Lecture 7: 26 April, 2021

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Data Mining and Machine Learning
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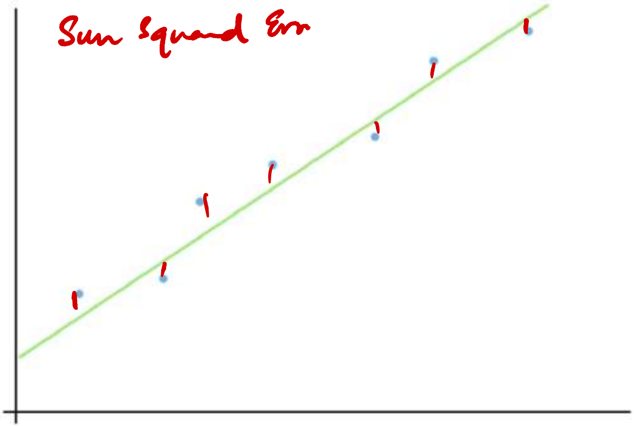
Linear regression

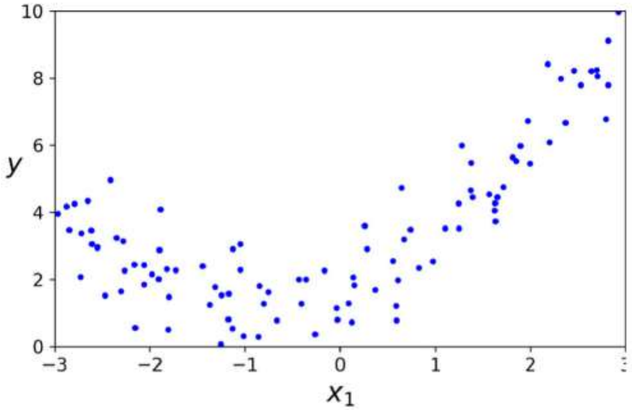
- Find the line that "fits" the data best
  - Normal equation
  - Gradient descent
- Linear: each parameter's contribution is independent
- Input $x : (x_1, x_2, \ldots, x_k)$
- $y = \theta_0 + \theta_1 x_1 + \cdots + \theta_k x_k$



Scaling x_i's to be compatible

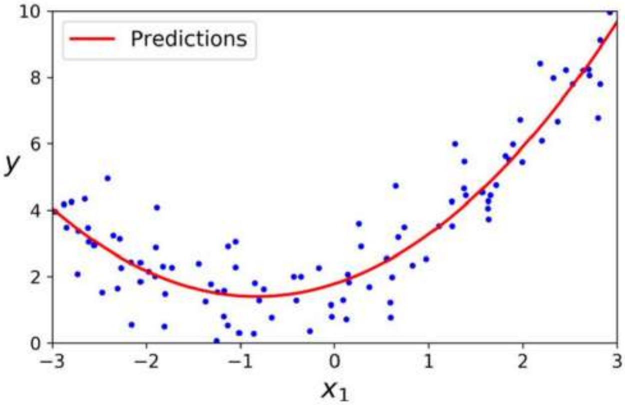
The non-linear case

- What if the relationship is not linear?



The non-linear case

- What if the relationship is not linear?
- Here the best possible explanation seems to be a quadratic



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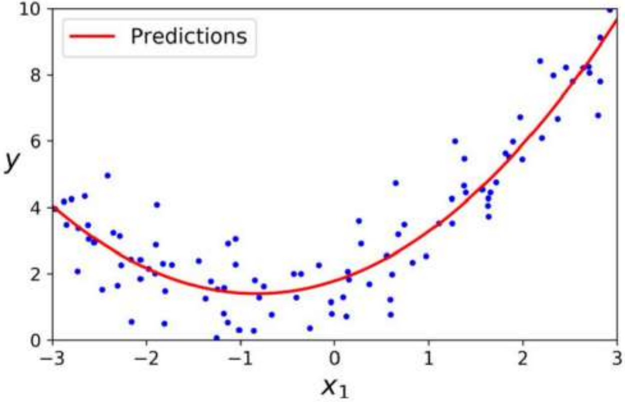
- Non-linear : cross dependencies



The non-linear case

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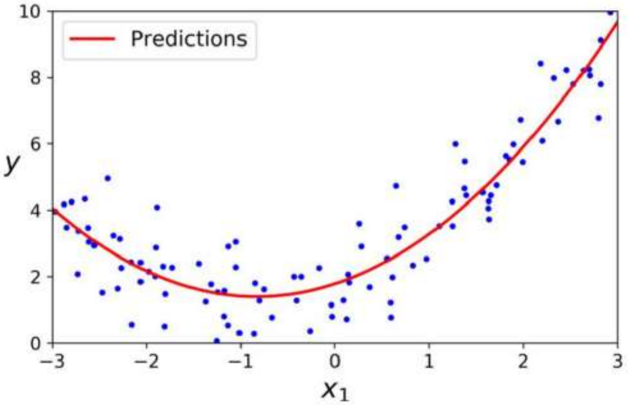
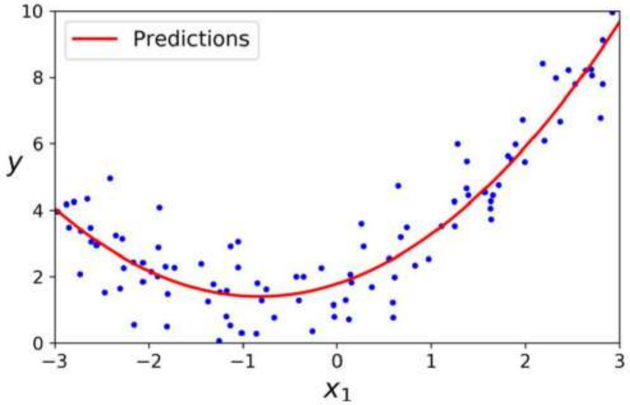
- Input $x_i : (x_{i_1}, x_{i_2})$



The non-linear case

- What if the relationship is not linear?
- Here the best possible explanation seems to be a quadratic
- Non-linear : cross dependencies
- Input $x_i : (x_{i_1}, x_{i_2})$
- Quadratic dependencies:

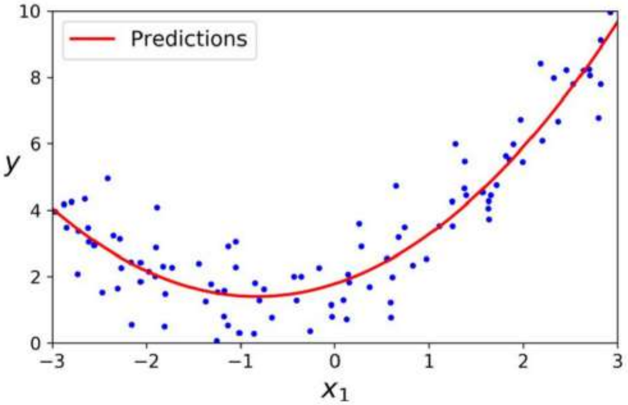
$$y = \theta_0 + \theta_1 x_{i_1} + \theta_2 x_{i_2} + \theta_{11} x_{i_1}^2 + \theta_{22} x_{i_2}^2 + \theta_{12} x_{i_1} x_{i_2}$$



The non-linear case

- Recall how we fit a line

$$\begin{bmatrix} 1 & x_i \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}$$



The non-linear case

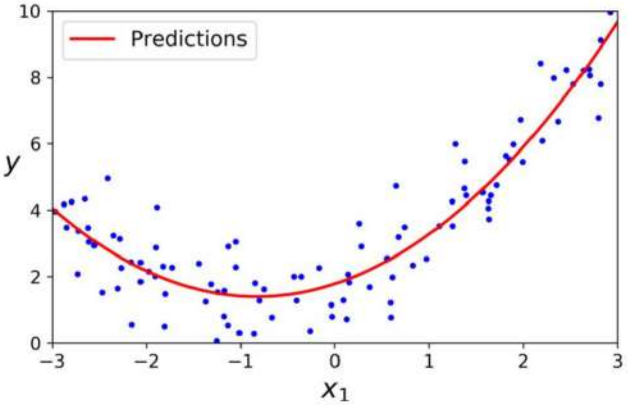
- Recall how we fit a line

$$\begin{bmatrix} 1 & x_i \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}$$

- For quadratic, add new coefficients and expand parameters

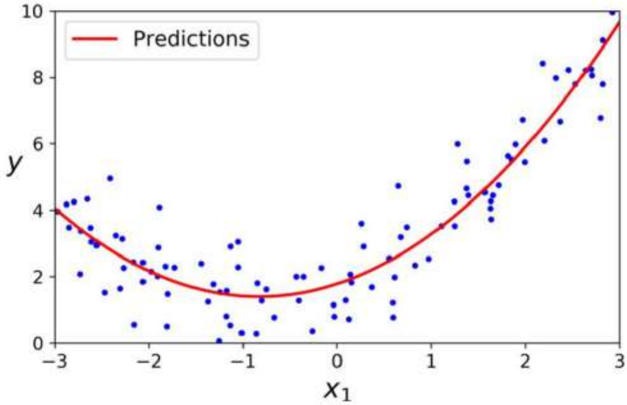
calculated

$$\begin{bmatrix} 1 & \boxed{x_i} & \underline{\underline{x_i^2}} \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix}$$



The non-linear case

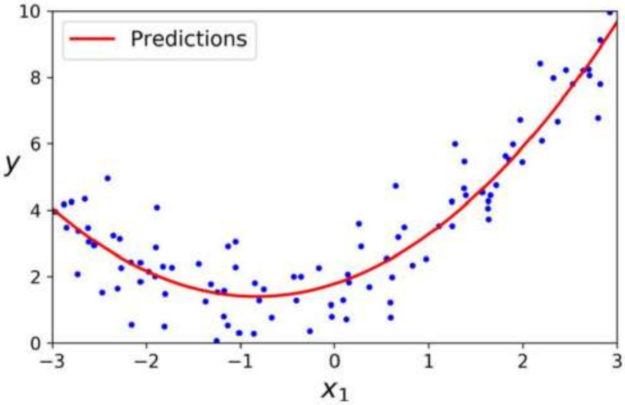
- Input (x_{i_1}, x_{i_2})



The non-linear case

- Input (x_{i_1}, x_{i_2})
- For the general quadratic case, we are adding new derived "features"

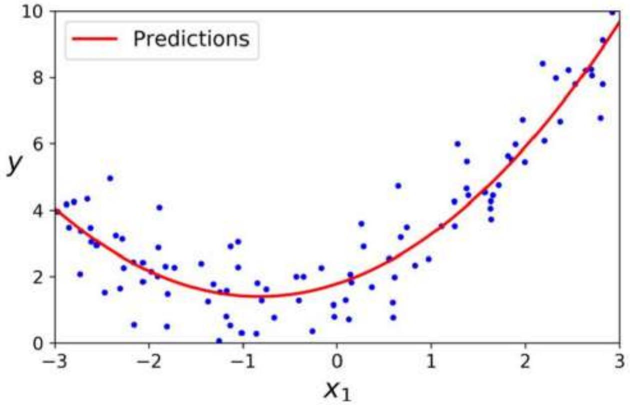
$$\begin{aligned} x_{i_3} &= x_{i_1}^2 \\ x_{i_4} &= x_{i_2}^2 \\ x_{i_5} &= x_{i_1} x_{i_2} \end{aligned}$$



The non-linear case

- Original input matrix

$$\begin{bmatrix} 1 & x_{1_1} & x_{1_2} \\ 1 & x_{2_1} & x_{2_2} \\ & \cdots & \\ 1 & x_{i_1} & x_{i_2} \\ & \cdots & \\ 1 & x_{n_1} & x_{2} \end{bmatrix}$$

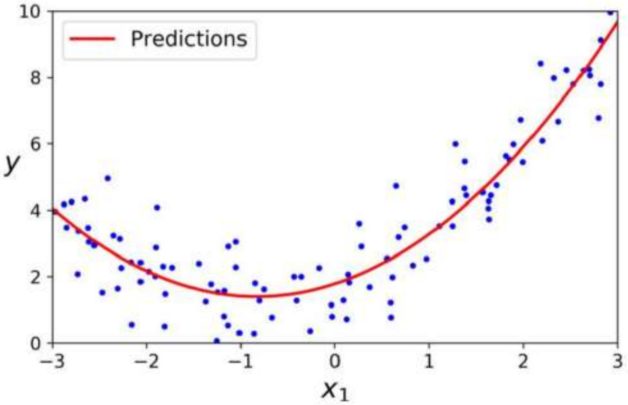


The non-linear case

Feature Engineering

- Expanded input matrix

$$
\begin{bmatrix}
1 & x_{1_1} & x_{1_2} & x_{1_1}^2 & x_{1_2}^2 & x_{1_1}x_{1_2} \\
1 & x_{2_1} & x_{2_2} & x_{2_1}^2 & x_{2_2}^2 & x_{2_1}x_{2_2} \\
 & \cdots & & & & \\
1 & x_{i_1} & x_{i_2} & x_{i_1}^2 & x_{i_2}^2 & x_{i_1}x_{i_2} \\
 & \cdots & & & & \\
1 & x_{n_1} & x_{n_2} & x_{n_1}^2 & x_{n_2}^2 & x_{n_1}x_{n_2}
\end{bmatrix}
$$



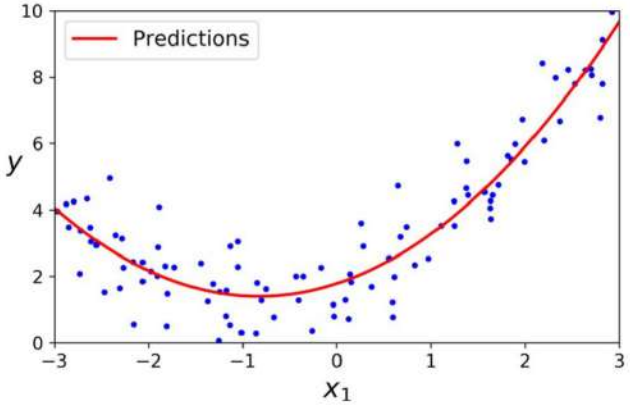
Height Weight $\rightsquigarrow$ BMI

The non-linear case

- Expanded input matrix

$$\begin{bmatrix} 1 & x_{1_1} & x_{1_2} & x_{1_1}^2 & x_{1_2}^2 & x_{1_1}x_{1_2} \\ 1 & x_{2_1} & x_{2_2} & x_{2_1}^2 & x_{2_2}^2 & x_{2_1}x_{2_2} \\ & \cdots & & & & \\ 1 & x_{i_1} & x_{i_2} & x_{i_1}^2 & x_{i_2}^2 & x_{i_1}x_{i_2} \\ & \cdots & & & & \\ 1 & x_{n_1} & x_{n_2} & x_{n_1}^2 & x_{n_2}^2 & x_{n_1}x_{n_2} \end{bmatrix}$$

- New columns are computed and filled in from original inputs



Exponential parameter blow-up

- Cubic derived features

a, b, c

$x_{i_1}^3,\ x_{i_2}^3,\ x_{i_3}^3,$

a^3

10

$x_{i_1}^2 x_{i_2},\ x_{i_1}^2 x_{i_3},$

$x_{i_2}^2 x_{i_1},\ x_{i_2}^2 x_{i_3},$

$x_{i_3}^2 x_{i_1},\ x_{i_3}^2 x_{i_2},$

$x_{i_1} x_{i_2} x_{i_3},$

b^3

c^3

$a^2 b$

$a^2 c$

$b^2 a$

$b^2 c$

abc

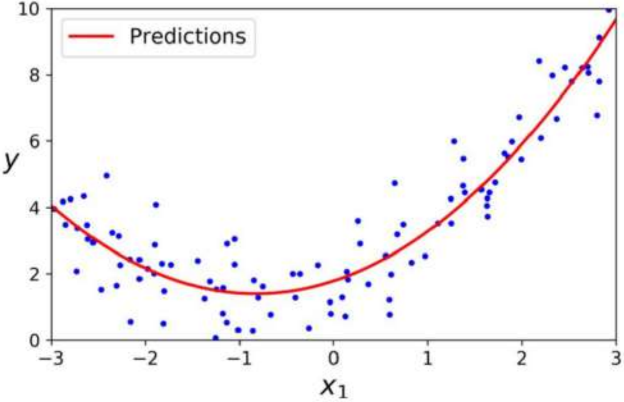
6

$x_{i_1}^2,\ x_{i_2}^2,\ x_{i_3}^2,$

$x_{i_1} x_{i_2},\ x_{i_1} x_{i_3},\ x_{i_2} x_{i_3},$

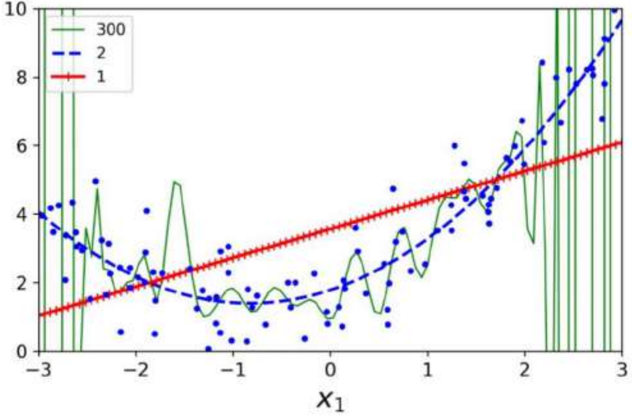
1

$x_{i_1},\ x_{i_2},\ x_{i_3}.$



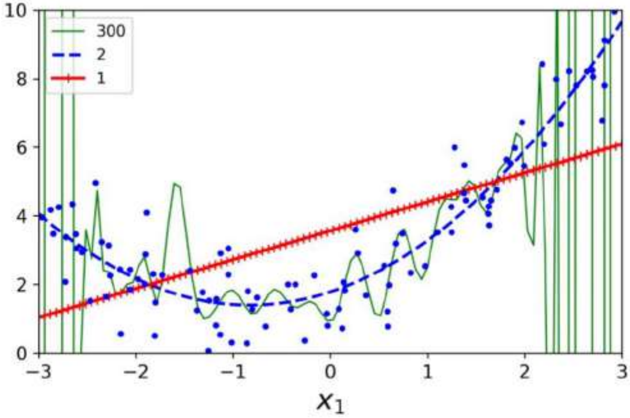
Higher degree polynomials

- How complex a polynomial should we try?



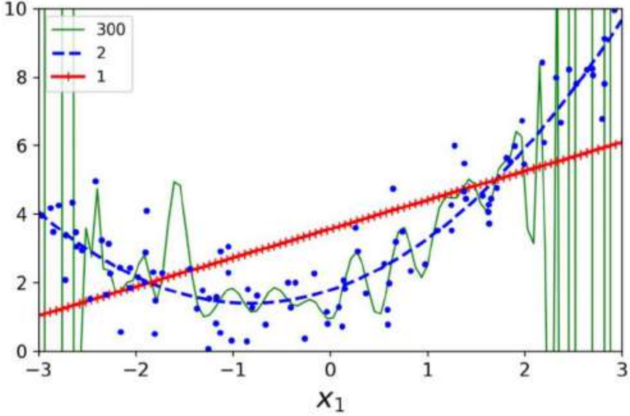
Higher degree polynomials

- How complex a polynomial should we try?
- Aim for degree that minimizes SSE



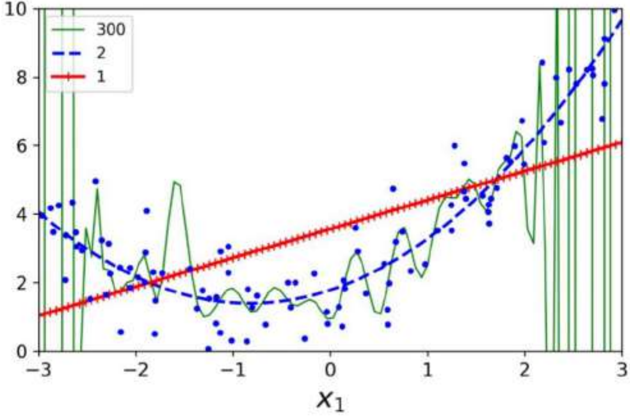
Higher degree polynomials

- How complex a polynomial should we try?
- Aim for degree that minimizes SSE
- As degree increases, features explode exponentially



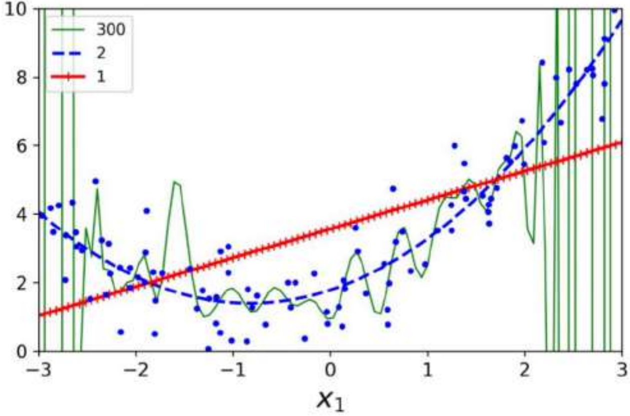
Overfitting

- Need to be careful about adding higher degree terms



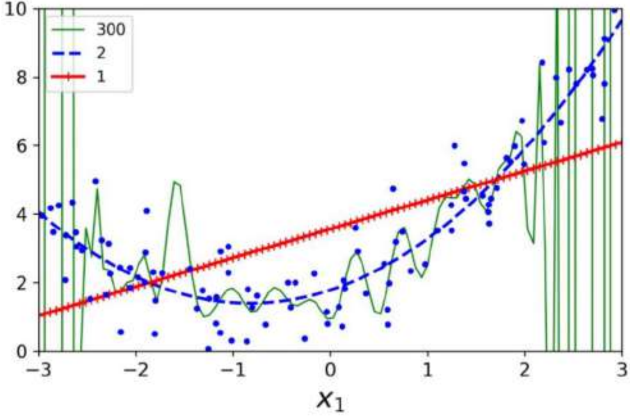
Overfitting

- Need to be careful about adding higher degree terms
- For n training points,can always fit polynomial of degree $(n-1)$ exactly
- However, such a curve would not generalize well to new data points



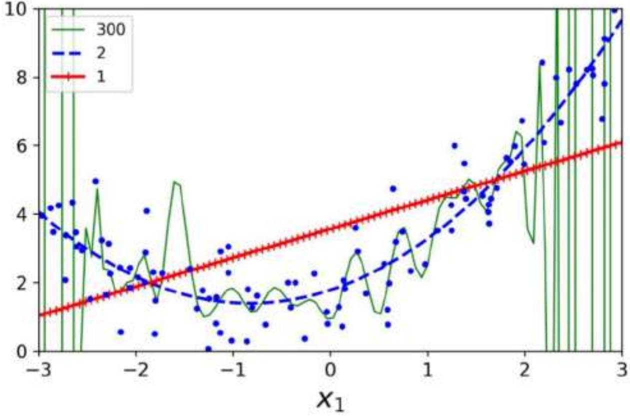
Overfitting

- Need to be careful about adding higher degree terms
- For n training points,can always fit polynomial of degree $(n-1)$ exactly
- However, such a curve would not generalize well to new data points
- Overfitting — model fits training data well, performs poorly on unseen data



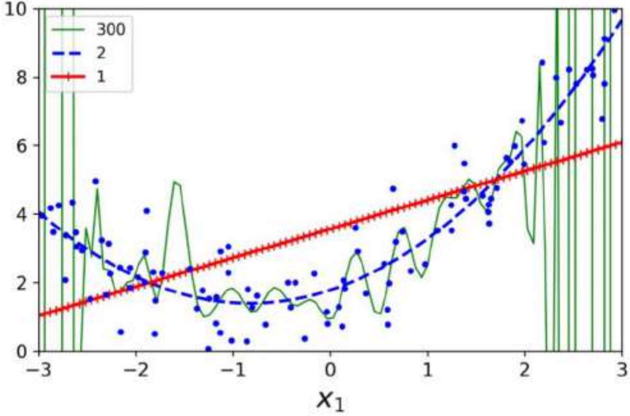
Regularization

- Need to trade off SSE against curve complexity



Regularization

- Need to trade off SSE against curve complexity
- So far, the only cost has been SSE



Regularization

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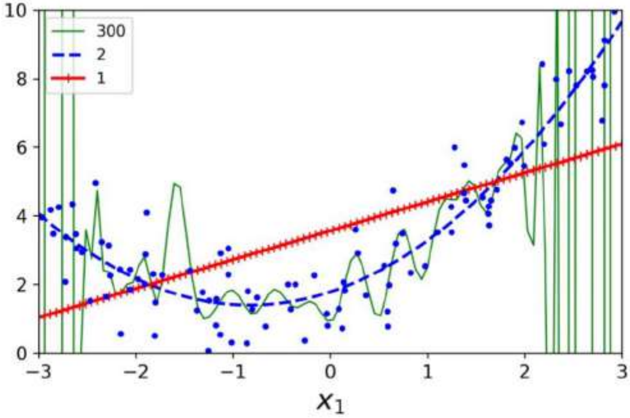
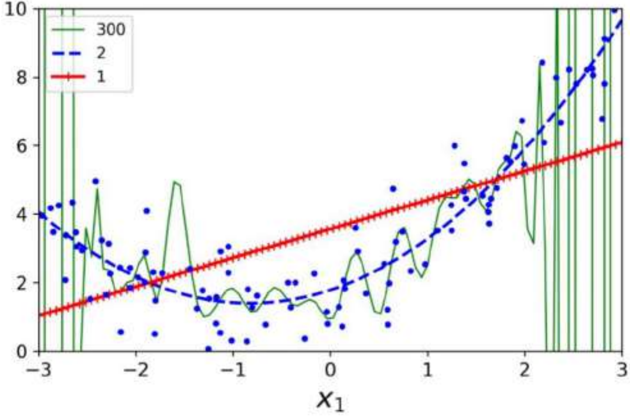
- Add a cost related to parameters $(\theta_0, \theta_1, \ldots, \theta_k)$



Regularization

- Need to trade off SSE against curve complexity
- So far, the only cost has been SSE
- Add a cost related to parameters $(\theta_0, \theta_1, \ldots, \theta_k)$
- Minimize, for instance

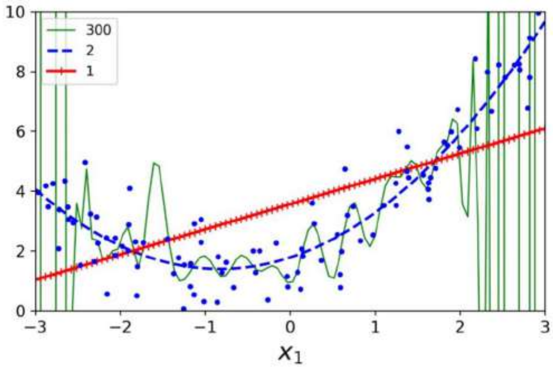
$$\frac{1}{2}\sum_{i=1}^{n}(z_i - y_i)^2 + \sum_{j=1}^{k}\theta_j^2$$



Regularization

$$\frac{1}{2}\sum_{i=1}^{n}(z_i - y_i)^2 + \sum_{j=1}^{k}\theta_j^2$$

- Second term penalizes curve complexity



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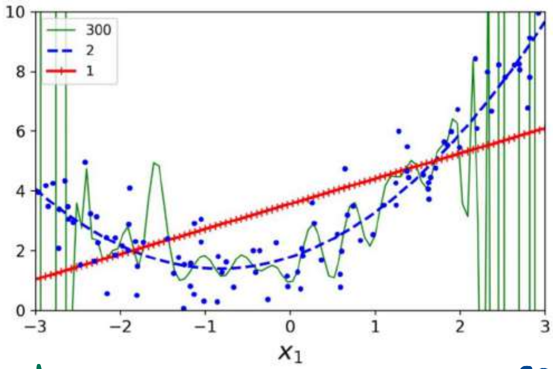


- Second term penalizes curve complexity
- Variations on regularatization
  - Ridge regression: $\sum_{j=1}^{k}\theta_j^2$
  - LASSO regression: $\sum_{j=1}^{k}|\theta_j|$
  - Elastic net regression: $\sum_{j=1}^{k}\lambda_1|\theta_j| + \lambda_2\theta_j^2$

$\lambda_1 + \lambda_2 = 1$

$x_1 \quad x_2 \quad \boxed{x_1^2 \quad x_2^2 \quad x_1x_2}$ SSE ↓

$\theta_3 \quad \theta_4 \quad \theta_5$ ↑ Reg.

Contradiction

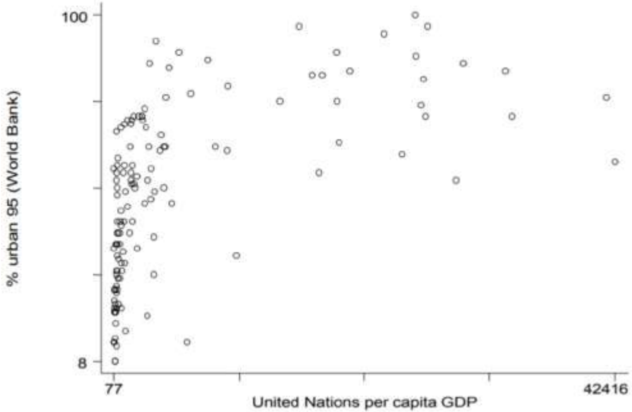
Training Data — Model to minimize training loss

Apply to general data

Minimize general loss

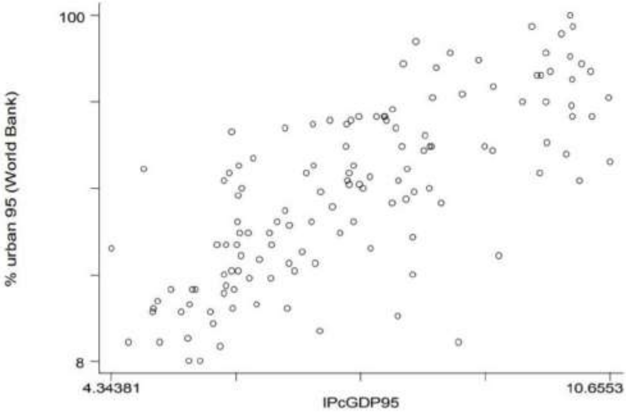
The non-polynomial case

- Percentage of urban population as a function of per capita GDP
- Not clear what polynomial would be reasonable



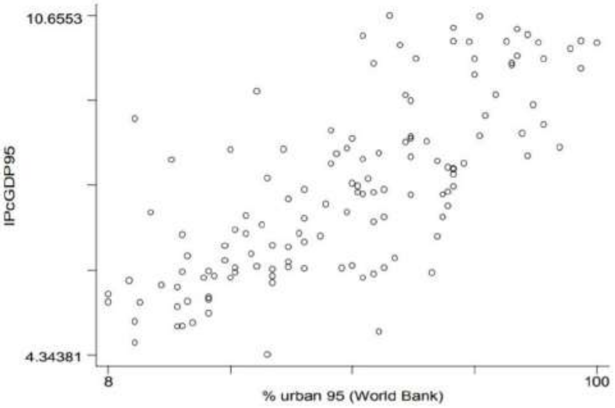
The non-polynomial case

- Percentage of urban population as a function of per capita GDP
- Not clear what polynomial would be reasonable
- Take log of GDP
- Regression we are computing is $y = \theta_0 + \theta_1 \log x_1$



The non-polynomial case

- Reverse the relationship
- Plot per capita GDP in terms of percentage of urbanization
- Now we take log of the output variable $\log y = \theta_0 + \theta_1 x_1$
- Log-linear transformation
- Earlier was linear-log
- Can also use log-log



Regression for classification

- Regression line

Estimate board exam marks

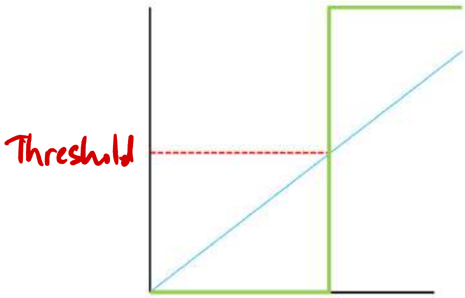
- Set a threshold

— 50%

- Classifier
  - Output below threshold : 0 (No)
  - Output above threshold : 1 (Yes)

Regression for classification

- Regression line
- Set a threshold
- Classifier
  - Output below threshold : 0 (No)
  - Output above threshold : 1 (Yes)
- Classifier output is a step function



Smoothen the step

- Sigmoid function

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

$z=0$ $e^0=1$ $\rightarrow \frac{1}{2}$

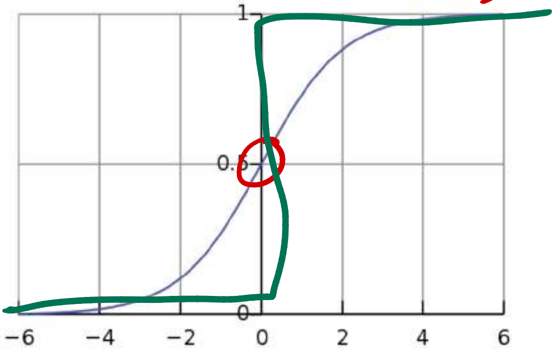
$z \rightarrow \infty$

$e^{-\infty}=0$

e^{∞}

$z \rightarrow -\infty$

$z \rightarrow \infty$



$z \rightarrow -\infty$

Smoothen the step

Adjusting θ_0 → shift the step

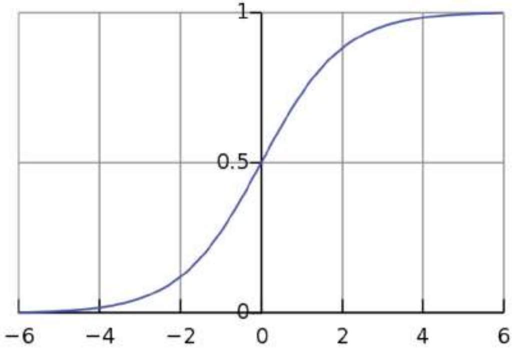
- Sigmoid function

$$\sigma(z) = \frac{1}{1+e^{-z}}$$

- Input z is output of our regression

$$\sigma(z) = \frac{1}{1+e^{-\underbrace{(\theta_0+\theta_1 x_1+\cdots+\theta_k x_k)}_{\downarrow\ 0}}}$$

0 at appropriate threshold



Smoothen the step

$x_i, \cancel{x}\ c_i$

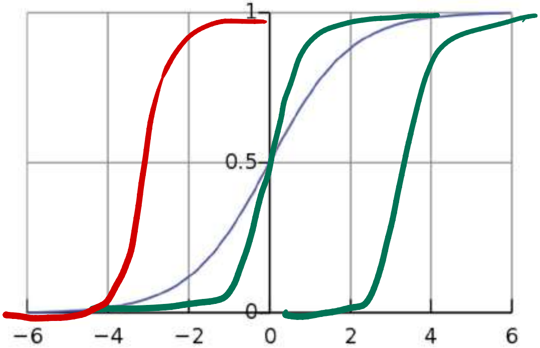
- Sigmoid function

$$\sigma(z) = \frac{1}{1+e^{-z}}$$

- Input z is output of our regression

$$\sigma(z) = \frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\cdots+\theta_k x_k)}}$$

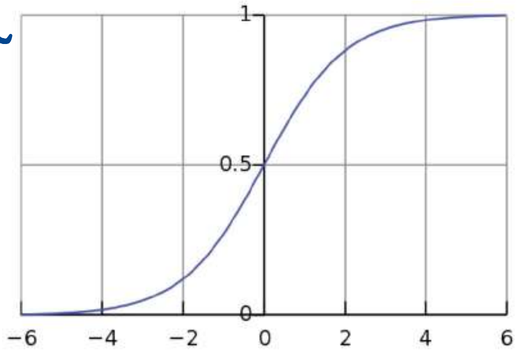
- Adjust parameters to fix horizontal position and steepness of step



Logistic regression

- Compute the coefficients?
- Solve by gradient descent

From classifier outputs

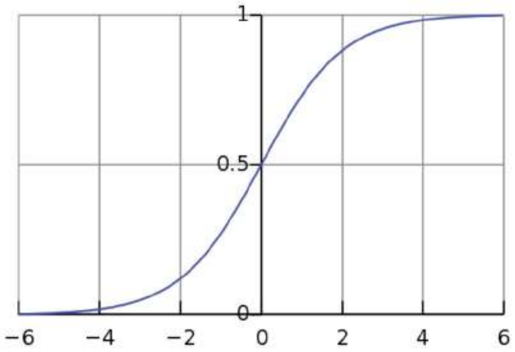


Logistic regression

Derivative wrt loss function

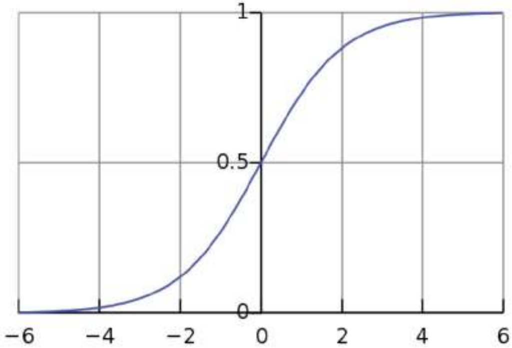
- Compute the coefficients?
- Solve by gradient descent
- Need derivatives to exist
  - Hence smooth sigmoid, not step function
  - $\underline{\sigma'(z) = \sigma(z)(1 - \sigma(z))}$ $\leftarrow \dfrac{\partial \sigma}{\partial z}$

$\sigma(z) = \dfrac{1}{1+e^{-z}}$



Logistic regression

- Compute the coefficients?
- Solve by gradient descent
- Need derivatives to exist
  - Hence smooth sigmoid, not step function
  - $\sigma'(z) = \sigma(z)(1 - \sigma(z))$
- Need a cost function to minimize



Loss function for logistic regression

- Goal is to maximize log likelihood

Loss function for logistic regression

- Goal is to maximize log likelihood
- Let $h_\theta(x_i) = \sigma(z_i)$.

$[0, 1]$

Loss function for logistic regression

$P(\text{outcome} \mid \text{parameters})$

- Goal is to maximize log likelihood
- Let $h_\theta(x_i) = \sigma(z_i)$. So, $P(y_i = 1 \mid x_i; \theta) = h_\theta(x_i)$,
  $P(y_i = 0 \mid x_i; \theta) = 1 - h_\theta(x_i)$

] 2 cases

- Combine as $P(y_i \mid x_i; \theta) = h_\theta(x_i)^{y_i} \cdot (1 - h_\theta(x_i))^{1-y_i}$

$y_i = 0, 1$

Loss function for logistic regression

- Goal is to maximize log likelihood
- Let $h_\theta(x_i) = \sigma(z_i)$. So, $P(y_i = 1 \mid x_i; \theta) = h_\theta(x_i)$, $P(y_i = 0 \mid x_i; \theta) = 1 - h_\theta(x_i)$
- Combine as $P(y_i \mid x_i; \theta) = h_\theta(x_i)^{y_i} \cdot (1 - h_\theta(x_i))^{1-y_i}$
- Likelihood: $\mathcal{L}(\theta) = \prod_{i=1}^{n} h_\theta(x_i)^{y_i} \cdot (1 - h_\theta(x_i))^{1-y_i}$

Loss function for logistic regression

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- Likelihood: $\mathcal{L}(\theta) = \prod_{i=1}^{n} \underline{h_\theta(x_i)^{y_i}} (1 - h_\theta(x_i))^{1-y_i}$
- Log-likelihood: $\ell(\theta) = \sum_{i=1}^{n} \underline{y_i \log h_\theta(x_i)} + (\underline{1 - y_i}) \log(1 - h_\theta(x_i))$ Maximize

Loss function for logistic regression

- Goal is to maximize log likelihood
- Let $h_\theta(x_i) = \underline{\sigma(z_i)}$. So, $P(y_i = 1 \mid x_i; \theta) = h_\theta(x_i)$,
  $P(y_i = 0 \mid x_i; \theta) = 1 - h_\theta(x_i)$

  $[0,1] \to \{0,1\}$
- Combine as $P(y_i \mid x_i; \theta) = h_\theta(x_i)^{y_i} \cdot (1 - h_\theta(x_i))^{1-y_i}$
- Likelihood: $\mathcal{L}(\theta) = \prod_{i=1}^{n} h_\theta(x_i)^{y_i} \cdot (1 - h_\theta(x_i))^{1-y_i}$
- Log-likelihood: $\ell(\theta) = -\sum_{i=1}^{n} y_i \log h_\theta(x_i) + (1 - y_i) \log(1 - h_\theta(x_i))$
- Minimize <u>cross entropy</u>: $-\sum_{i=1}^{n} y_i \cancel{\log} h_\theta(x_i) + (1 - y_i) \log(1 - h_\theta(x_i))$

Max $-\Sigma$ SSE

Min Σ SSE

Decision Trees

Entropy

$-\Sigma p_i \log p_i$

minimizing encoding

MSE for logistic regression and gradient descent

- Suppose we take mean sum-squared error as the loss function.
- Consider two inputs $x = (x_1, x_2)$

$$C = \frac{1}{n}\sum_{i=1}^{n}(y_i - \sigma(z_i))^2, \text{ where } z_i = \theta_0 + \theta_1 x_{i_1} + \theta_2 x_{i_2}$$

MSE for logistic regression and gradient descent

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$2\,\underline{(*)}^2 \times \underline{d*}$

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$$\frac{\partial C}{\partial \theta_j} = \frac{2}{n}\sum_{i=1}^{n}(y_i - \sigma(z_i)) \cdot -\frac{\partial \sigma(z_i)}{\partial \theta_j} = \frac{2}{n}\sum_{i=1}^{n}(\sigma(z_i) - y_i)\,\underline{\frac{\partial \sigma(z_i)}{\partial z_i}\frac{\partial z_i}{\partial \theta_j}}$$

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MSE for logistic regression and gradient descent . . .

- For $j = 1, 2$, $\dfrac{\partial C}{\partial \theta_j} = \dfrac{2}{n}\sum_{i=1}^{n}(\sigma(z_i) - y_i)\sigma'(z_i)x_j^i$, and $\dfrac{\partial C}{\partial \theta_0} = \dfrac{2}{n}\sum_{i=1}^{n}(\sigma(z_i) - y_i)\sigma'(z_i)$
- Each term in $\dfrac{\partial C}{\partial \theta_1}, \dfrac{\partial C}{\partial \theta_2}, \dfrac{\partial C}{\partial \theta_0}$ is proportional to $\sigma'(z_i)$

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MSE for logistic regression and gradient descent . . .

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$\theta_i + \alpha \dfrac{\partial C}{\partial \theta_i}$

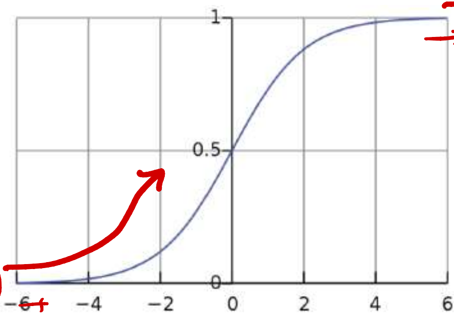
- Ideally, gradient descent should take large steps when $\boxed{\sigma(z) - y}$ is large

y_i

- $\sigma(z)$ is flat at both extremes

- If $\sigma(z)$ is completely wrong, $\sigma(z) \approx (1 - y)$, we still have $\sigma'(z) \approx 0$

- Learning is slow even when current model is far from optimal



$\sigma(z_i)$

Cross entropy and gradient descent

- $C = -[y \ln(\sigma(z)) + (1-y)\ln(1-\sigma(z))]$

Cross entropy and gradient descent

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Cross entropy and gradient descent

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- The greater the error, the faster the learning rate