Instituto de Computação
UNIVERSIDADE ESTADUAL DE CAMPINAS

Capacitação profissional em tecnologias de Inteligência Artificial

Machine Learning Overview

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Institute of Computing - UNICAMP

Common ML Algorithms

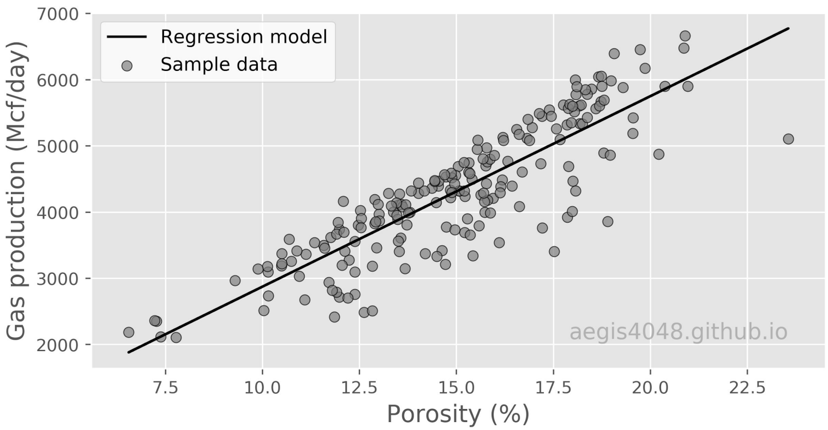
- **Machine learning**
  - **Supervised Learning**
    - Classification
      - Logistic regression
      - SVM
      - Neural Network
      - Decision Tree
      - Random Forest
      - GBDT
      - KNN
      - Naive Bayes
    - Regression
      - Linear regression
      - SVM
      - Neural Network
      - Decision Tree
      - Random Forest
      - GBDT
  - **Unsupervised Learning**
    - Clustering
      - K-means
      - Hierarchical clustering
      - Density-based clustering
    - Others
      - Correlation rule
      - Principal component analysis (PCA)
      - Gaussian mixture models (GMM)

Linear Regression

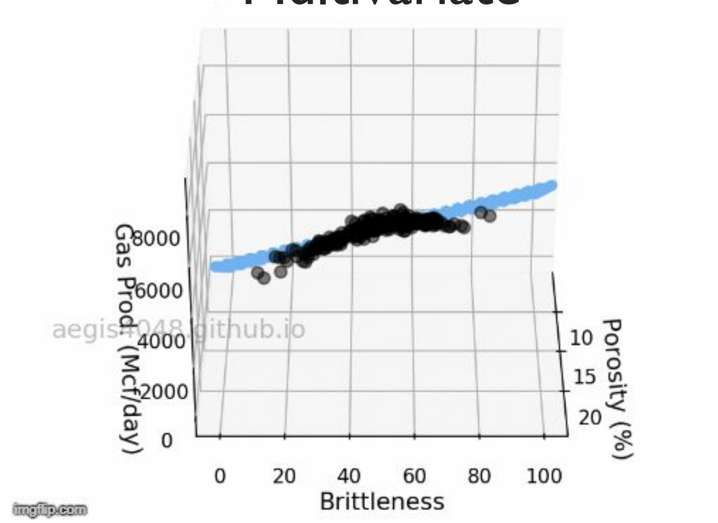
Linear regression

- Statistical analysis method to determine linear relationships between a scalar response (output variable or label) and one or more explanatory variables (input variables or features)

Univariate



Multivariate



Source: https://aegis4048.github.io/mutiple_linear_regression_and_visualization_in_python

Linear regression

Let:

- θ: Set of model parameters. $\theta = \{\theta_0, \theta_1, \ldots, \theta_n\}$
- x: Set of input variables. $x = \{x_1, x_2, \ldots, x_n\}$
- $\hat{y}$: model output (predicted value)
- $\hat{y} = \theta_0 + \theta_1 \cdot x_1 + \ldots + \theta_n \cdot x_n$
- $\hat{y} = \theta_0 + \theta_1 \cdot x_1$
- $h_\theta(x) = \theta_0 + \theta_1 \cdot x_1 + \ldots + \theta_n \cdot x_n$

Multivariate linear model

Univariate linear model

Also known has hypothesis!

Linear regression

Linear model

- $h_\theta(x) = \theta_0 + \theta_1 \cdot x_1 + \ldots + \theta_n \cdot x_n$

Linear regression

Linear model

- $h_{\theta}(x) = \theta_0 + \theta_1 \cdot x_1 + \ldots + \theta_n \cdot x_n$

Also explained as:

- $h_w(x) = \mathbf{b} + \boldsymbol{w_1} \cdot x_1 + \ldots + \boldsymbol{w_n} \cdot x_n$
- $h(x) = \mathbf{intercept} + \boldsymbol{coef_1} \cdot x_1 + \ldots + \boldsymbol{coef_n} \cdot x_n$

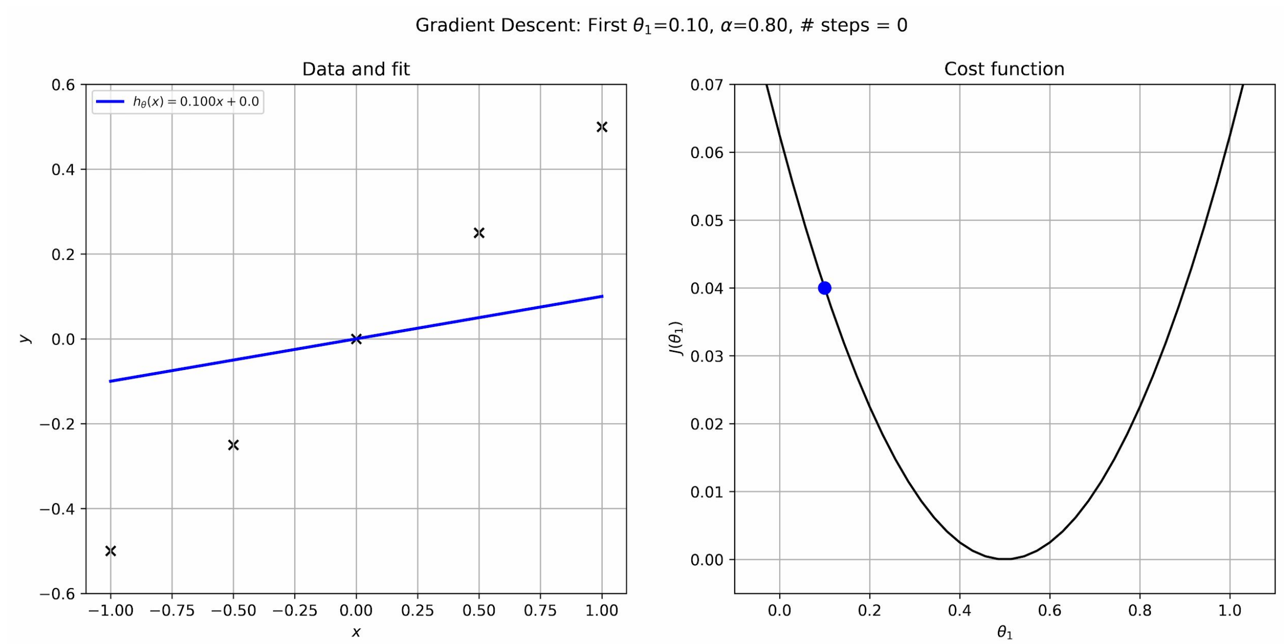
Linear regression

Linear model

- $h_\theta(x) = \theta_0 + \theta_1 \cdot x_1 + \ldots + \theta_n \cdot x_n$

Training

Select θ so that the cost function is minimized



Linear regression

Linear model

- $h_\theta(x) = \theta_0 + \theta_1 \cdot x_1 + \ldots + \theta_n \cdot x_n$

Cost function:

- Usually the Mean Squared Error (MSE)

$$J(\theta) = \underbrace{\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2}_{\mathrm{MSE}(X, h_\theta)}$$

Linear regression

Can also be the Mean Absolute Error (MAE)

Linear model

- $h_\theta(x) = \theta_0 + \theta_1 \cdot x_1 + \ldots + \theta_n \cdot x_n$

Cost function:

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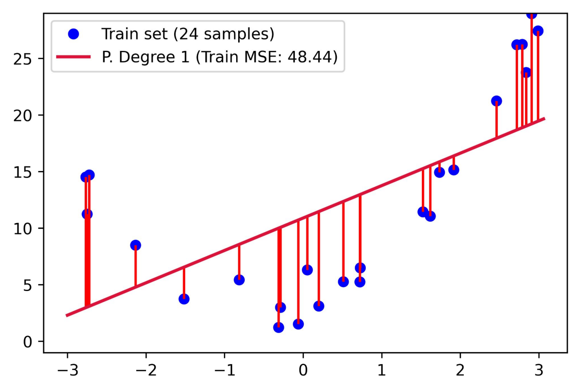
Polynomial regression

Similar to linear regression.

<u>Polynomial model</u>

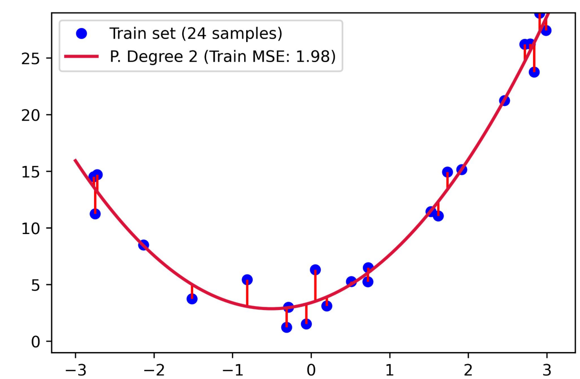
- $h_\theta(x) = \theta_0 + \theta_1 \cdot x_1 + \theta_2 \cdot x_1^{\,2} + \theta_3 \cdot x_1^{\,3} + \ldots + \theta_n \cdot x_1^{\,n}$

Linear model



$f(x) = 10.895022 + 2.863998\, x$

Poly. degree = 2



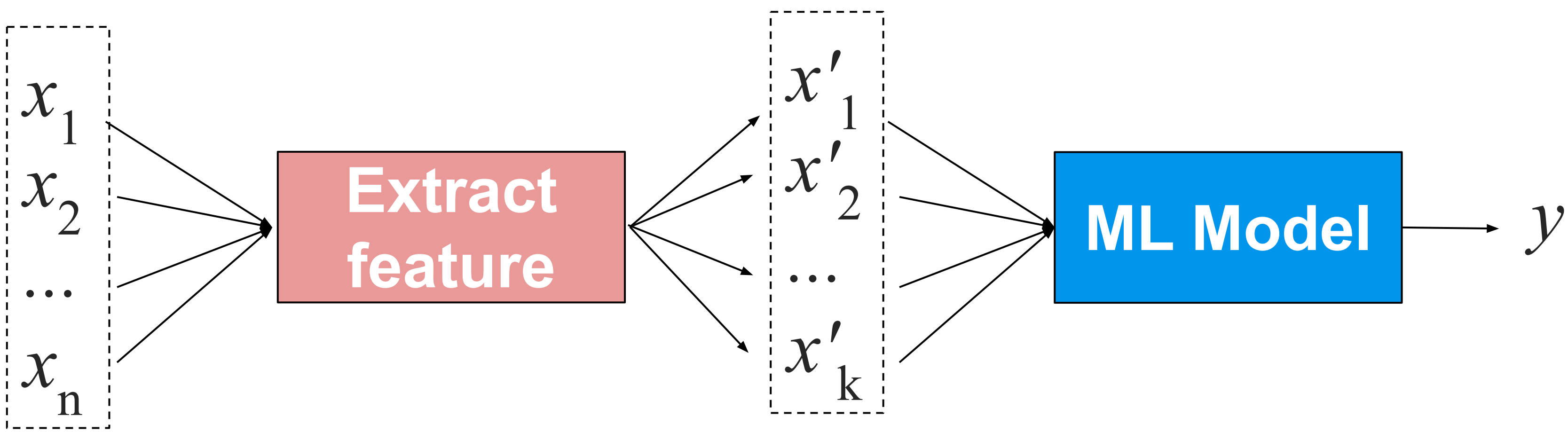
$f(x) = 3.403875 + 2.122188\, x + 2.099980\, x^2$

Polynomial regression

Similar to linear regression.

<u>Polynomial model</u>

- $h_\theta(x) = \theta_0 + \theta_1 \cdot x_1 + \theta_2 \cdot x_1^{\,2} + \theta_3 \cdot x_1^{\,3} + \ldots + \theta_n \cdot x_1^{\,n}$



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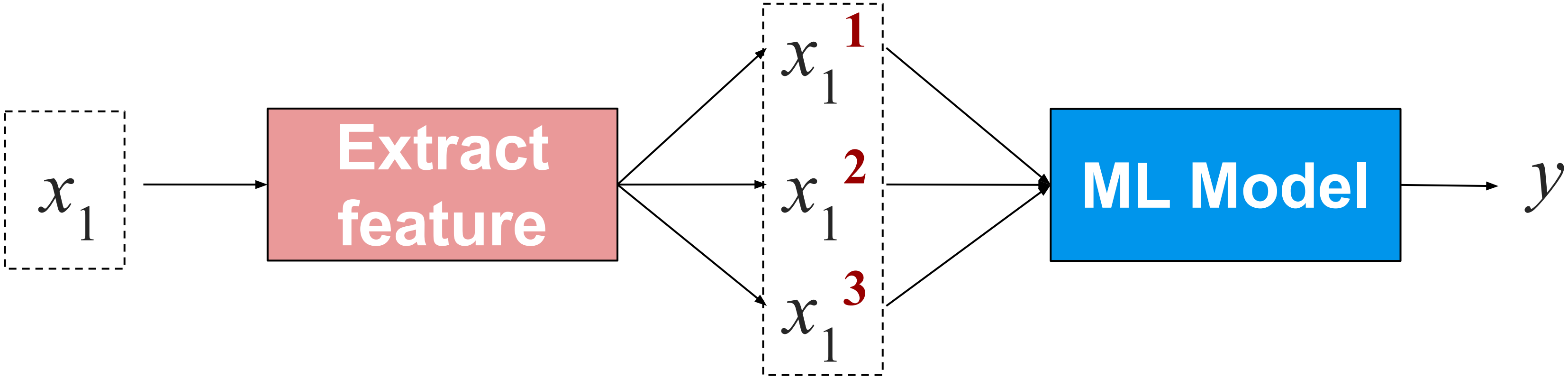

Polynomial regression

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<u>Polynomial model</u>

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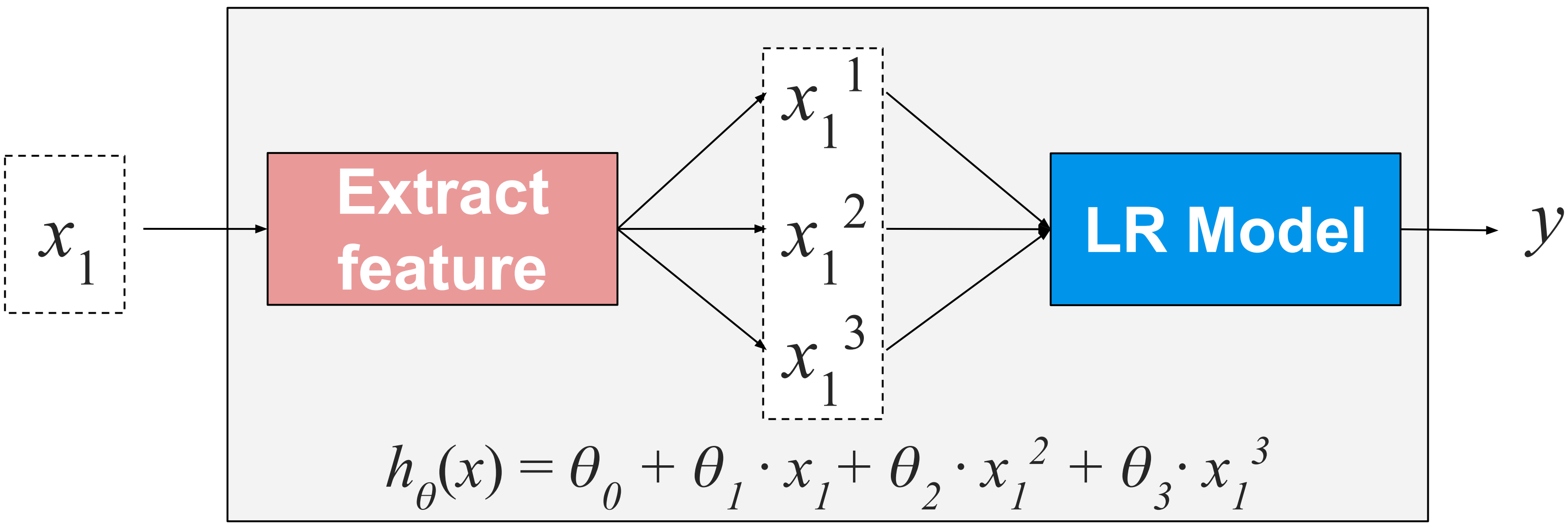


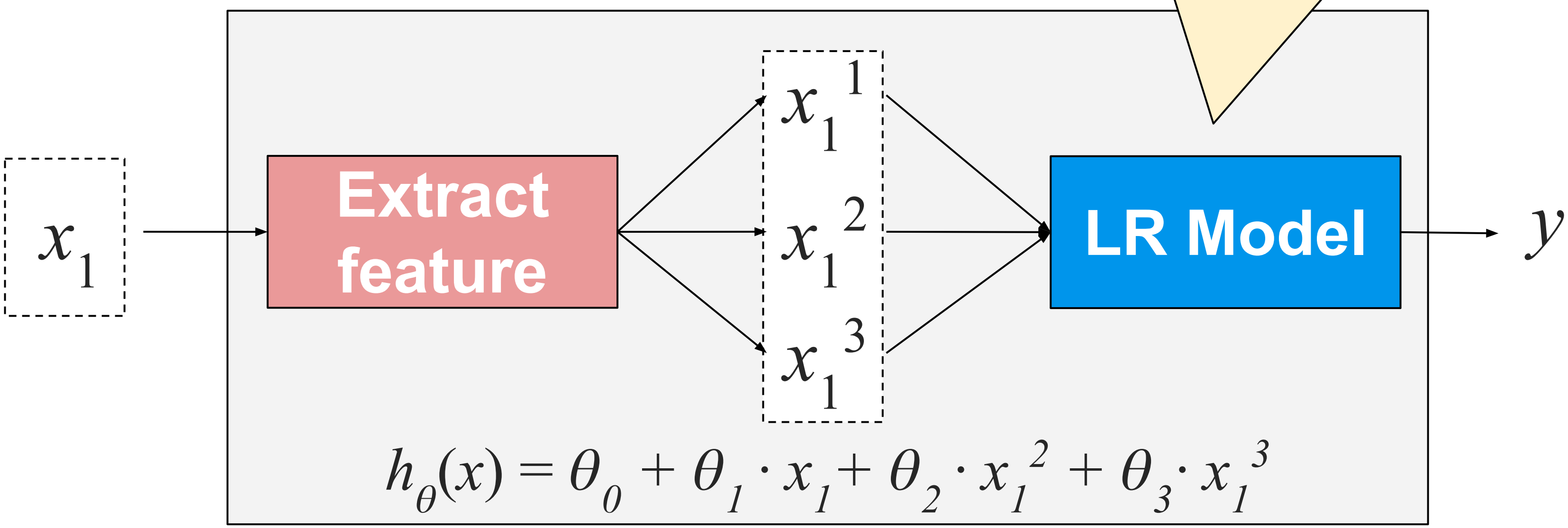
Polynomial regression

Similar to linear reg

Polynomial model

- $h_\theta(x) = \theta_0 + \theta_1 \cdot x_1 + \theta_2 \cdot x_1^2 + \theta_3 \cdot x_1^3 + \ldots + \theta_n$

Train in the same way we train linear regression models!



Supervised Learning Algorithms
Linear Regression

Polynomial regression

Similar to linear reg

<u>Polynomial model</u>

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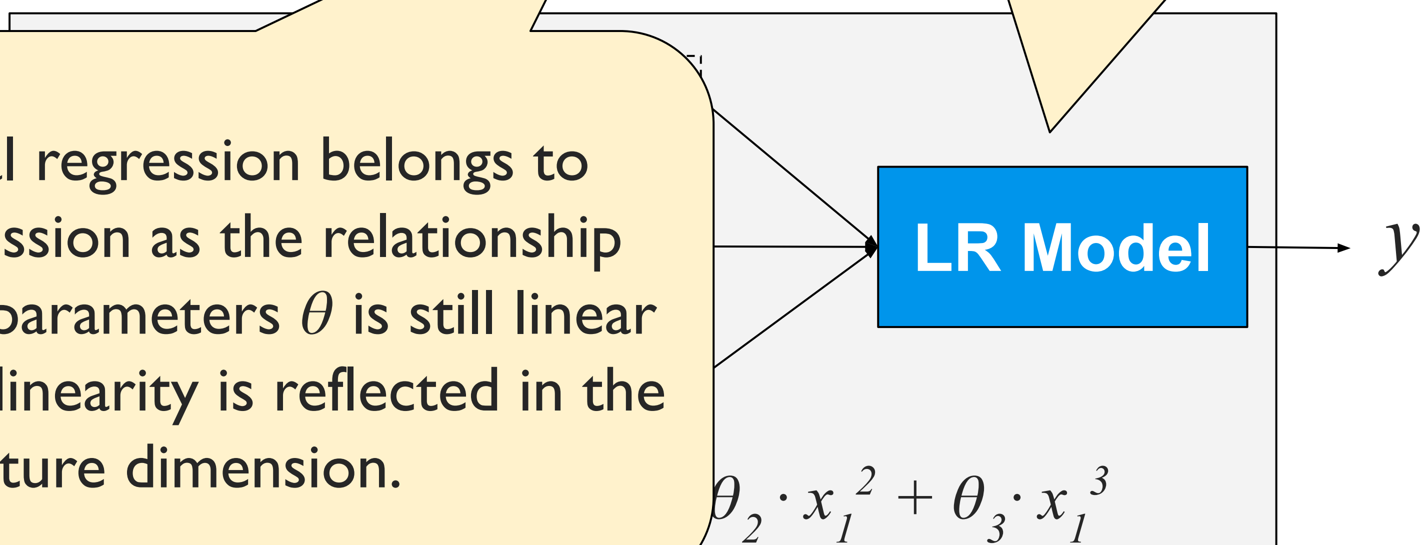


Polynomial regression belongs to linear regression as the relationship between its parameters θ is still linear while its nonlinearity is reflected in the feature dimension.

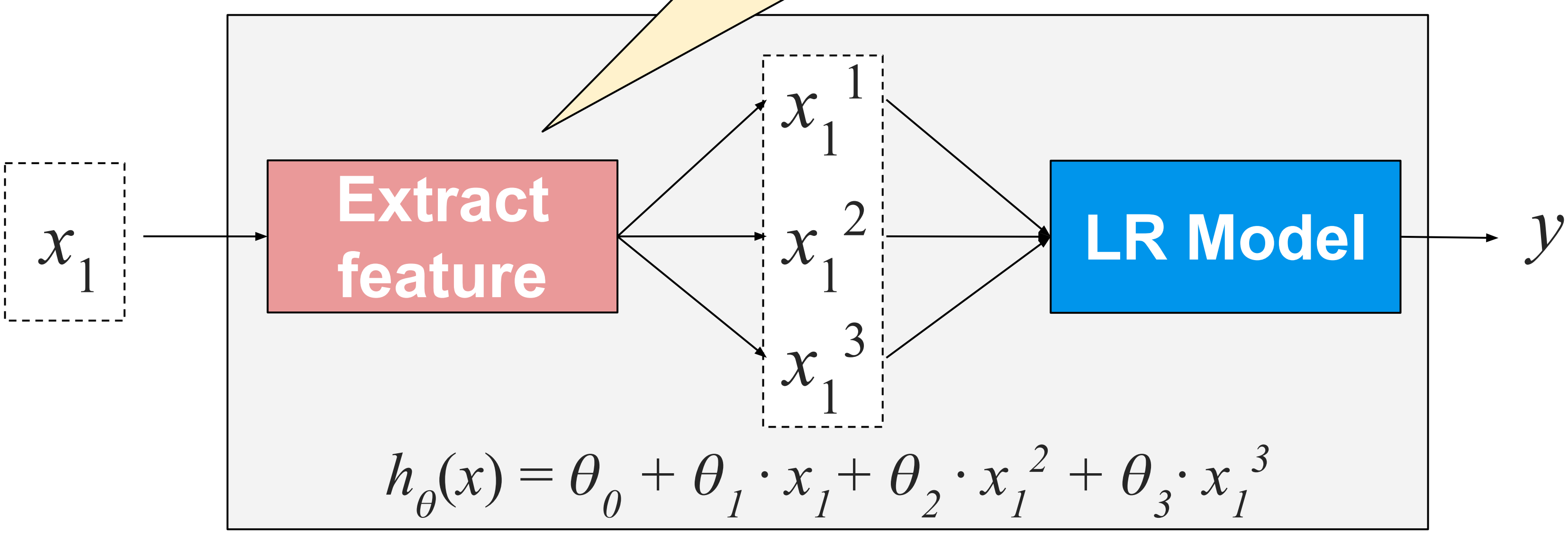
Polynomial regression

Scikit Learn
PolynomialFeatures module

Similar to linear regressi

Polynomial model

- $h_\theta(x) = \theta_0 + \theta_1 \cdot x_1 + \theta_2 \cdot x_1^2 + \ldots + \theta_n \cdot x_1^n$



Ridge/Lasso regression

In linear (and polynomial) regression, the more input variables, the more parameters the model will have, and the greater the chance of overfitting the training data

Ridge/Lasso regression

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An approach to minimize overfit is to tweak the training process to produce a model with small parameter (θ) values

Supervised Learning Algorithms
Linear Regression

Ridge/Lasso regression

In linear (and polynomial) regression, the more input variables, the ... have, and the greater the ... e of overfitting the training data

This is called regularization!

An approach to minimize overfit is to tweak the training process to produce a model with small parameter (θ) values

Ridge/Lasso regression

How do we tweak the training process to produce a model with small parameter (θ) values?

Ridge/Lasso regression

How do we tweak the training process to produce a model with small parameter (θ) values?

- By penalizing the cost function with θ values!

$$J(\theta) = \underbrace{\frac{1}{\mathrm{m}} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2}_{\mathrm{MSE}(\mathrm{X}, h_\theta)} + \boxed{(\theta_1^{\ 2} + \theta_2^{\ 2} + \ldots + \theta_n^{\ 2})}$$

Ridge/Lasso regression

How do we tweak the training process to produce a model with small parameter (θ) values?

- By penalizing the cost function with θ values!

θ_0 (a.k.a. bias) is not penalized

$$J(\theta) = \underbrace{\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2}_{\mathrm{MSE}(X,h_\theta)} + \boxed{(\theta_1^{\,2} + \theta_2^{\,2} + \ldots + \theta_n^{\,2})}$$

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$$J(\theta) = \underbrace{\frac{1}{\mathrm{m}} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2}_{\mathrm{MSE}(\mathrm{X}, h_\theta)} + \boxed{\alpha \,.\, (\theta_1^{\,2} + \theta_2^{\,2} + \ldots + \theta_n^{\,2})}$$

α: hyperparameter

Ridge/Lasso regression

How do we tweak the training process to produce
a model with small par

- By penalizing the co

Assuming w = $\{\theta_1, \ldots, \theta_n\}$,
then, $(\theta_1^{\,2} + \theta_2^{\,2} + \ldots + \theta_n^{\,2}) = ||\mathrm{w}||_2^{\,2}$

$$J(\theta) = \underbrace{\frac{1}{\mathrm{m}} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2}_{\mathrm{MSE}(\mathrm{X}, h_\theta)} + \boxed{\alpha \,.\, (\theta_1^{\,2} + \theta_2^{\,2} + \ldots + \theta_n^{\,2})}$$

Ridge/Lasso regression

How do we tweak the training process to produce a model with small par…

- By penalizing the co…

Assuming w = $\{\theta_1, \ldots, \theta_n\}$,
then, $(|\theta_1| + |\theta_2| + \ldots + |\theta_n|) = ||w||_1$

$$J(\theta) = \underbrace{\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2}_{\mathrm{MSE}(X, h_\theta)} + \boxed{\alpha \cdot (|\theta_1| + |\theta_2| + \ldots + |\theta_n|)}$$

Ridge/Lasso regression

$$J(\theta) = \underbrace{\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2}_{\text{MSE}(X,h_\theta)} + \boxed{\alpha \,.\, (\theta_1^{\,2} + \theta_2^{\,2} + \ldots + \theta_n^{\,2})}$$

Ridge regression

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Lasso regression

Supervised Learning Algorithms

Line

Ridge/Lasso regre

Tends to produce small parameter values (close to zero), but not zero.

$$J(\theta) = \underbrace{\frac{1}{\mathrm{m}} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2}_{\mathrm{MSE}(\mathrm{X}, h_\theta)} + \boxed{\alpha \;.\; (\theta_1^{\,2} + \theta_2^{\,2} + \ldots + \theta_n^{\,2})}$$

Ridge regression

$$J(\theta) = \frac{1}{\mathrm{m}} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 + \boxed{\alpha \;.\; (|\theta_1| + |\theta_2| + \ldots + |\theta_n|)}$$

Tends to zero-out parameters associated with non-informative features! Can be used to simplify models!

$$h_\theta(x) = \theta_0 + \theta_1 \cdot x_1 + \ldots + \theta_n \cdot x_n$$

Ridge/Lasso regression

$$J(\theta) = \underbrace{\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2}_{\mathrm{MSE}(\mathrm{X},h_\theta)} + \boxed{\alpha \,.\, (\theta_1^{\,2} + \theta_2^{\,2} + \ldots + \theta_n^{\,2})}$$

Make sure you perform feature scaling if using Ridge/Lasso regression

Elastic Net regression

- Combines both Ridge and Lasso regression
- Hyperparameter r: mix ratio

r: mix ratio

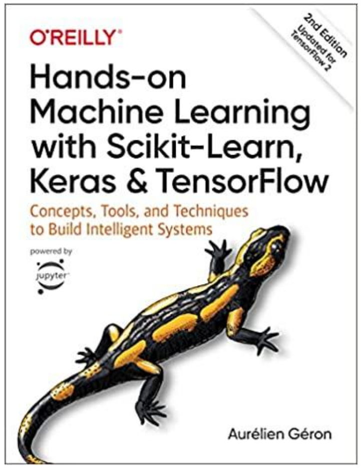
$$J(\theta) = \underbrace{\frac{1}{\mathrm{m}} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2}_{\mathrm{MSE}(\mathrm{X}, h_\theta)} + \underbrace{r.\alpha.\sum_{i=1}^{n} |\theta_i|}_{\text{Lasso Regularization Term}} + (1\text{-}r).\alpha.\underbrace{\sum_{i=1}^{n} (\theta_i)^2}_{\text{Ridge Regularization Term}}$$

General recommendations

- It is usually preferable to have at least a little bit of regularization: Avoid plain LR!
- Make sure you perform feature scaling if using Ridge/Lasso/Elastic Net regression
- Ridge is a good default, but if you suspect only a few features are actually useful, you should prefer Lasso or Elastic Net
  - Both tend to reduce the useless features' weights down to zero.

Supervised Learning Algorithms
Linear Regression

References



- Aurelien Geron. Hands-on Machine Learning with Scikit-Learn, Keras, and TensorFlow: Concepts, Tools, and Techniques to Build Intelligent Systems - 2019
  - Chapter 4

- Logistic Regression on the scikit-learn website:
  - https://scikit-learn.org/stable/modules/linear_model.html

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Video Index

Video lessons	Length	Start	Length	Subtopics	
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		0:03:30	0:02:35		Linear model
		0:06:05	0:02:26		Training / Cost function
		0:08:31	0:05:23	Polynomial Regression	Polynomial regression
		0:13:54	0:06:27	Ridge/Lasso regression	Ridge/Lasso regression
		0:20:21	0:02:13	Elastic Net regression	Elastic Net regression
		0:22:34	0:02:01	General recommendations	General recommendations
		0:24:35			