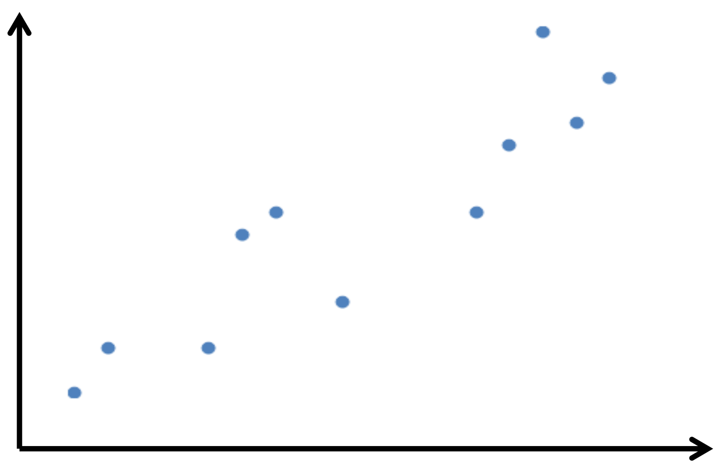
$$f(x) = w_0 + w_1 h_1(x) + w_2 h_2(x) + w_3 h_3(x)$$
$$\text{where, } h_1(x) = x,\ h_2(x) = x^2,\ \ h_3(x) = x^3$$



Additive Linear Model

- **Example**

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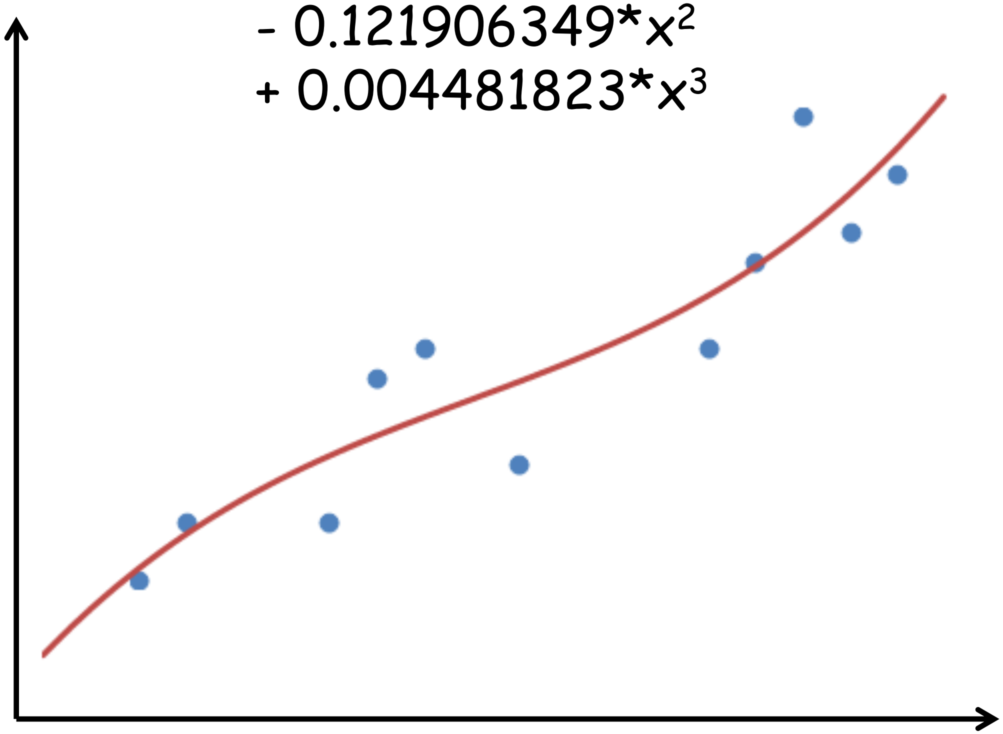
(17, 14)
(18, 16)

$$f(x) = -0.63143704 + 1.713506327*x - 0.121906349*x^2 + 0.004481823*x^3$$



Additive Linear Model

- **Example**
  - You think that the given data are periodic

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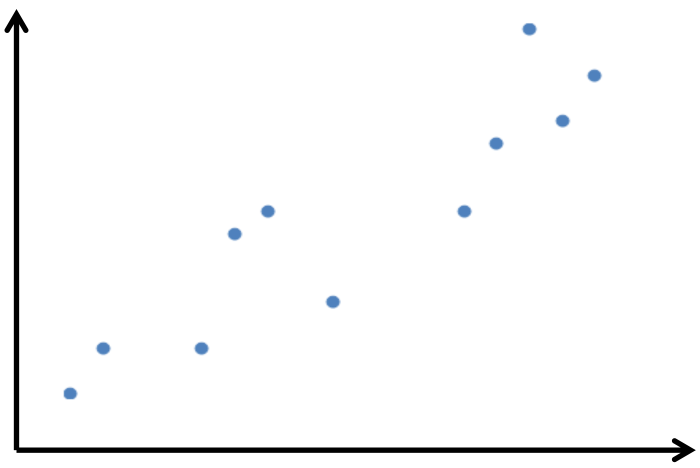
$$f(x) = w_0 + w_1 h_1(x) + w_2 h_2(x)$$
$$\text{where, } h_1(x) = x, h_2(x) = \sin(ax)$$



Additive Linear Model

- **Example**

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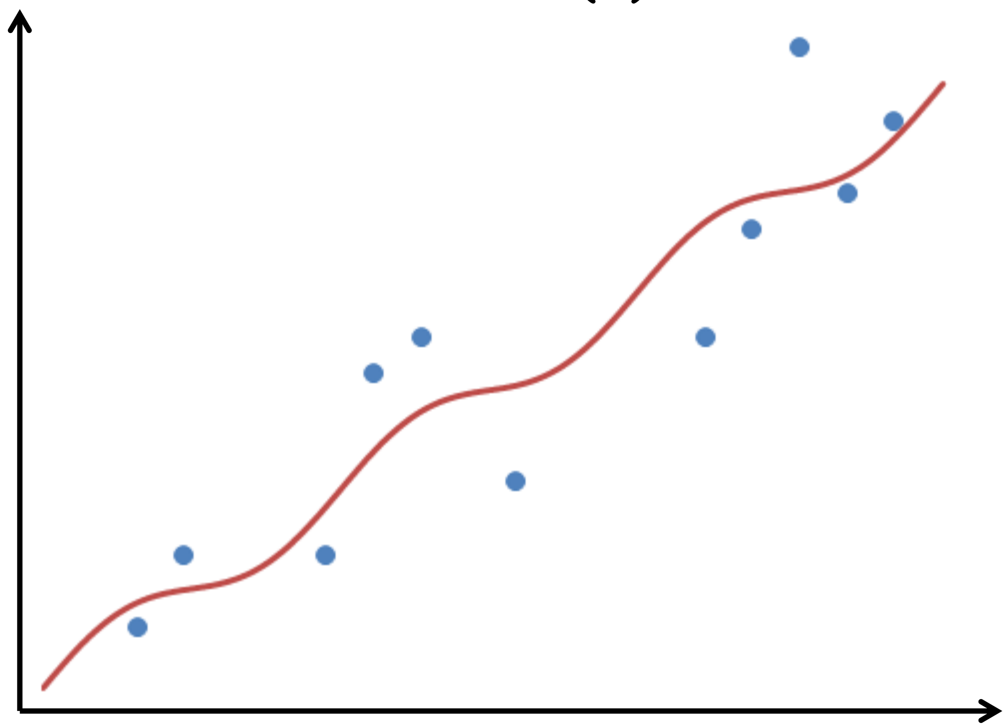
(17, 14)
(18, 16)

$$f(x) = 0.328770262 + 0.873739195 * x + 0.680191174 * \sin(x)$$



Additive Linear Model

- **Example: Kernel Regression**
  - You can find a linear combination of given kernel functions

(2, 2)
(3, 4)
(6, 4)
(7, 9)
(8, 10)
(10, 6)
(14, 10)
(15, 13)
(16, 18)
(17, 14)
(18, 16)

$$f(x) = w_0 + w_1 h_1(x) + w_2 h_2(x) + w_3 h_3(x)$$

$$\text{where, } h_1(x) = \exp\left(\frac{-(x-1)^2}{18}\right), h_2(x) = \exp\left(\frac{-(x-9)^2}{18}\right),$$

$$h_3(x) = \exp\left(\frac{-(x-18)^2}{18}\right)$$

Additive Linear Model

- **Example**

$$f(x) = 5.76 - 3.64\exp\left(\frac{-(x-1)^2}{18}\right) + 2.40\exp\left(\frac{-(x-9)^2}{18}\right) + 10.82\exp\left(\frac{-(x-18)^2}{18}\right)$$

(2, 2)
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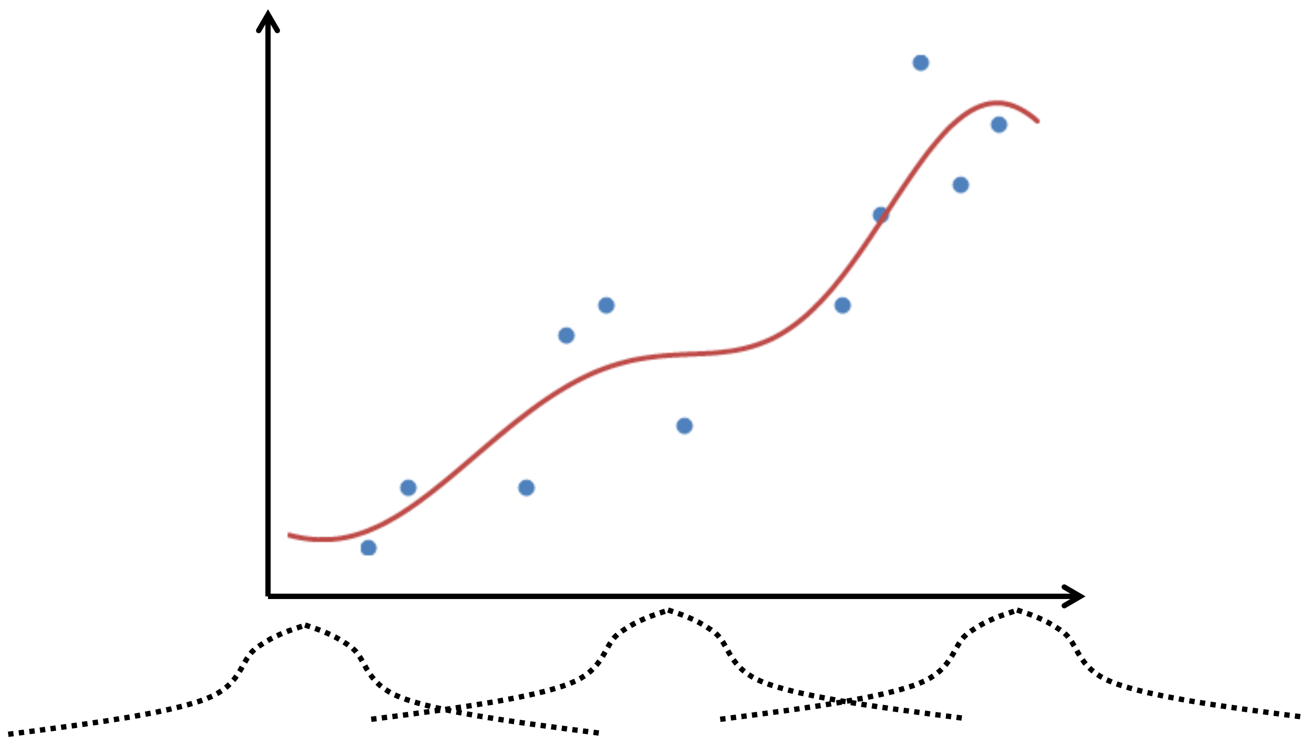
(18, 16)



Another Approaches

- **Solving Linear Equations**
  - Simplest Approach for Linear Regression

- **Another Approaches to Solve Linear Regression**
  - Gradient Descent Approach
  - Maximum Likelihood Estimation Approach

  => Both give the same solution as SLE gives

- **Then, Why?**
  - Both are well-known, useful and important methods to solve problems in ML domain