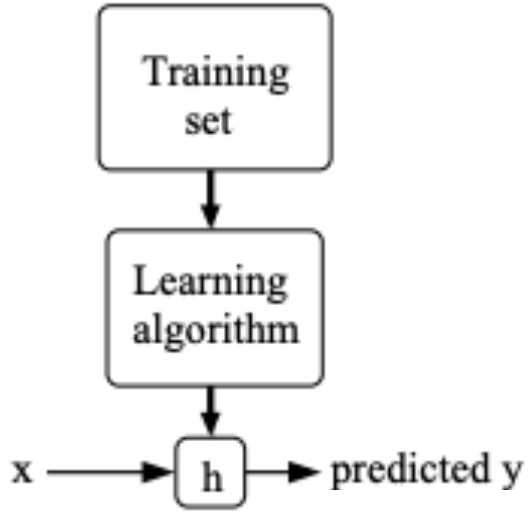
COMP [56]630– Machine Learning

Lecture 4 – Linear Regression Pt. 2

The basics

- Input: a set of inputs X = {x_1, x_2, … x_n}, also called ***features***
- Output: a set of expected outputs or ***targets*** Y = {y_1, y_2, … y_n}
- Goal: to learn a function $h : X \rightarrow Y$ such that the function $h(x_i)$ is a good predictor of the corresponding value y_i
  - h(x) is called the ***hypothesis***
- If the target is continuous the problem setting is called ***regression.***
- If the target is discrete or categorical, the problem is called ***classification.***



Example

- Suppose we have a dataset giving the living areas and prices of 47 houses from Stillwater, OK

Living area (ft^2)	# bedrooms	Price (1000$s)
1643	4	256
1356	3	202
1678	3	287
…	…	…
3000	4	400

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Features (X)

Targets (Y)

Targets are continuous valued! => Task is *regression*

Linear Regression

- Goal: formulate a hypothesis function h(x) which will model the 2-d input feature (size, # bedrooms) and produce the expected target value (the house price in 1000$s).
- We can say that the hypothesis function could be a linear function of x:

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2$$

- Here, θ_i represent the ***parameters*** or ***weights*** of the linear model characterizing X→Y
- A more simpler model then will be $$h(x) = \sum_{i=0}^{n} \theta_i x_i = \theta^T x,$$

Linear Regression (cntd.)

- **Learning:** Given this formulation, we will need to identify a way to find the values of θ.
- We will need to use the ***training*** data to learn these parameters. This process is called ***learning***
- **What do we need to achieve this?**
- We will define a function that measures the quality of predictions for each value of θ.
- This is called the **cost function or objective function**

$$h(x) = \sum_{i=0}^{n} \theta_i x_i = \theta^T x,$$

How to obtain parameter matrix using this objective function?

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2.$$

Ordinary least squares regression model

Learning

- Goal: To find a set of parameters θ that will minimize the cost function J(θ).
- Common approach: *gradient descent*
- What does it do?
  - Start with an initial “guess” for θ
  - Update values of θ that will gradually move towards the “optimal solution”
  - What is the optimal solution?
  - The value of θ that minimizes the cost function
- How do we do it computationally?

Gradient Descent

- How do we do it computationally?

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

- α is the learning rate
  - Modulates how much of the change that we need to propagate at each instant
- Each update of θ will be a step in the *steepest decrease of the cost function J(*θ)
- How to Compute the derivative of the cost function J(θ)?

Gradient Descent

- Hence each update is given by

$$\theta_j := \theta_j + \alpha \left(y^{(i)} - h_\theta(x^{(i)}) \right) x_j^{(i)}$$

- This is called the **LMS** update rule or the ***Least Mean Squares*** update rule.
  - Also known as the ***Widrow-Hoff*** learning rule.

Gradient Descent

- Has several properties:
  - Magnitude of update is proportional to the error (y – h(x))
    - What does this mean?
    - If we have a very good prediction i.e. h(x)≈ y, then the update is very small.
    - Conversely, if the prediction is very far off i.e. h(x)≫ y or h(x)≪ y then the update will be large.
- For learning over the complete training set, we iteratively update the parameters as below

Repeat until convergence {

$$\theta_j := \theta_j + \alpha \sum_{i=1}^{m} \left(y^{(i)} - h_\theta(x^{(i)})\right) x_j^{(i)} \qquad \text{(for every } j\text{)}.$$

}

Is there a non-iterative solution?

- Yes! We can directly find the solution using “Normal Equations”.
- It is an analytical approach used for optimization
- Can be done as follows:
  - Set the partial derivatives of the cost function J(θ) to zero
  - Then you can estimate the parameters as follows:

$$\nabla_\theta J(\theta) = 0$$

$$X^T X \theta = X^T \vec{y}$$

$$\Theta = (X^T X)^{-1} X^T y$$

  - Where X is the input feature vector
  - y is the expected target value

Linear Regression with Basis Functions

Basis Functions

- Sometimes, you will need to have some fixed pre-processing of the input data.
  - Also called feature extraction
- Linearity is often a good assumption when many inputs influence the output
  - Natural examples include $F = ma$

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How do we handle non-linear relationships?

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How do we handle non-linear relationships?

- Simple! In addition to the original features, add more features that are deterministic functions of the original features

Basis Functions

- If the original variables comprise the vector x, then the features can be expressed in terms of basis functions $\{\phi_j(x)\}$
- By using nonlinear basis functions, we allow the hypothesis function h(x,w) to be a nonlinear function of the input vector x
  - They are linear functions of parameters, yet are nonlinear with respect to the input variables
- You can have multiple basis functions to model different non-linearities

$$y(\mathrm{x},\mathrm{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathrm{x})$$

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Basis Functions

- More generally,

$$y(\mathrm{x},\mathrm{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathrm{x}) = \mathrm{w}^T \phi(\mathrm{x})$$

where $w=(w_0,w_1,..,w_{M-1})$ and $\Phi=(\phi_0,\phi_1,..,\phi_{M-1})^T$

- We now need M weights for basis functions instead of D weights for features

Types of Basis Functions

- Linear Basis function:

$$y(x,\mathrm{w}) = \sum_{j=0}^{M-1} w_j \phi_j(x) = \mathrm{w}^T \phi(x)$$

- Polynomial Basis Function:
  - Model with M-1 degree polynomial $\boxed{\phi_j(x) = x^j}$
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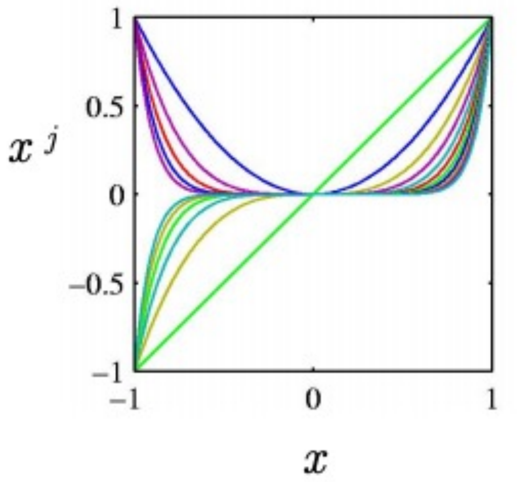

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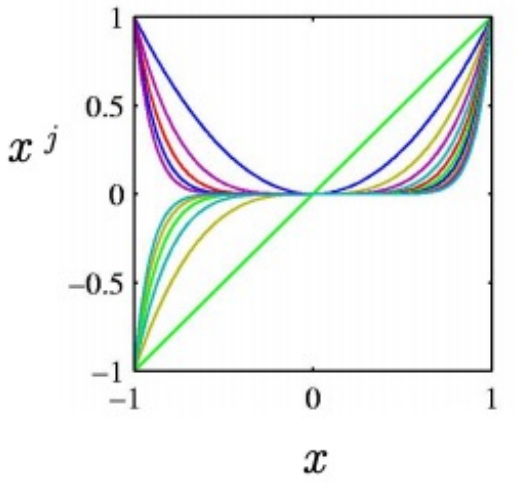
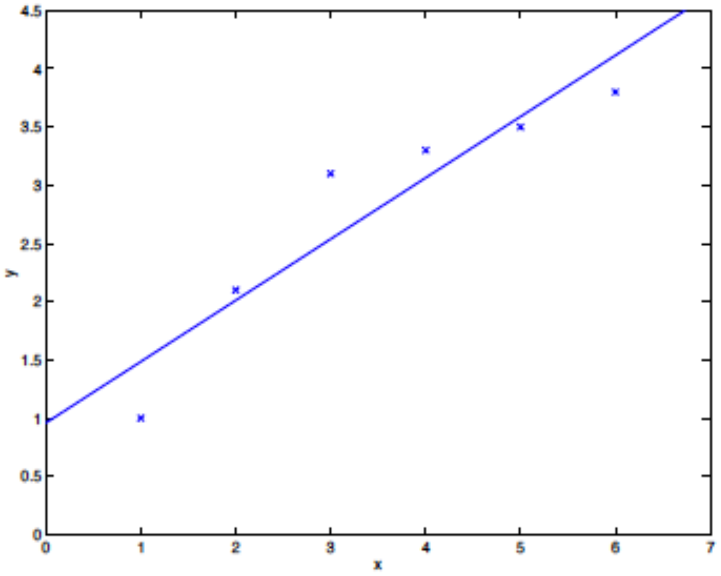
  - Model with M-1 degree polynomial $\boxed{\phi_j(x) = x^j}$
  - Works really well for 1-d feature vector i.e. only modelling one variable *x*
- Disadvantage
  - Global:
    - changes in one region of input space affects others
  - Difficult to formulate
    - Number of polynomials increases exponentially with M
  - Can divide input space into regions
    - use different polynomials in each region
    - equivalent to spline functions



Example



Linear Basis Function

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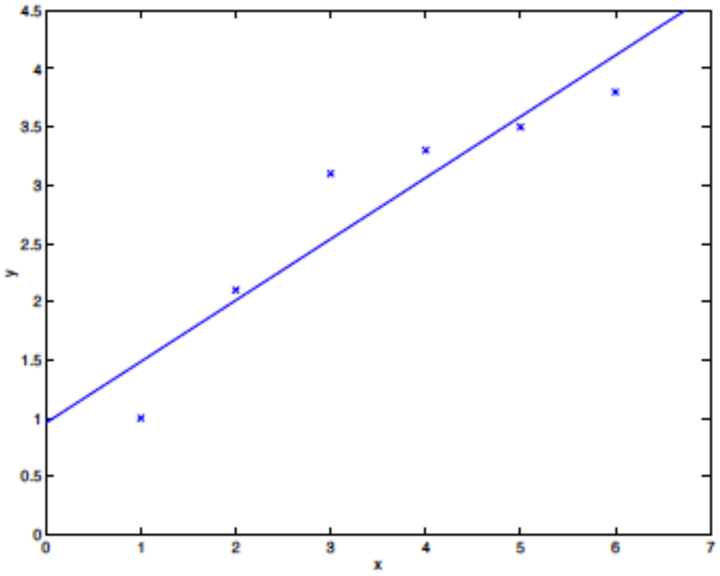

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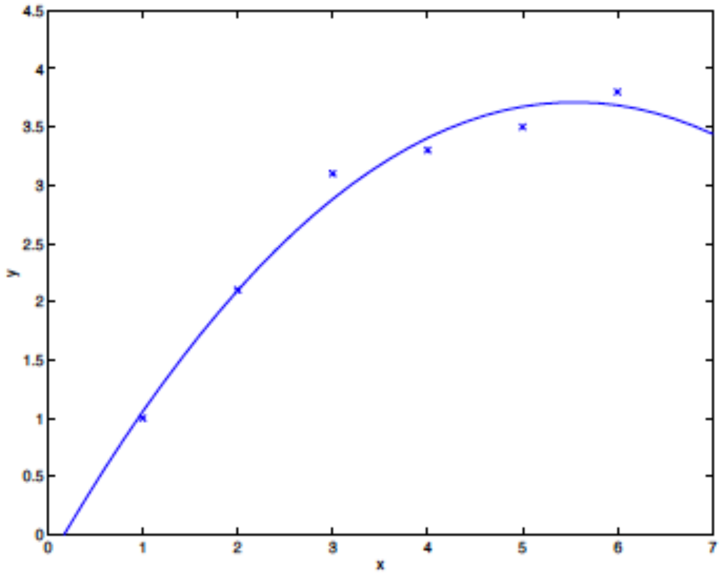
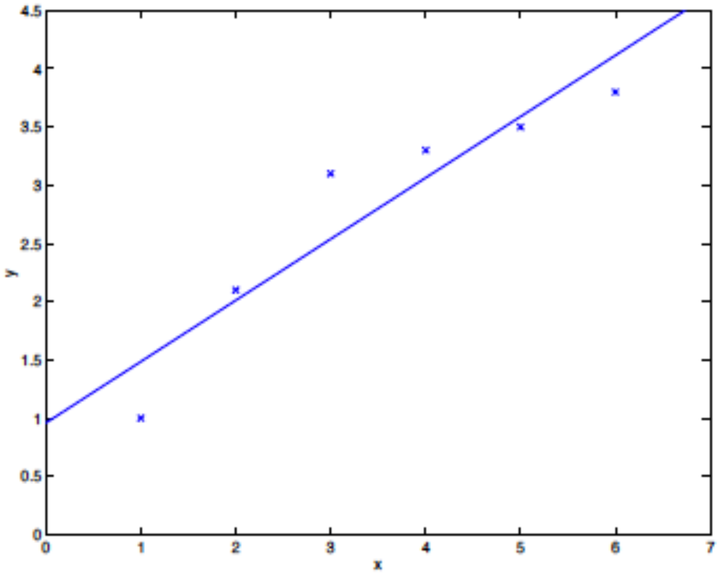


2nd order basis Function
i.e. add x^2 feature

Example



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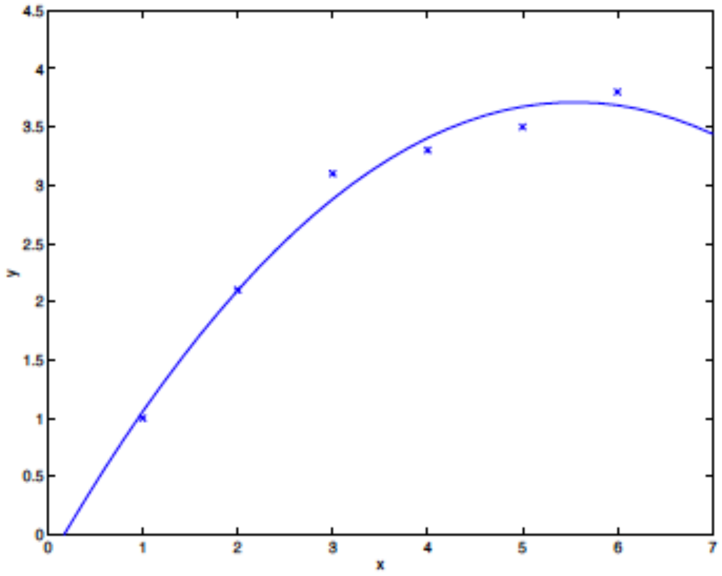

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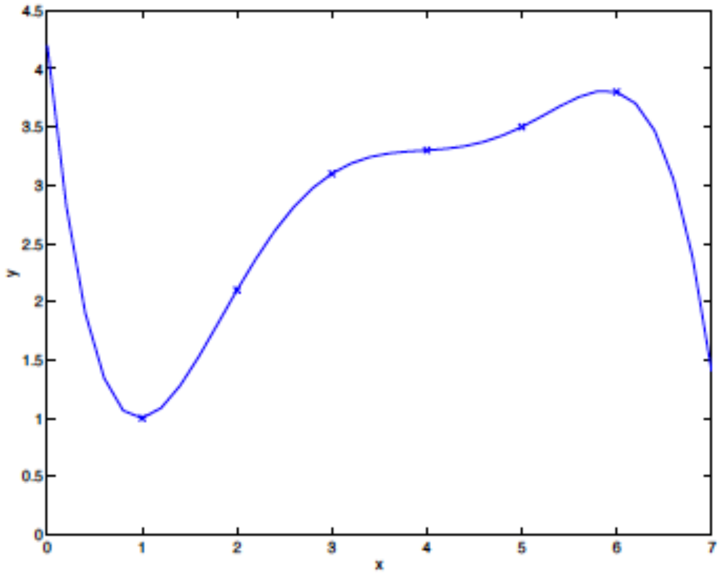

5^{th} order basis Function
i.e. add up to x^5 feature

$$y = \sum_{j=0}^{5} \theta_j x^j$$

Other Basis Functions

- Gaussian Radial Basis function:
  - μ_j govern the locations of the basis functions
    - Can be an arbitrary set of points within the range of the data
      - Can choose some representative data points
  - σ governs the spatial scale
    - Could be chosen from the data set e.g., average variance

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

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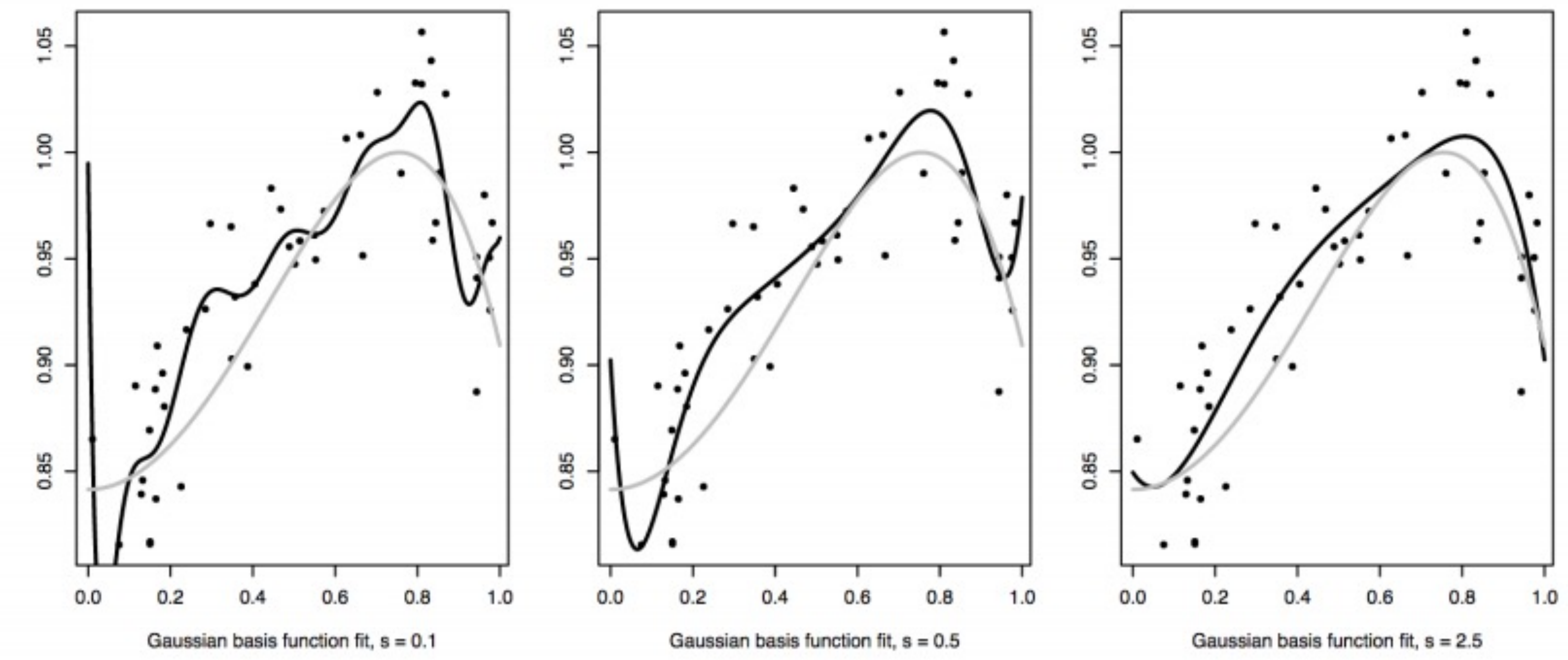

Other Basis Functions

- Sigmoid: $\phi_j(x) = \sigma\left(\frac{x - \mu_j}{s}\right)$
- Fourier
  - Expansion in sinusoidal functions
- Signal Processing
  - Also called *wavelets*
    - Functions grounded in time and frequency
- Linear
  - $\phi(x) = x$

Does more features always mean better?

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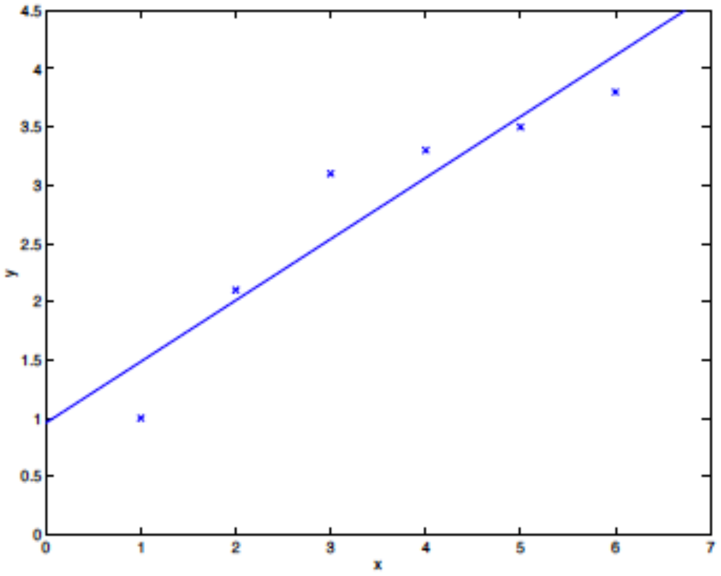

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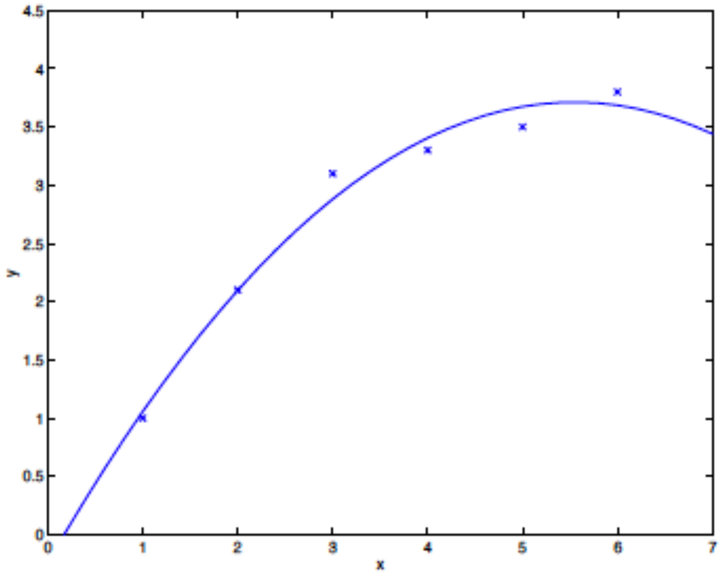

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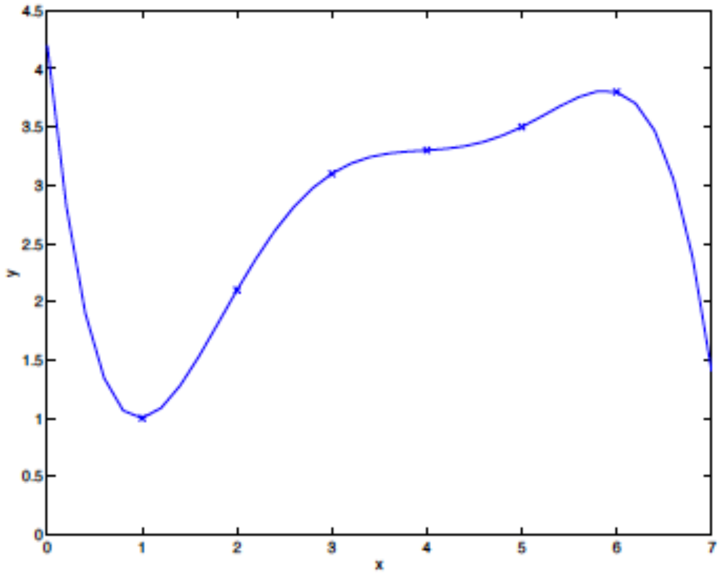

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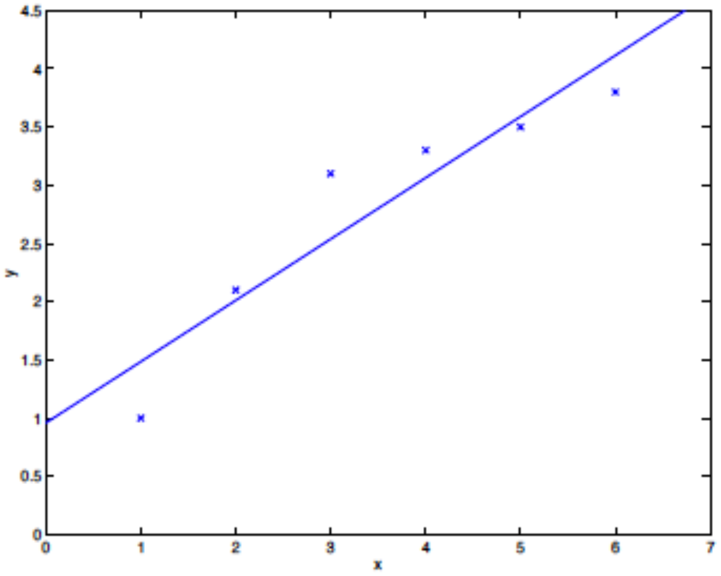

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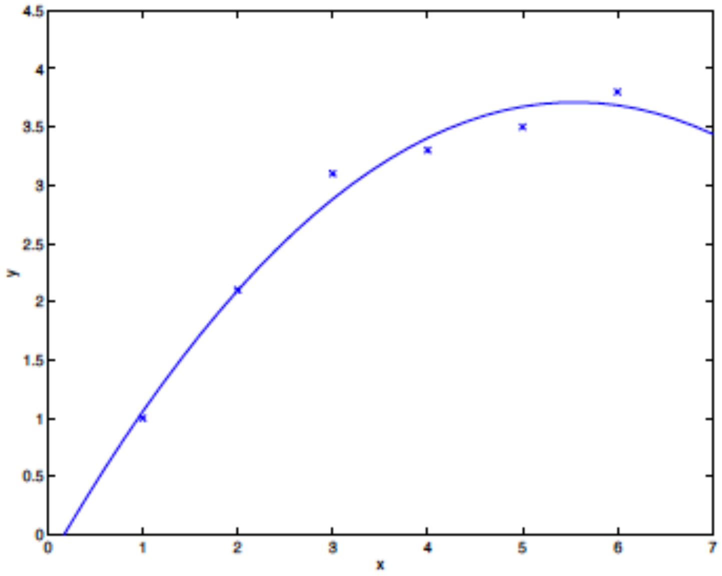

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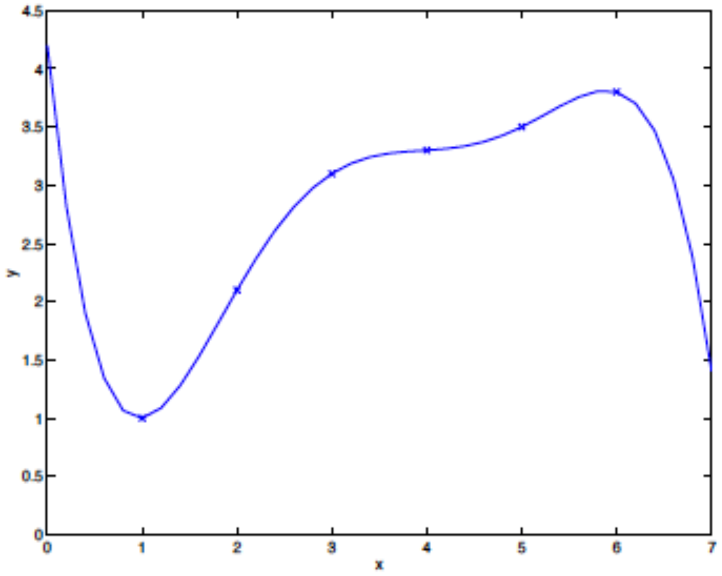

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NO!

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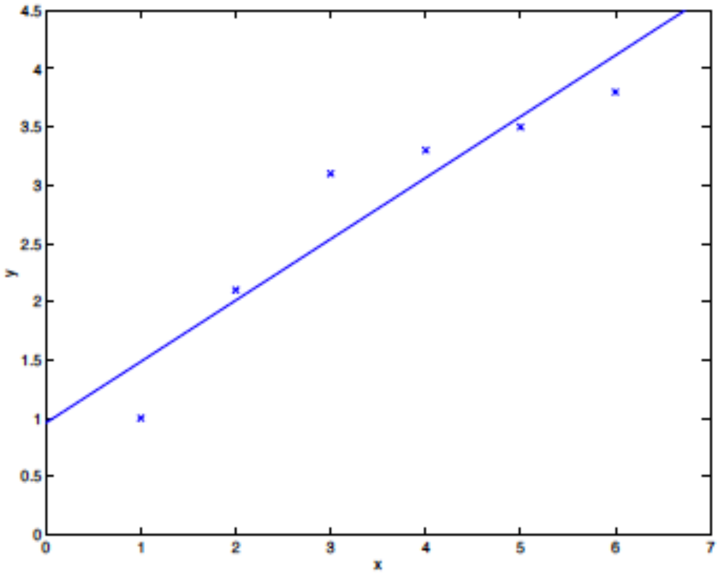

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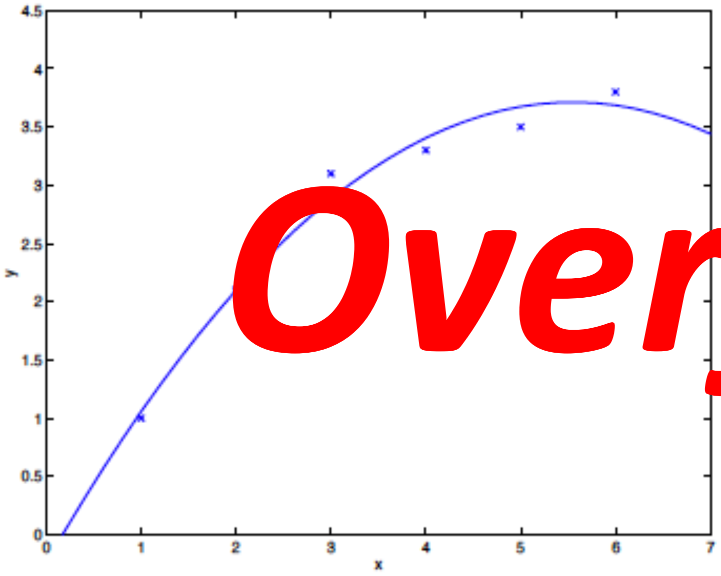

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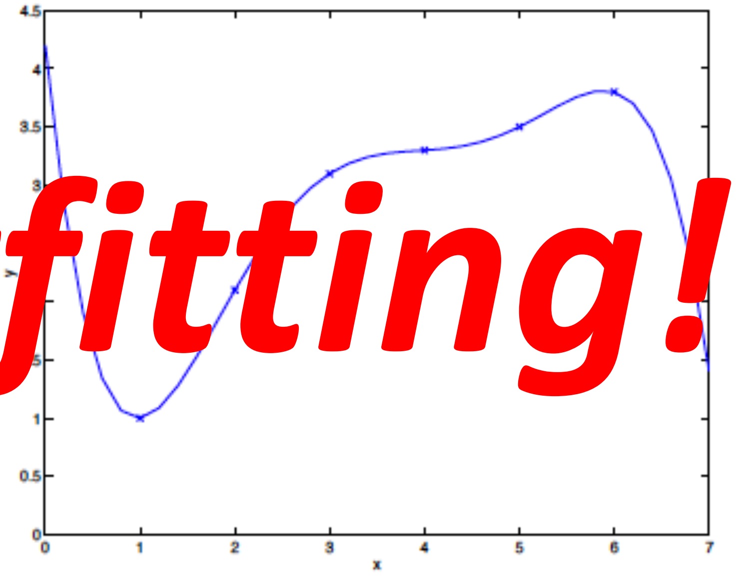

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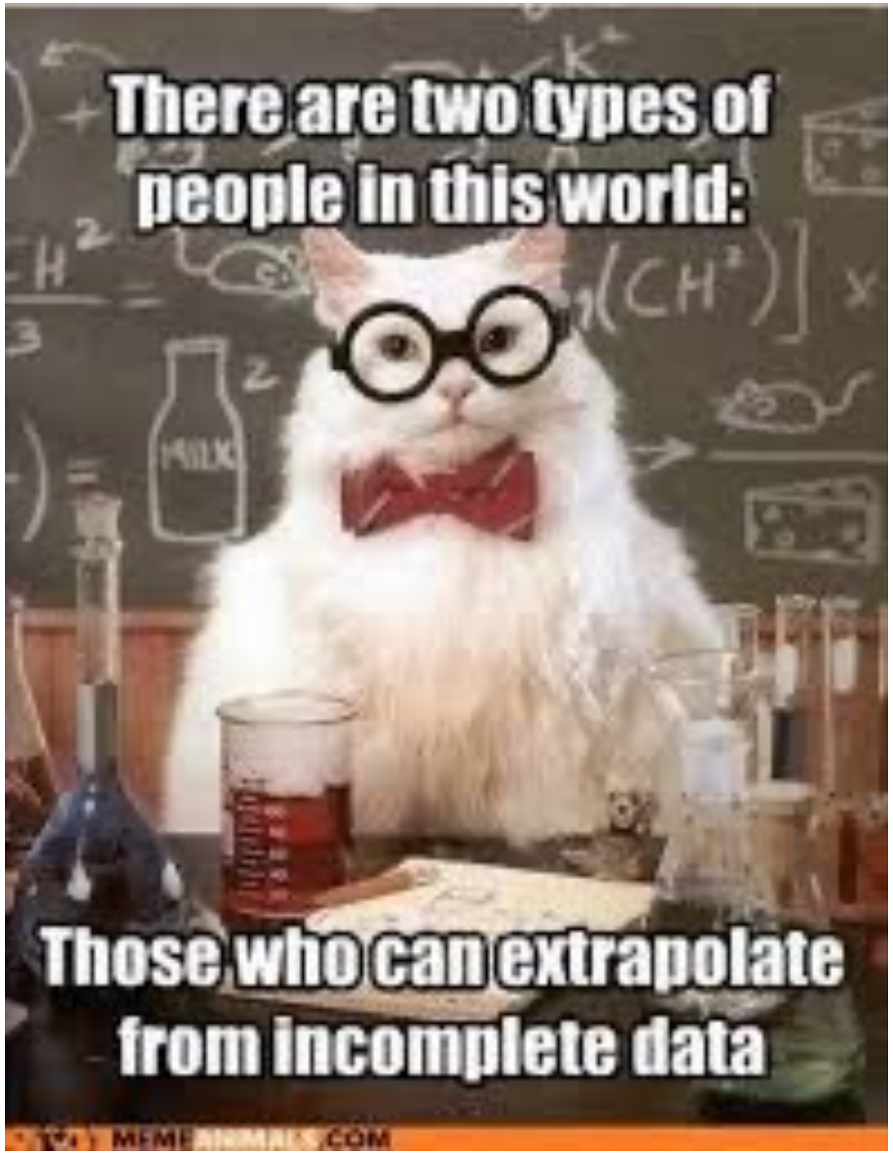
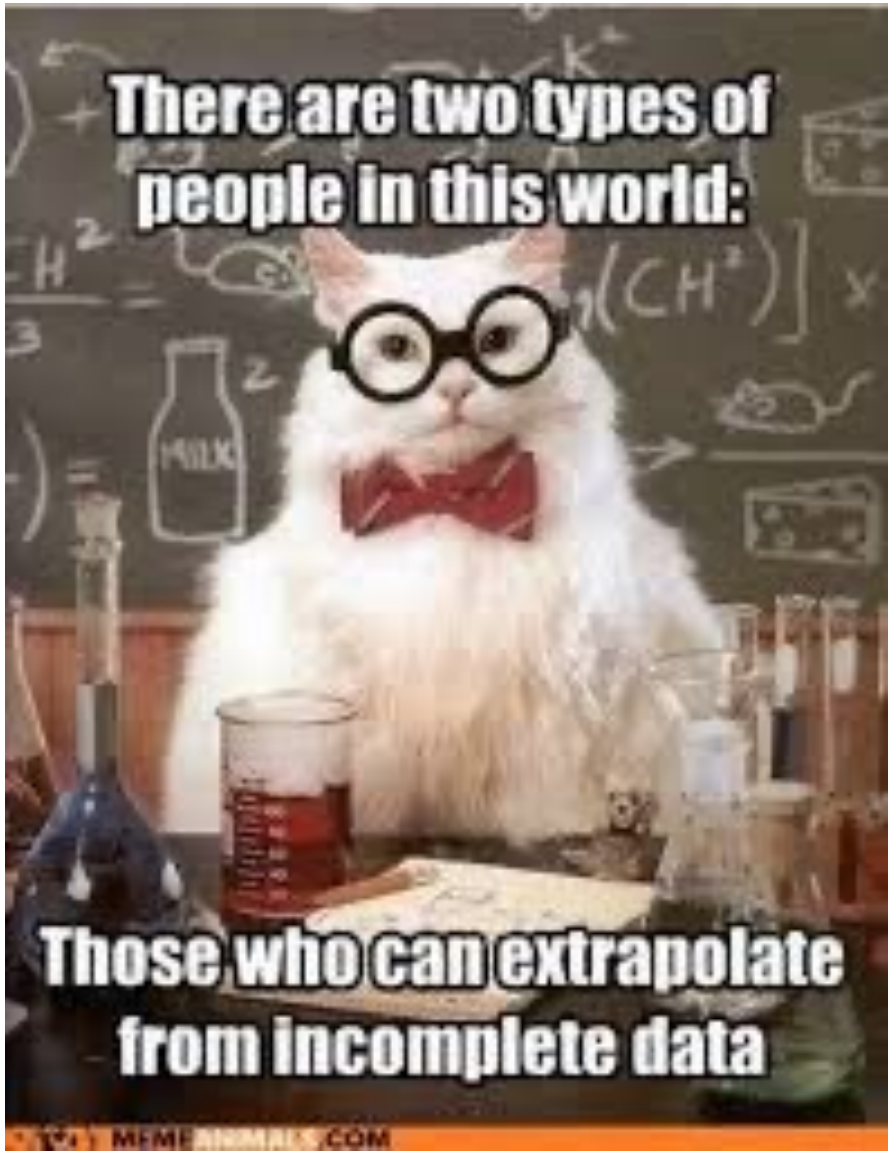
Overfitting!

NO!


There are two types of people in this world:
Those who can extrapolate from incomplete data



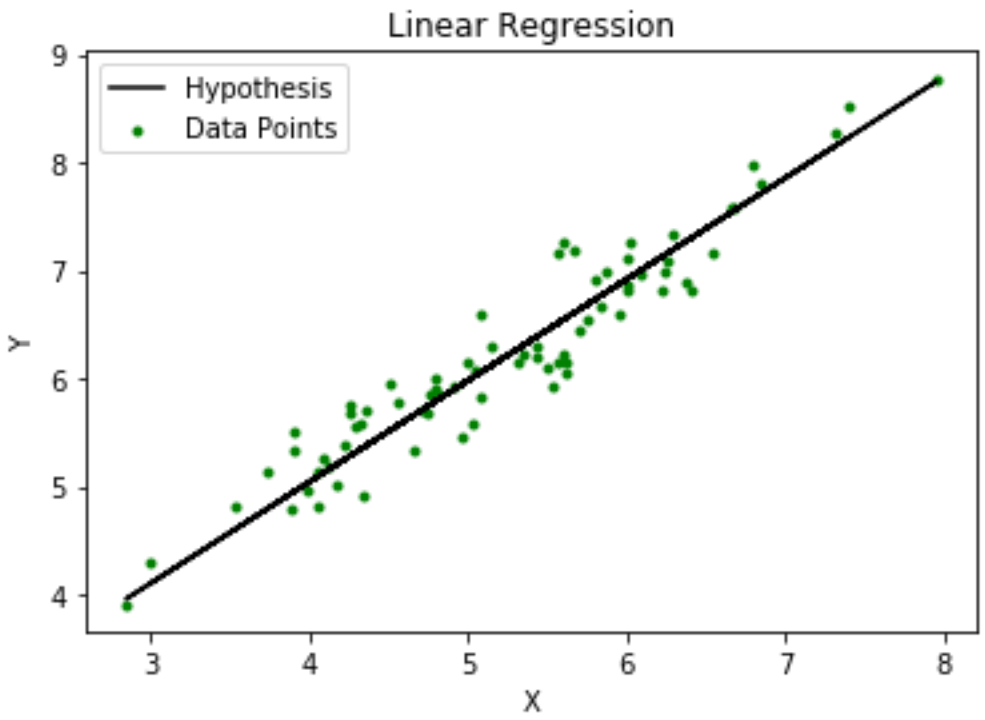
You don't want your model to be other kind!

☺

Locally Weighted Linear Regression

Who needs parameters or learning, anyway?

Non-linear Data



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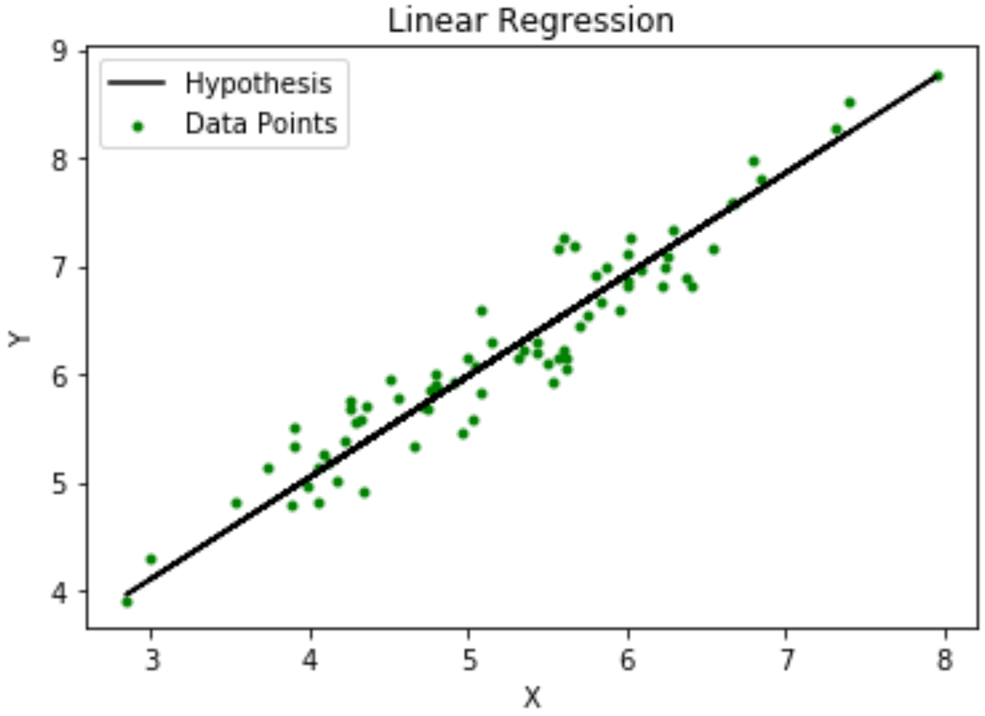

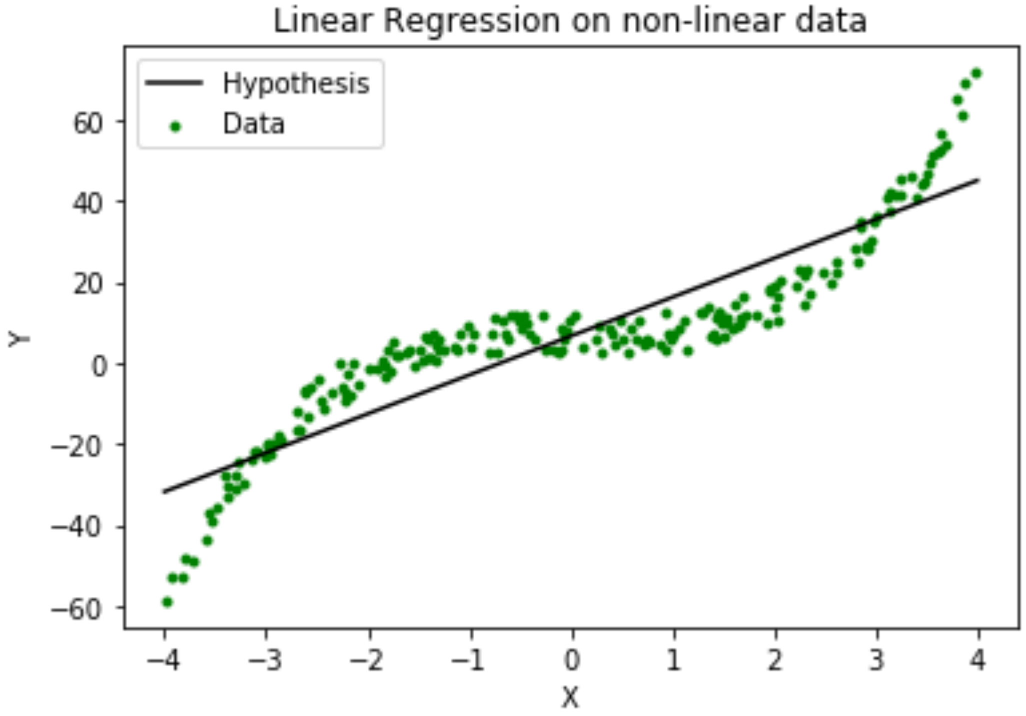

Locally weighted LR

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$$\sum_i w^{(i)}(y^{(i)} - \theta^T x^{(i)})^2$$

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$$\sum_i \underbrace{w^{(i)}}_{\text{Weights for each example in training set}} (y^{(i)} - \theta^T x^{(i)})^2$$

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$$w^{(i)} = \exp\left(-\frac{(x^{(i)} - x)^2}{2\tau^2}\right)$$

τ is called the **bandwidth** parameter.

- If $x^{(i)}$ is closer to the query value x , then w is almost 1. If it is farther away, then *w* will be small.

Example

- Input value: x = 5.0
- Two values in training set: x_1=4.9, x_2=3.0
- What would the values of w_1 and w_2 be, if $\tau = 0.5$?

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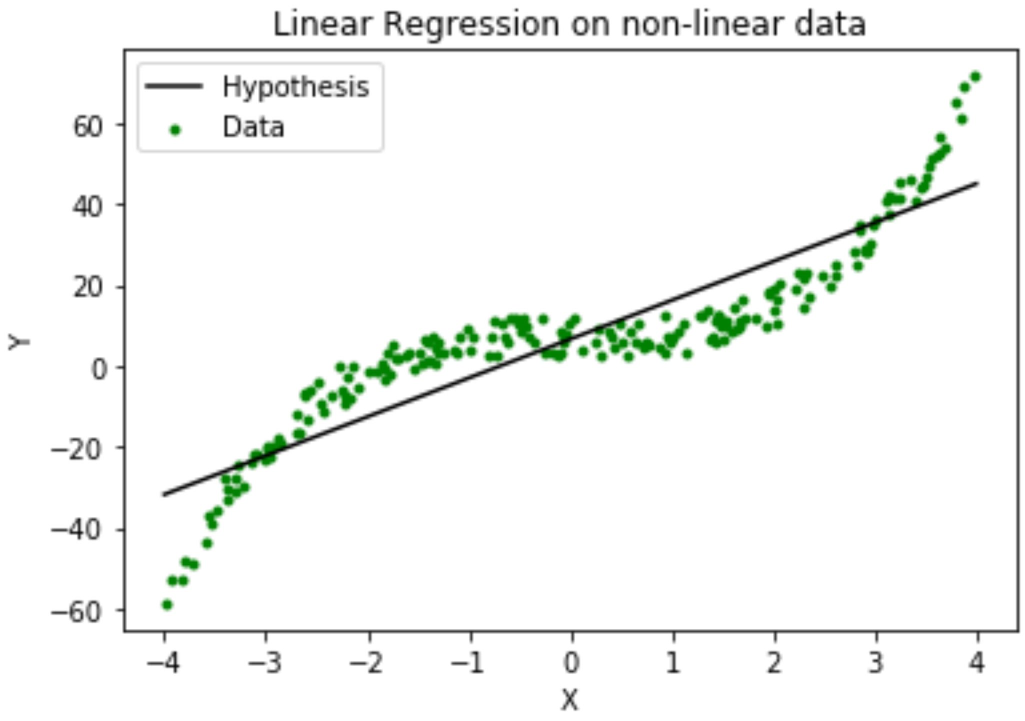
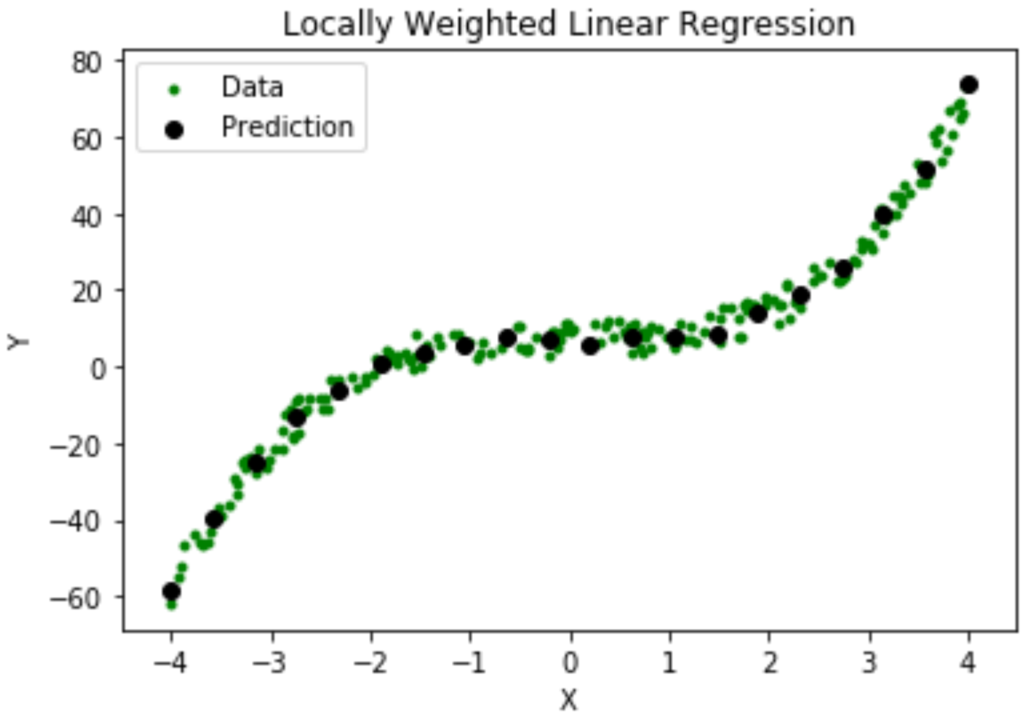
$$J(\theta) = 0.9802 * (\theta^T x^{(1)} - y^{(1)}) + 0.000335 * (\theta^T x^{(2)} - y^{(2)})$$

Non-linear Data





How to learn $\boldsymbol{\theta}$?

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{m} w^i(\theta^T x^i - y^i)^2$$
$$= \frac{1}{2}\sum_{i=1}^{m} (\theta^T x^i - y^i) w^i (\theta^T x^i - y^i)$$
$$= \frac{1}{2}(X\theta - y)^T W (X\theta - y)$$

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\begin{aligned}
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Hence the gradient is given by $\nabla_\theta J = X^T W (X\theta - Y)$

Set the gradient to 0 to get the normal equations

$$
\begin{aligned}
\nabla_\theta J &= 0 \\
X^T W (X\theta - Y) &= 0 \\
X^T W X \theta &= X^T W Y \\
\theta &= (X^T W X)^{-1} X^T W Y
\end{aligned}
$$

Practical Implementation

- Use Normal Equations approach
- Compute Weight Matrix
  - Diagonal matrix
  - Each element in the diagonal is the weight for that point given by

$$w^{(i)} = \exp\left(-\frac{(x^{(i)} - x)^2}{2\tau^2}\right)$$

  - Have to compute Theta for every point you want to predict.
    - So to predict 100 points → Compute theta for that point, and then predict using

$$h(x) = \sum_{i=0}^{n} \theta_i x_i = \theta^T x,$$

$$\theta = (X^T W X)^{-1} X^T W Y$$

Do Non-Parametric models overfit?


NONPARAMETRIC CAT
HAS BEEN OVERFITTED
force
ROFLBOT