Linear Regression

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Regression

Given:

- Data \( X = \{ x^{(1)}, \ldots, x^{(n)} \} \) where \( x^{(i)} \in \mathbb{R}^d \)

- Corresponding labels \( Y = \{ y^{(1)}, \ldots, y^{(n)} \} \) where \( y^{(i)} \in \mathbb{R} \)

Linear Regression

• Hypothesis:

\[ y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_d x_d = \sum_{j=0}^{d} \theta_j x_j \]

Assume \( x_0 = 1 \)

• Fit model by minimizing sum of squared errors

Figures are courtesy of Greg Shakhnarovich
Least Squares Linear Regression

• Cost Function

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

• Fit by solving \( \min_\theta J(\theta) \)
Intuition Behind Cost Function

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

For insight on $J()$, let’s assume $x \in \mathbb{R}$ so $\theta = [\theta_0, \theta_1]$
Intuition Behind Cost Function

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Based on example by Andrew Ng
Intuition Behind Cost Function

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

For insight on \( J() \), let’s assume \( x \in \mathbb{R} \) so \( \theta = [\theta_0, \theta_1] \)

\[ h_\theta(x) \]
(for fixed \( \theta_1 \), this is a function of \( x \))

\[ J(\theta_1) \]
(function of the parameter \( \theta_1 \))

Based on example by Andrew Ng
Intuition Behind Cost Function

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

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Based on example by Andrew Ng
Intuition Behind Cost Function
Intuition Behind Cost Function

$h_\theta(x)$
(for fixed $\theta_0$, $\theta_1$, this is a function of $x$)

$J(\theta_0, \theta_1)$
(function of the parameters $\theta_0$, $\theta_1$)

Slide by Andrew Ng
Intuition Behind Cost Function

\( h_\theta(x) \)
(for fixed \( \theta_0, \theta_1 \), this is a function of \( x \))

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Intuition Behind Cost Function

$h_{\theta}(x)$
(for fixed $\theta_0$, $\theta_1$, this is a function of $x$)

$J(\theta_0, \theta_1)$
(function of the parameters $\theta_0$, $\theta_1$)
Basic Search Procedure

- Choose initial value for $\theta$
- Until we reach a minimum:
  - Choose a new value for $\theta$ to reduce $J(\theta)$

\[ J(\theta_0, \theta_1) \]

Figure by Andrew Ng
Basic Search Procedure

• Choose initial value for $\theta$
• Until we reach a minimum:
  – Choose a new value for $\theta$ to reduce $J(\theta)$
Basic Search Procedure

• Choose initial value for $\theta$
• Until we reach a minimum:
  – Choose a new value for $\theta$ to reduce $J(\theta)$

Since the least squares objective function is convex (concave), we don’t need to worry about local minima
Gradient Descent

- Initialize $\theta$
- Repeat until convergence

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

Simultaneous update for $j = 0 \ldots d$

Learning rate (small) e.g., $\alpha = 0.05$
Gradient Descent

- Initialize $\theta$
- Repeat until convergence

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

Simultaneous update for $j = 0 \ldots d$

For Linear Regression:

$$ \frac{\partial}{\partial \theta_j} J(\theta) = \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left( h_{\theta}(x^{(i)}) - y^{(i)} \right)^2 $$
Gradient Descent

- Initialize $\theta$
- Repeat until convergence

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

Simultaneous update for $j = 0 \ldots d$

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$$= \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left( \sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right)^2$$
Gradient Descent

- Initialize $\theta$
- Repeat until convergence

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

simultaneous update for $j = 0 \ldots d$

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$$= \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left( \sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right)^2$$

$$= \frac{1}{n} \sum_{i=1}^{n} \left( \sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right) \times \frac{\partial}{\partial \theta_j} \left( \sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right)$$
Gradient Descent

• Initialize $\theta$
• Repeat until convergence

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

simultaneous update for $j = 0 \ldots d$

For Linear Regression:

$$
\frac{\partial}{\partial \theta_j} J(\theta) = \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left( h_\theta(x^{(i)}) - y^{(i)} \right)^2
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= \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left( \sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right)^2
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$$

$$
= \frac{1}{n} \sum_{i=1}^{n} \left( \sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right) x_j^{(i)}
$$
Gradient Descent for Linear Regression

- Initialize $\theta$
- Repeat until convergence

$$
\theta_j \leftarrow \theta_j - \alpha \frac{1}{n} \sum_{i=1}^{n} \left( h_\theta \left( x^{(i)} \right) - y^{(i)} \right) x_j^{(i)}
$$

To achieve simultaneous update
- At the start of each GD iteration, compute $h_\theta \left( x^{(i)} \right)$
- Use this stored value in the update step loop

Assume convergence when

$$
\left\| \theta_{new} - \theta_{old} \right\|_2 < \epsilon
$$

L2 norm:

$$
\|v\|_2 = \sqrt{\sum_i v_i^2} = \sqrt{v_1^2 + v_2^2 + \ldots + v_{|v|}^2}
$$
Gradient Descent

\[ h_\theta(x) \]
(for fixed \( \theta_0, \theta_1 \), this is a function of \( x \))

\[ J(\theta_0, \theta_1) \]
(function of the parameters \( \theta_0, \theta_1 \))

\[ h(x) = -900 - 0.1 \times x \]
Gradient Descent

$h_\theta(x)$
(for fixed $\theta_0$, $\theta_1$, this is a function of $x$)

$J(\theta_0, \theta_1)$
(function of the parameters $\theta_0$, $\theta_1$)

Slide by Andrew Ng
Gradient Descent

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(for fixed \( \theta_0, \theta_1 \), this is a function of \( x \))

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Gradient Descent

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Slide by Andrew Ng
Choosing $\alpha$

$\alpha$ too small
- slow convergence

$\alpha$ too large
- Increasing value for $J(\theta)$
  - May overshoot the minimum
  - May fail to converge
  - May even diverge

To see if gradient descent is working, print out $J(\theta)$ each iteration
- The value should decrease at each iteration
- If it doesn’t, adjust $\alpha$
Extending Linear Regression to More Complex Models

• The inputs $X$ for linear regression can be:
  – Original quantitative inputs
  – Transformation of quantitative inputs
    • e.g. log, exp, square root, square, etc.
  – Polynomial transformation
    • example: $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$
  – Basis expansions
  – Dummy coding of categorical inputs
  – Interactions between variables
    • example: $x_3 = x_1 \cdot x_2$

This allows use of linear regression techniques to fit non-linear datasets.
Linear Basis Function Models

• Generally,
\[ h_\theta(x) = \sum_{j=0}^{d} \theta_j \phi_j(x) \]

• Typically, \( \phi_0(x) = 1 \) so that \( \theta_0 \) acts as a bias
• In the simplest case, we use linear basis functions:
\[ \phi_j(x) = x_j \]
Linear Basis Function Models

• Polynomial basis functions:
  \[ \phi_j(x) = x^j \]
  – These are global; a small change in \( x \) affects all basis functions

• Gaussian basis functions:
  \[ \phi_j(x) = \exp \left\{ -\frac{(x - \mu_j)^2}{2s^2} \right\} \]
  – These are local; a small change in \( x \) only affect nearby basis functions. \( \mu_j \) and \( s \) control location and scale (width).

Based on slide by Christopher Bishop (PRML)
Linear Basis Function Models

- Sigmoidal basis functions:

\[ \phi_j(x) = \sigma \left( \frac{x - \mu_j}{s} \right) \]

where

\[ \sigma(a) = \frac{1}{1 + \exp(-a)} \]

- These are also local; a small change in \( x \) only affects nearby basis functions. \( \mu_j \) and \( s \) control location and scale (slope).
Example of Fitting a Polynomial Curve with a Linear Model

\[ y = \theta_0 + \theta_1 x + \theta_2 x^2 + \ldots + \theta_p x^p = \sum_{j=0}^{p} \theta_j x^j \]
Linear Basis Function Models

- Basic Linear Model: \( h_\theta(\mathbf{x}) = \sum_{j=0}^{d} \theta_j x_j \)

- Generalized Linear Model: \( h_\theta(\mathbf{x}) = \sum_{j=0}^{d} \theta_j \phi_j(\mathbf{x}) \)

- Once we have replaced the data by the outputs of the basis functions, fitting the generalized model is exactly the same problem as fitting the basic model
  - Unless we use the kernel trick – more on that when we cover support vector machines
  - Therefore, there is no point in cluttering the math with basis functions

Based on slide by Geoff Hinton
**Linear Algebra Concepts**

- **Vector** in $\mathbb{R}^d$ is an ordered set of $d$ real numbers
  - e.g., $v = [1,6,3,4]$ is in $\mathbb{R}^4$
  - “[1,6,3,4]” is a column vector:
  - as opposed to a row vector:

\[
\begin{pmatrix}
1 \\
6 \\
3 \\
4
\end{pmatrix}
\quad \quad
\begin{pmatrix}
1 \\
6 \\
3 \\
4
\end{pmatrix}
\]

- An $m$-by-$n$ **matrix** is an object with $m$ rows and $n$ columns, where each entry is a real number:

\[
\begin{pmatrix}
1 & 2 & 8 \\
4 & 78 & 6 \\
9 & 3 & 2
\end{pmatrix}
\]

Based on slides by Joseph Bradley
Linear Algebra Concepts

• Transpose: reflect vector/matrix on line:

\[
\begin{pmatrix}
a \\
b
\end{pmatrix}^T = (a \ b) \quad \begin{pmatrix}
a & b \\
c & d
\end{pmatrix}^T = \begin{pmatrix}
a & c \\
b & d
\end{pmatrix}
\]

– Note: \((Ax)^T = x^TA^T\) (We’ll define multiplication soon…)

• Vector norms:
  – \(L_p\) norm of \(v = (v_1, \ldots, v_k)\) is
  \[
  \left( \sum_i |v_i|^p \right)^{\frac{1}{p}}
  \]
  – Common norms: \(L_1, L_2\)
  – \(L_{\infty}\) = \(\max_i |v_i|\)

• Length of a vector \(v\) is \(L_2(v)\)

Based on slides by Joseph Bradley
Linear Algebra Concepts

• Vector dot product: \[ u \cdot v = (u_1 \quad u_2) \cdot (v_1 \quad v_2) = u_1 v_1 + u_2 v_2 \]

  – Note: dot product of \( u \) with itself = length\((u)\)^2 = \( ||u||^2 \)

• Matrix product:

\[
A = \begin{pmatrix}
a_{11} & a_{12} \\
a_{21} & a_{22}
\end{pmatrix}, \quad
B = \begin{pmatrix}
b_{11} & b_{12} \\
b_{21} & b_{22}
\end{pmatrix}
\]

\[
AB = \begin{pmatrix}
a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} \\
a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22}
\end{pmatrix}
\]

Based on slides by Joseph Bradley
Linear Algebra Concepts

• Vector products:
  – Dot product: \[ u \cdot v = u^T v = \begin{pmatrix} u_1 & u_2 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = u_1 v_1 + u_2 v_2 \]

  – Outer product:
    \[ uv^T = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \begin{pmatrix} v_1 & v_2 \end{pmatrix} = \begin{pmatrix} u_1 v_1 & u_1 v_2 \\ u_2 v_1 & u_2 v_2 \end{pmatrix} \]
Vectorization

• Benefits of vectorization
  – More compact equations
  – Faster code (using optimized matrix libraries)

• Consider our model:

\[ h(x) = \sum_{j=0}^{d} \theta_j x_j \]

• Let

\[
\theta = \begin{bmatrix}
\theta_0 \\
\theta_1 \\
\vdots \\
\theta_d
\end{bmatrix} \quad \mathbf{x}^T = \begin{bmatrix}
1 & x_1 & \ldots & x_d
\end{bmatrix}
\]

• Can write the model in vectorized form as \( h(x) = \theta^T \mathbf{x} \)
Vectorization

• Consider our model for \( n \) instances:

\[
h \left( x^{(i)} \right) = \sum_{j=0}^{d} \theta_j x^{(i)}_j
\]

• Let

\[
\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix} \quad X = \begin{bmatrix} 1 & x^{(1)}_1 & \ldots & x^{(1)}_d \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x^{(i)}_1 & \ldots & x^{(i)}_d \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x^{(n)}_1 & \ldots & x^{(n)}_d \end{bmatrix}
\]

\( \mathbb{R}^{(d+1) \times 1} \)

\( \mathbb{R}^{n \times (d+1)} \)

• Can write the model in vectorized form as

\[
h_\theta(x) = X \theta
\]
Vectorization

• For the linear regression cost function:

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

\[
= \frac{1}{2n} \sum_{i=1}^{n} \left( \theta^T x^{(i)} - y^{(i)} \right)^2
\]

\[
= \frac{1}{2n} (X \theta - y)^T (X \theta - y)
\]

Let:

\[
y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{bmatrix}
\]

\[
X \in \mathbb{R}^{n \times (d+1)}
\]

\[
\theta \in \mathbb{R}^{(d+1) \times 1}
\]

\[
y \in \mathbb{R}^{1 \times n}
\]

\[
\theta \in \mathbb{R}^{n \times 1}
\]
Closed Form Solution

• Instead of using GD, solve for optimal $\theta$ analytically
  – Notice that the solution is when $\frac{\partial}{\partial \theta} J(\theta) = 0$

• Derivation:

$$J(\theta) = \frac{1}{2n} (X\theta - y)^T (X\theta - y)$$

$$\propto \theta^T X^T X \theta - y^T X \theta - \theta^T X^T y + y^T y$$

Take derivative and set equal to 0, then solve for $\theta$:

$$\frac{\partial}{\partial \theta} (\theta^T X^T X \theta - 2\theta^T X^T y + y^T y) = 0$$

$$(X^T X)\theta - X^T y = 0$$

$$(X^T X)\theta = X^T y$$

Closed Form Solution: $\theta = (X^T X)^{-1} X^T y$
Closed Form Solution

• Can obtain $\theta$ by simply plugging $X$ and $y$ into

$$\theta = (X^TX)^{-1}X^Ty$$

$$X = \begin{bmatrix}
1 & x_1^{(1)} & \cdots & x_d^{(1)} \\
\vdots & \vdots & \ddots & \vdots \\
1 & x_1^{(i)} & \cdots & x_d^{(i)} \\
\vdots & \vdots & \ddots & \vdots \\
1 & x_1^{(n)} & \cdots & x_d^{(n)}
\end{bmatrix} \quad y = \begin{bmatrix}
y^{(1)} \\
y^{(2)} \\
\vdots \\
y^{(n)}
\end{bmatrix}$$

• If $X^TX$ is not invertible (i.e., singular), may need to:
  – Use pseudo-inverse instead of the inverse
    • In python, `numpy.linalg.pinv(a)`
  – Remove redundant (not linearly independent) features
  – Remove extra features to ensure that $d \leq n$
# Gradient Descent vs Closed Form Solution

<table>
<thead>
<tr>
<th>Gradient Descent</th>
<th>Closed Form Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Requires multiple iterations</td>
<td>Non-iterative</td>
</tr>
<tr>
<td>Need to choose $\alpha$</td>
<td>No need for $\alpha$</td>
</tr>
<tr>
<td>Works well when $n$ is large</td>
<td>Slow if $n$ is large</td>
</tr>
<tr>
<td>Can support incremental learning</td>
<td>– Computing $(X^TX)^{-1}$ is roughly $O(n^3)$</td>
</tr>
</tbody>
</table>
Improving Learning: Feature Scaling

- **Idea:** Ensure that feature have similar scales

- Makes gradient descent converge *much* faster
Feature Standardization

• Rescales features to have zero mean and unit variance
  
  – Let $\mu_j$ be the mean of feature $j$:
    \[
    \mu_j = \frac{1}{n} \sum_{i=1}^{n} x_j^{(i)}
    \]
  
  – Replace each value with:
    \[
    x_j^{(i)} \leftarrow \frac{x_j^{(i)} - \mu_j}{s_j}
    \]
    \[
    \text{for } j = 1 \ldots d
    \]
    \[
    \text{(not } x_0!\text{)}
    \]

  • $s_j$ is the standard deviation of feature $j$
  • Could also use the range of feature $j$ ($\max_j - \min_j$) for $s_j$

• Must apply the same transformation to instances for both training and prediction

• Outliers can cause problems
Quality of Fit

Overfitting:

- The learned hypothesis may fit the training set very well ($J(\theta) \approx 0$)
- ...but fails to generalize to new examples

Underfitting (high bias)

Correct fit

Overfitting (high variance)

Based on example by Andrew Ng
Regularization

• A method for automatically controlling the complexity of the learned hypothesis

• **Idea:** penalize for large values of $\theta_j$
  – Can incorporate into the cost function
  – Works well when we have a lot of features, each that contributes a bit to predicting the label

• Can also address overfitting by eliminating features (either manually or via model selection)
Regularization

• Linear regression objective function

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

- $\lambda$ is the regularization parameter ($\lambda \geq 0$)
- No regularization on $\theta_0$!
Understanding Regularization

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

- Note that \[ \sum_{j=1}^{d} \theta_j^2 = \| \theta_{1:d} \|_2^2 \]
  - This is the magnitude of the feature coefficient vector!

- We can also think of this as:
  \[ \sum_{j=1}^{d} (\theta_j - 0)^2 = \| \theta_{1:d} - \overline{0} \|_2^2 \]
  - L₂ regularization pulls coefficients toward 0
Understanding Regularization

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

- What happens if we set \( \lambda \) to be huge (e.g., 10^{10})?

Price

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

Size

Based on example by Andrew Ng
Understanding Regularization

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

- What happens if we set \( \lambda \) to be huge (e.g., \( 10^{10} \))? 

Based on example by Andrew Ng
Regularized Linear Regression

- Cost Function

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

- Fit by solving \( \min_\theta J(\theta) \)

- Gradient update:

\[
\begin{align*}
\frac{\partial}{\partial \theta_0} J(\theta) &= \theta_0 - \alpha \frac{1}{n} \sum_{i=1}^{n} \left( h_\theta (x^{(i)}) - y^{(i)} \right) \\
\frac{\partial}{\partial \theta_j} J(\theta) &= \theta_j - \alpha \frac{1}{n} \sum_{i=1}^{n} \left( h_\theta (x^{(i)}) - y^{(i)} \right) x_j^{(i)} - \lambda \theta_j
\end{align*}
\]
Regularized Linear Regression

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

\[
\theta_0 \leftarrow \theta_0 - \alpha \frac{1}{n} \sum_{i=1}^{n} \left( h_{\theta} \left( x^{(i)} \right) - y^{(i)} \right)
\]

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

- We can rewrite the gradient step as:

\[
\theta_j \leftarrow \theta_j \left( 1 - \alpha \lambda \right) - \alpha \frac{1}{n} \sum_{i=1}^{n} \left( h_{\theta} \left( x^{(i)} \right) - y^{(i)} \right) x_j^{(i)}
\]
Regularized Linear Regression

• To incorporate regularization into the closed form solution:

\[ \theta = \left( X^T X \right)^{-1} X^T y \]
Regularized Linear Regression

• To incorporate regularization into the closed form solution:

\[
\theta = \left( X^\top X + \lambda \begin{bmatrix} 0 & 0 & 0 & \ldots & 0 \\ 0 & 1 & 0 & \ldots & 0 \\ 0 & 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & 1 \end{bmatrix} \right)^{-1} X^\top y
\]

• Can derive this the same way, by solving \( \frac{\partial}{\partial \theta} J(\theta) = 0 \)

• Can prove that for \( \lambda > 0 \), inverse exists in the equation above