# Data Mining:
## Overfitting & Regularization

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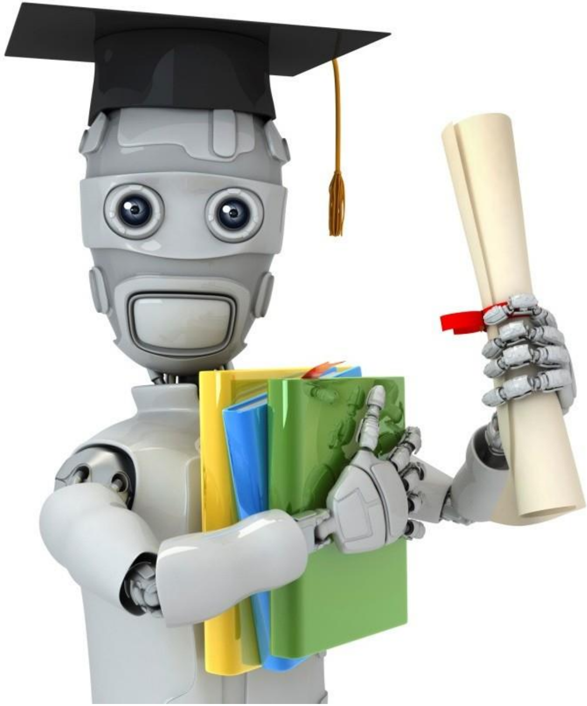
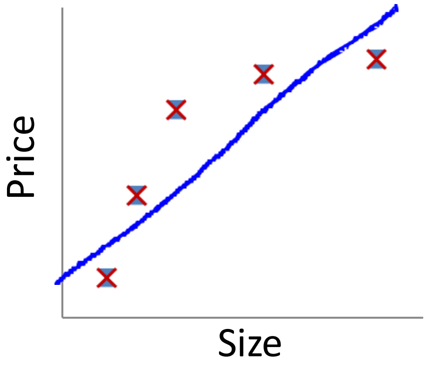


Machine Learning

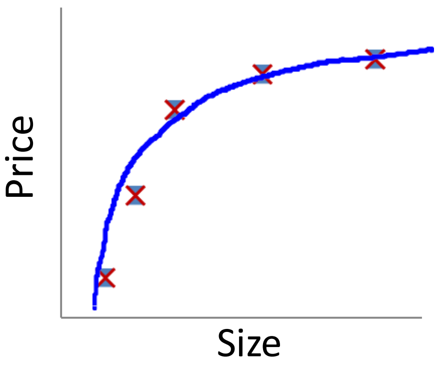
# Regularization

## The problem of overfitting

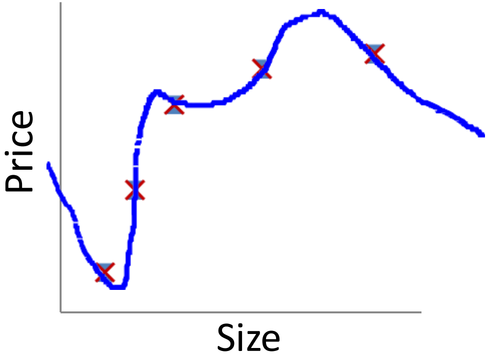
# Example: Linear regression (housing prices)




$\theta_0 + \theta_1 x$




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




$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

**Overfitting:** If we have too many features, the learned hypothesis may fit the training set very well ($J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 \approx 0$), but fail to generalize to new examples (predict prices on new examples).

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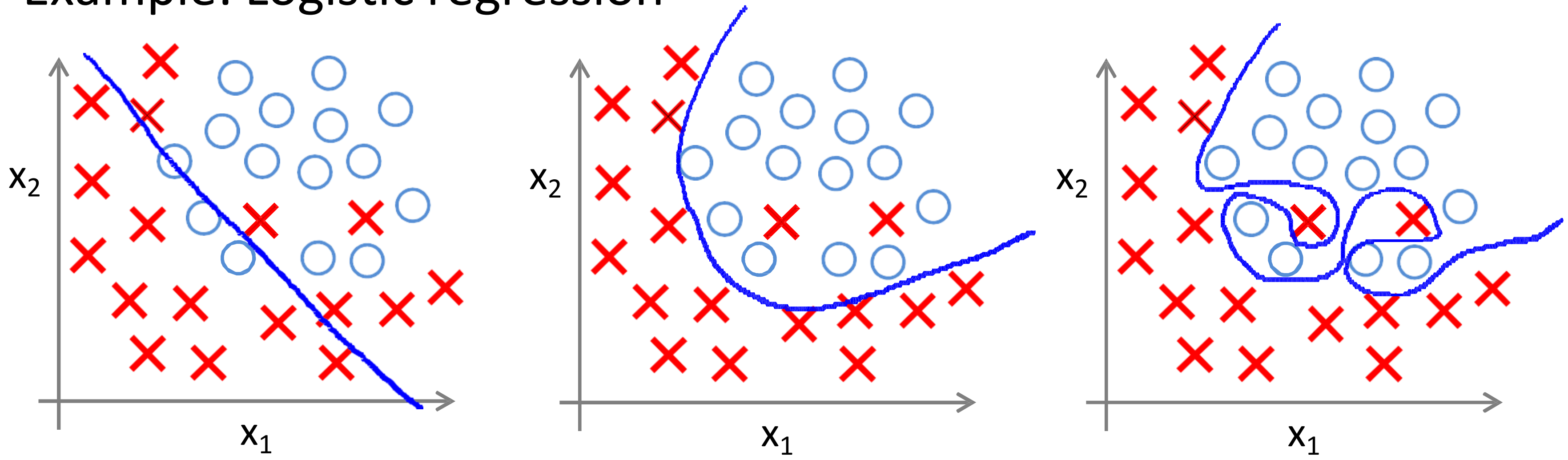
# Example: Logistic regression




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

( $g$ = sigmoid function)

$$g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2 + \theta_5 x_1 x_2)$$

$$g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 + \theta_5 x_1^2 x_2^3 + \theta_6 x_1^3 x_2 + \dots)$$

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Consider the medical diagnosis problem of classifying tumors as malignant or benign. If a hypothesis $h_\theta(x)$ has overfit the training set, it means that:

- It makes accurate predictions for examples in the training set and generalizes well to make accurate predictions on new, previously unseen examples.
- It does not make accurate predictions for examples in the training set, but it does generalize well to make accurate predictions on new, previously unseen examples.
- It makes accurate predictions for examples in the training set, but it does not generalize well to make accurate predictions on new, previously unseen examples.
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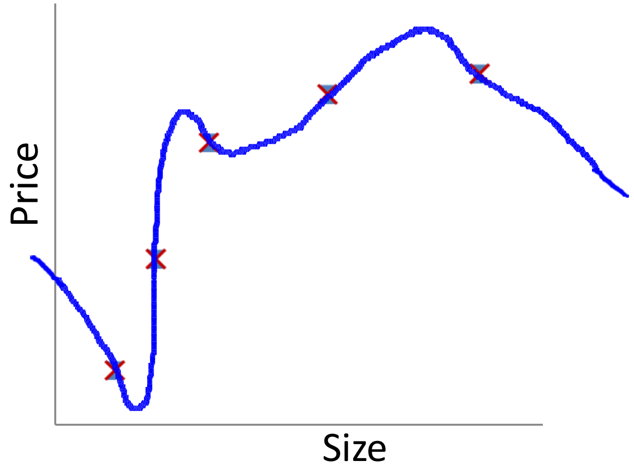
## Addressing overfitting:

$x_1 =$ size of house
$x_2 =$ no. of bedrooms
$x_3 =$ no. of floors
$x_4 =$ age of house
$x_5 =$ average income in neighborhood
$x_6 =$ kitchen size

$\vdots$

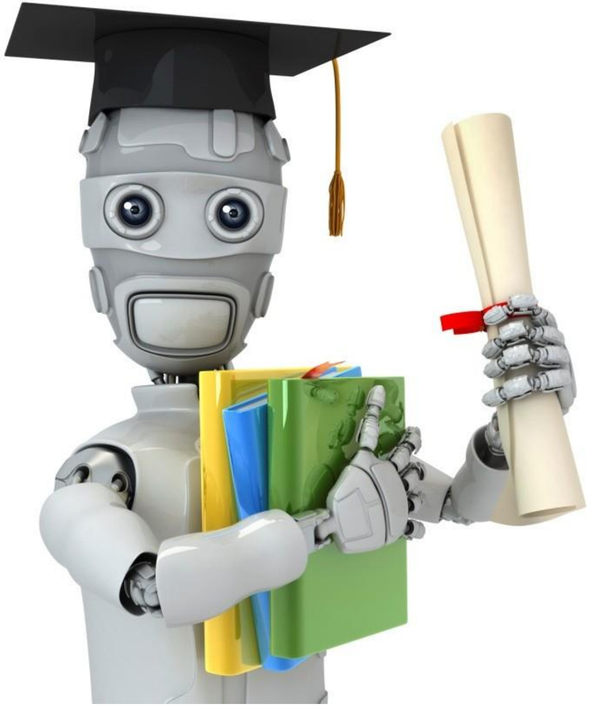
$x_{100}$



## Addressing overfitting:

Options:

1. Reduce number of features.
   - Manually select which features to keep.
   - Model selection algorithm (later in course).
2. Regularization.
   - Keep all the features, but reduce magnitude/values of parameters $\theta_j$.
   - Works well when we have a lot of features, each of which contributes a bit to predicting $y$.



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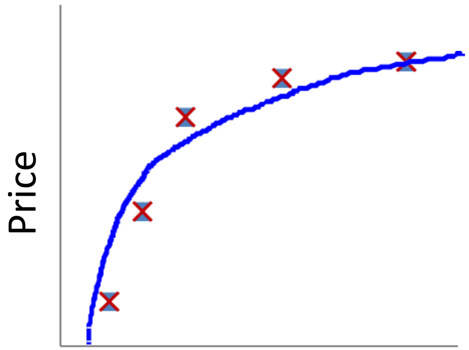
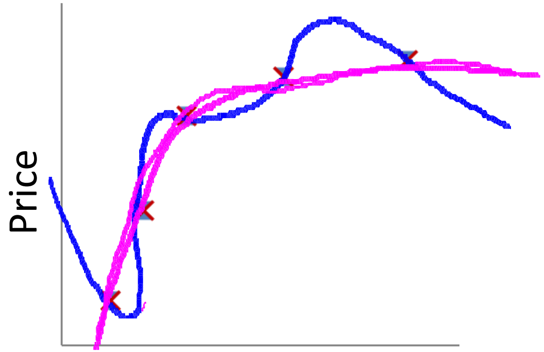
# Regularization

## Cost function

# Intuition




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




$$\theta_0 + \theta_1 x + \theta_2 x^2 + \cancel{\theta_3 x^3} + \cancel{\theta_4 x^4}$$

Suppose we penalize and make $\theta_3, \theta_4$ really small.

$$\min_\theta \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 + 1000\,\theta_3^2 + 1000\,\theta_4^2$$

# Regularization.

Small values for parameters $\theta_0, \theta_1, \ldots, \theta_n$

— "Simpler" hypothesis

— Less prone to overfitting

Housing:

— Features: $x_1, x_2, \ldots, x_{100}$

— Parameters: $\theta_0, \theta_1, \theta_2, \ldots, \theta_{100}$

$$J(\theta) = \frac{1}{2m} \left[ \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 \qquad\qquad \right]$$

## Regularization.

Small values for parameters $\theta_0, \theta_1, \ldots, \theta_n$

- "Simpler" hypothesis
- Less prone to overfitting

Housing:

- Features: $x_1, x_2, \ldots, x_{100}$
- Parameters: $\theta_0, \theta_1, \theta_2, \ldots, \theta_{100}$

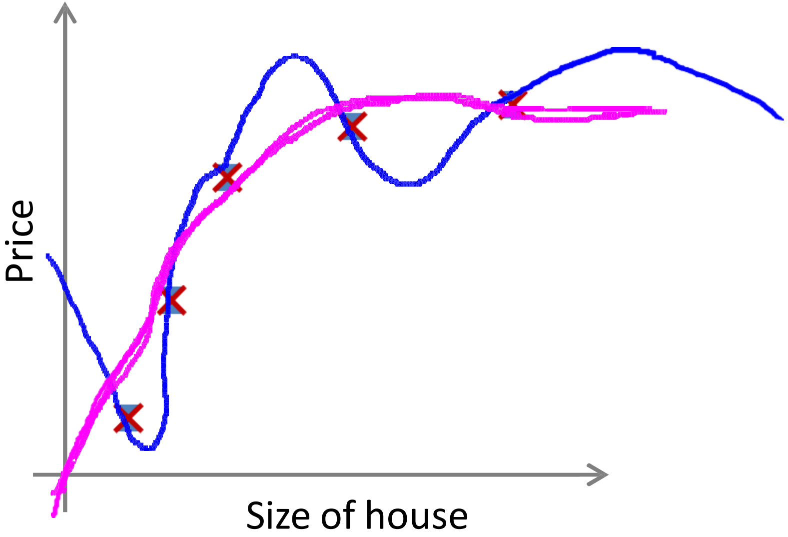
$$J(\theta) = \frac{1}{2m} \left[ \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n} \theta_j \right]$$

# Regularization.

Positive regularization parameter

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda\sum_{j=1}^{n}\theta_j^2\right]$$

$$\min_\theta J(\theta)$$



In regularized linear regression, we choose $\theta$ to minimize

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda\sum_{j=1}^{n}\theta_j^2\right]$$

What if $\lambda$ is set to an extremely large value (perhaps for too large for our problem, say $\lambda = 10^{10}$)?

- Algorithm works fine; setting $\lambda$ to be very large can’t hurt it
- Algortihm fails to eliminate overfitting.
- Algorithm results in underfitting. (Fails to fit even training data well).
- Gradient descent will fail to converge.

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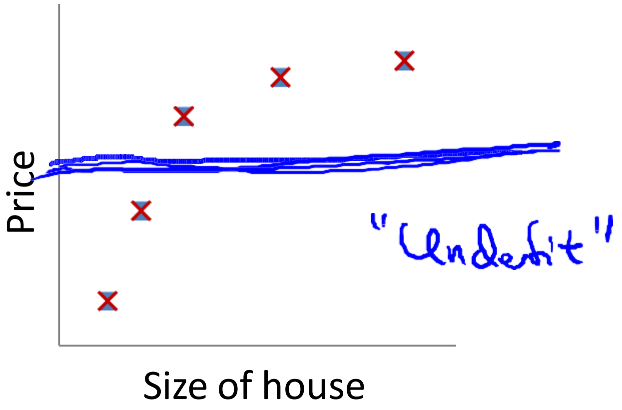


$\underline{\theta_1}, \underline{\theta_2}, \underline{\theta_3}, \underline{\theta_4}$

$\theta_1 \approx 0, \theta_2 \approx 0$

$\theta_3 \approx 0, \theta_4 \approx 0$

$$\boxed{h_\theta(x) = \theta_0}$$

$h_\theta(x)$

$$\theta_0 + \cancel{\theta_1 x} + \cancel{\theta_2 x^2} + \cancel{\theta_3 x^3} + \cancel{\theta_4 x^4}$$

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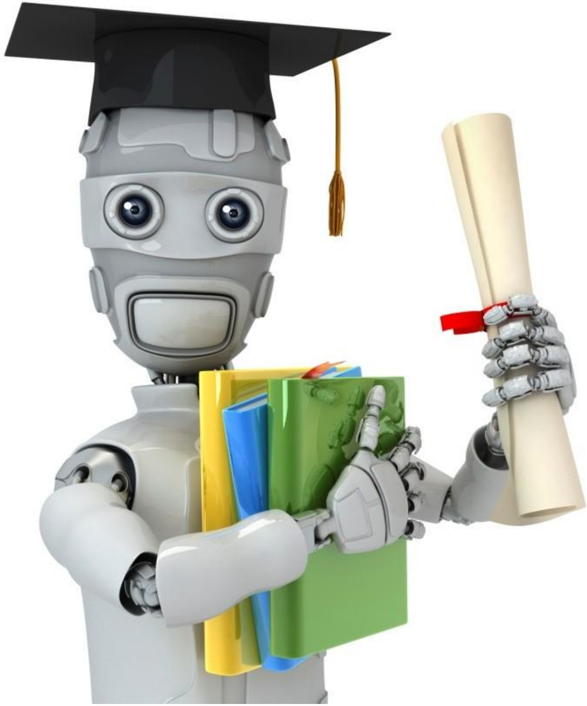

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# Regularization

## Regularized linear regression

# Regularized linear regression

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda\sum_{j=1}^{n}\theta_j^2\right]$$

$$\min_\theta \underline{J(\theta)}$$

# Gradient descent

Repeat $\{$

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \left[ \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j \right]$$

$$(j = \cancel{0}, \underline{1, 2, 3, \ldots, n})$$

$\}$

$J(\theta)$

$$\theta_j := \theta_j (1 - \alpha \frac{\lambda}{m}) - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

# Normal equation

$$X = \begin{bmatrix} (x^{(1)})^T \\ \vdots \\ (x^{(m)})^T \end{bmatrix} \qquad y = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(m)} \end{bmatrix} \quad \mathbb{R}^m$$

$m \times (n+1)$

$$\rightarrow \min_\theta J(\theta)$$

$$\theta = \Big( X^T X + \lambda \underbrace{\begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & & & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}}_{(n+1)\times(n+1)} \Big)^{-1} X^T y$$

E.g. $n = 2$ $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

# Non-invertibility (optional/advanced).

Suppose $m \leq n$,
(#examples) (#features)

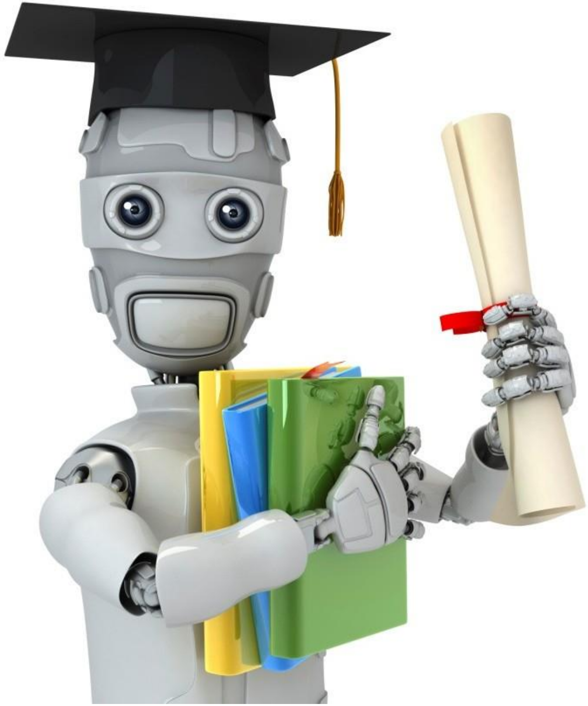
$$\theta = (X^T X)^{-1} X^T y$$

Non-invertible or singular

If $\lambda > 0$,

$$\theta = \left( X^T X + \lambda \begin{bmatrix} 0 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix} \right)^{-1} X^T y$$

Invertible



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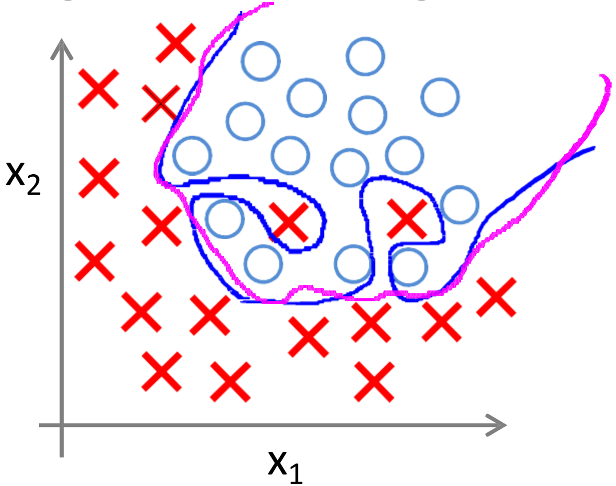
# Regularization

## Regularized logistic regression

# Regularized logistic regression.




$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 + \theta_5 x_1^2 x_2^3 + \dots)$$

Cost function:

$$\rightarrow J(\theta) = -\left[\frac{1}{m}\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))\right]$$

$$+ \frac{\lambda}{2m} \sum_{j=1}^{n} \theta_j^2$$

$\boxed{\theta_1, \theta_2, \dots, \theta_n}$

# Gradient descent

Repeat $\{$

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \underbrace{\left[ \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j \right]}_{\frac{\partial}{\partial \theta_j} J(\theta)}$$

$$(j = \cancel{0}, \underbrace{1, 2, 3, \ldots, n}_{\theta_1 \ldots \theta_n})$$

$\}$

$$h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$$

# Unified Formulation

- General cost function

$$J(\boldsymbol{\theta}) = \lambda R(\boldsymbol{\theta}) + \frac{1}{m}\sum_{i=1}^{m} L\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right), y^{(i)}\right)$$

  - Loss function $L$ measures the cost to pay for inaccuracy prediction, e.g.,
    - Square loss, Logistic loss, Hinge loss, etc.
  - Regularization function $R$ to make the prediction model simple or prevent overfitting, e.g.,
    - L2 norm (Tikhonov regularization): $R(\boldsymbol{\theta}) = \frac{1}{2}\|\boldsymbol{\theta}\|_2^2$
    - L1 norm (LASSO): $R(\boldsymbol{\theta}) = \|\boldsymbol{\theta}\|_1$
    - Elastic net: $R(\boldsymbol{\theta}) = \frac{\alpha}{2}\|\boldsymbol{\theta}\|_2^2 + (1-\alpha)\|\boldsymbol{\theta}\|_1, 0 < \alpha < 1$

# References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- Robert Tibshirani, "Regression shrinkage and selection via the lasso." Journal of the Royal Statistical Society. Series B (Methodological) (1996): 267-288.
- Hui Zou, and Trevor Hastie. "Regularization and variable selection via the elastic net." Journal of the Royal Statistical Society: Series B (Statistical Methodology) 67.2 (2005): 301-320.