Linear Regression

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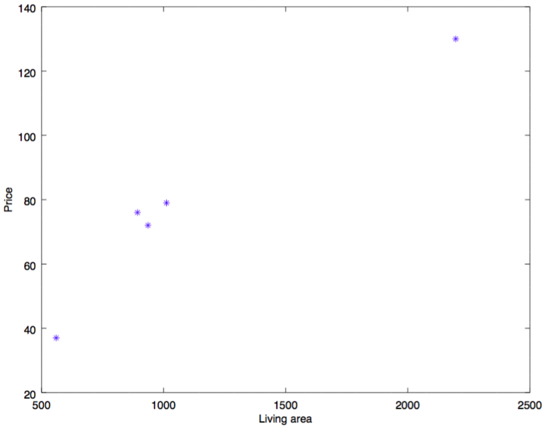
Housing Data

Suppose we have the following housing data:

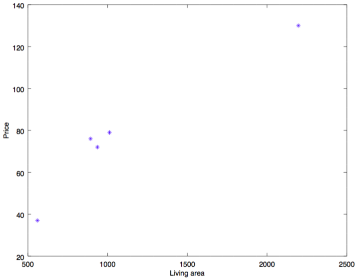
Living area (feet square)	Price (USD)
560	37
1012	79
893	76
2196	130
936	72
⋮	⋮

Housing Data



One Dimensional Regression Problem

Living area (x_1)	Price (y)
560	37
1012	79
893	76
2196	130
936	72
⋮	⋮



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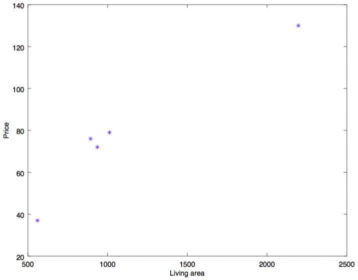

We are looking for something like: $h_\theta(\mathbf{x}) = \theta_0 + \theta_1 x_1$

Two Dimensional Regression Problem

Living area (x_1)	Bedrooms (x_2)	Price (y)
560	2	37
1012	3	79
893	3	76
2196	4	130
936	3	72
$\vdots$	$\vdots$	$\vdots$

Now, we are looking for something like: $h_\theta(\mathbf{x}) = \theta_0 + \theta_1 x_1 + \theta_2 x_2$

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Letting $x_0 = 1$ we have: $h(\mathbf{x}) = \sum_{j=0}^{n} \theta_j x_j$

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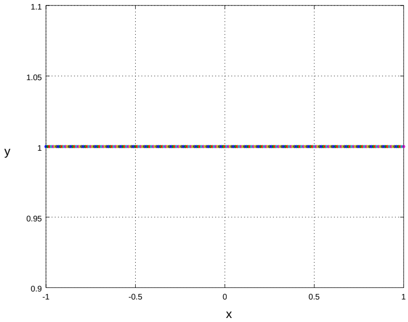
This is the dot product: $\theta^\top \mathbf{x}$

Polynomial Functions

$$y = 1$$

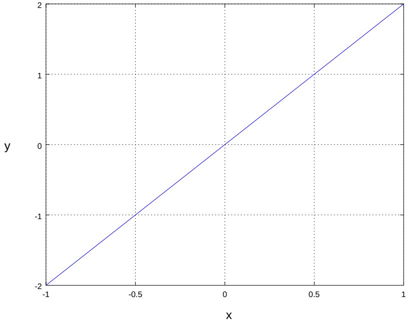
$$y = \theta_0$$



Polynomial Functions

$$y = 2x$$

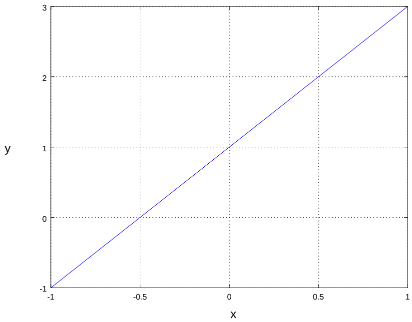
$$y = \theta_1 x$$



Polynomial Functions

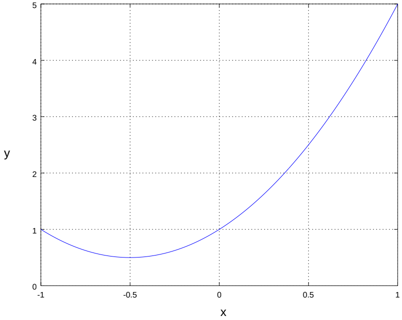
$$y = 1 + 2x$$

$$y = \theta_0 + \theta_1 x$$



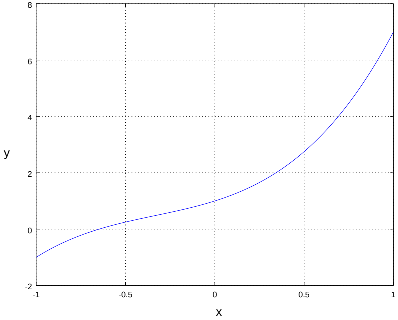
Polynomial Functions

$$y = 1 + 2x + 2x^2$$
$$y = \theta_0 + \theta_1 x + \theta_2 x^2$$



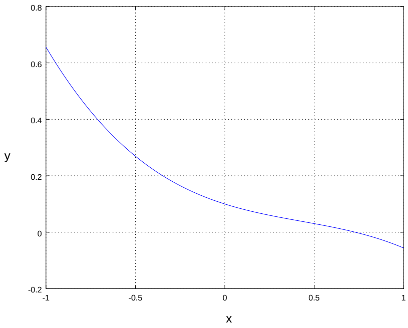
Polynomial Functions

$$y = 1 + 2x + 2x^2 + 2x^3$$
$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3$$



Polynomial Functions

$$y = 0.1 - 0.2x + 0.2x^2 - 0.156x^3$$
$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3$$



How do we pick θ?

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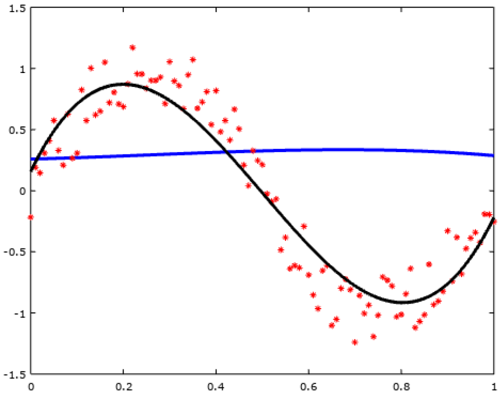
- We can initialize randomly θ and use the gradient descent algorithm to find the θ that minimizes $J(\theta)$.
- $\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$.

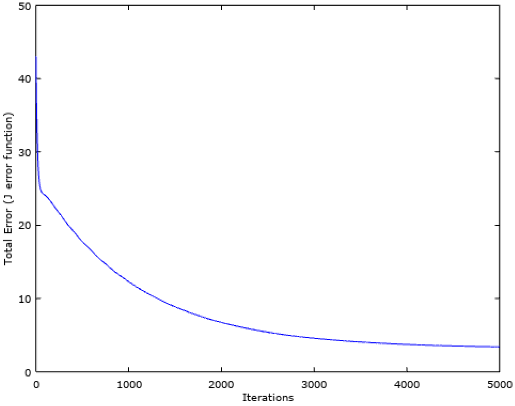
Estimating parameters

In blue, the initial $h_\theta(x)$ function, with randomly generated θ's. In black, the final $h_\theta(x)$ function.

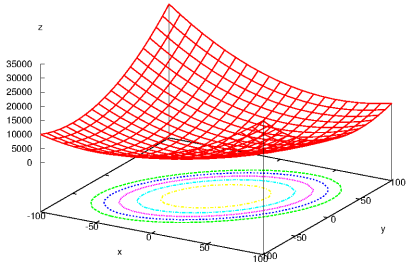


Graph of the error

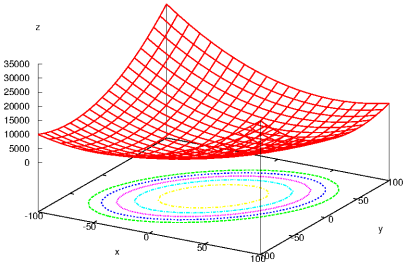
Plot of the error $J(\theta) = \frac{1}{2}\sum_{i=1}^{m}\left[h_\theta(x^{(i)}) - y^{(i)}\right]^2$, after each iteration of stochastic gradient descent.

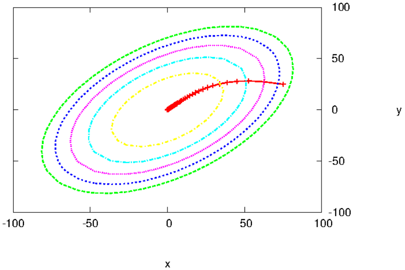


Gradient Descent



Gradient Descent





Deriving the LMS Learning Rule

$$\frac{\partial}{\partial\theta_j} J(\theta) = \frac{\partial}{\partial\theta_j} \frac{1}{2}(h_\theta(x) - y)^2$$

Deriving the LMS Learning Rule

$$\begin{aligned}
\frac{\partial}{\partial \theta_j} J(\theta) &= \frac{\partial}{\partial \theta_j} \frac{1}{2} (h_\theta(x) - y)^2 \\
&= 2 \cdot \frac{1}{2} (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} (h_\theta(x) - y)
\end{aligned}$$

Deriving the LMS Learning Rule

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\begin{aligned}
\frac{\partial}{\partial \theta_j} J(\theta) &= \frac{\partial}{\partial \theta_j} \frac{1}{2} (h_\theta(x) - y)^2 \\
&= 2 \cdot \frac{1}{2} (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} (h_\theta(x) - y) \\
&= (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} \left(\sum_{i=0}^{n} \theta_i x_i - y \right)
\end{aligned}
$$

Deriving the LMS Learning Rule

$$
\begin{aligned}
\frac{\partial}{\partial\theta_j}J(\theta) &= \frac{\partial}{\partial\theta_j}\frac{1}{2}(h_\theta(x)-y)^2 \\
&= 2\cdot\frac{1}{2}(h_\theta(x)-y)\cdot\frac{\partial}{\partial\theta_j}(h_\theta(x)-y) \\
&= (h_\theta(x)-y)\cdot\frac{\partial}{\partial\theta_j}\left(\sum_{i=0}^{n}\theta_i x_i - y\right) \\
&= (h_\theta(x)-y)x_j
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&= (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} \left(\sum_{i=0}^{n} \theta_i x_i - y \right) \\
&= (h_\theta(x) - y) x_j
\end{aligned}$$

For a single example, the rule is:

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

LMS Algorithms

Batch Gradient Descent

Repeat until convergence {

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

}

LMS Algorithms

Batch Gradient Descent

Repeat until convergence $\{$

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$\}$

Stochastic Gradient Descent

Loop $\{$

for $i = 1$ to m $\{$

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

$\}$

$\}$

LMS Algorithms

Mini-Batch Gradient Descent

Repeat until convergence $\{$

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

$\}$

Here we use mini-batches containing 10 to 1000 examples. This is $k \in [10, 1000]$.

Matrix of Training Examples

Given a training set of m examples, with each example consisting of n variables, then we can construct a $m \times (n+1)$ matrix:

$$\mathbf{X} = \begin{bmatrix} x_0^{(1)} & x_1^{(1)} & \cdots & x_n^{(1)} \\ x_0^{(2)} & x_1^{(2)} & \cdots & x_n^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ x_0^{(m)} & x_1^{(m)} & \cdots & x_n^{(m)} \end{bmatrix} = \begin{bmatrix} [\mathbf{x}^{(1)}]^\top \\ [\mathbf{x}^{(2)}]^\top \\ \vdots \\ [\mathbf{x}^{(m)}]^\top \end{bmatrix}$$

Vector of Training Target Values

Let $\mathbf{y}$ be the m-dimensional vector containing the target values from the training set:

$$\mathbf{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

Cost Function $J(\theta)$

We can write the $J(\theta)$ cost function as follows:

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

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& \frac{1}{2}(\mathbf{X}\theta - \mathbf{y})^\top(\mathbf{X}\theta - \mathbf{y})
\end{aligned}
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and the $\nabla_\theta J(\theta)$ can be written as:

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\end{aligned}
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\begin{aligned}
\nabla_\theta J(\theta) &= \nabla_\theta \frac{1}{2}(\mathbf{X}\theta - \mathbf{y})^\top(\mathbf{X}\theta - \mathbf{y}) \\
\nabla_\theta J(\theta) &= \mathbf{X}^\top\mathbf{X}\theta - \mathbf{X}^\top\mathbf{y} \\
0 &= \mathbf{X}^\top\mathbf{X}\theta - \mathbf{X}^\top\mathbf{y} \\
\mathbf{X}^\top\mathbf{X}\theta &= \mathbf{X}^\top\mathbf{y} \\
\theta &= (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}.
\end{aligned}
$$

Computing Directly θ

For an n by n square matrix A, the trace of A is defined to be the sum of its diagonal entries

$$\text{tr}\, A = \sum_{i=1}^{n} A_{ii}$$

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If a is a real number, then

$$\text{tr } a = a$$

Computing Directly θ

For matrices A, B, C and D, we have that

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$$\text{tr } ABCD = \text{tr } DABC = \text{tr } CDAB = \text{tr } BCDA$$

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For matrices A and B, and real number a, we have that

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$$\nabla_{A^\top} f(A) = (\nabla_A f(A))^\top$$

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$$\nabla_{A^\top} f(A) = (\nabla_A f(A))^\top$$

$$\nabla_{A^\top} \operatorname{tr} ABA^\top C = B^\top A^\top C^\top + BA^\top C$$

Computing Directly θ

$$\nabla_\theta J(\theta) \quad = \quad \nabla_\theta \frac{1}{2}(\mathbf{X}\theta - \mathbf{y})^\top (\mathbf{X}\theta - \mathbf{y}).$$

Computing Directly θ

$$\begin{aligned}
\nabla_\theta J(\theta) &= \nabla_\theta \frac{1}{2}(\mathbf{X}\theta - \mathbf{y})^\top(\mathbf{X}\theta - \mathbf{y}). \\
&= \nabla_\theta \frac{1}{2}(\theta^\top \mathbf{X}^\top - \mathbf{y}^\top)(\mathbf{X}\theta - \mathbf{y}).
\end{aligned}$$

Computing Directly θ

$$
\begin{aligned}
\nabla_\theta J(\theta) &= \nabla_\theta \tfrac{1}{2}(\mathbf{X}\theta - \mathbf{y})^\top(\mathbf{X}\theta - \mathbf{y}). \\
&= \nabla_\theta \tfrac{1}{2}(\theta^\top \mathbf{X}^\top - \mathbf{y}^\top)(\mathbf{X}\theta - \mathbf{y}). \\
&= \tfrac{1}{2}\nabla_\theta(\theta^\top \mathbf{X}^\top \mathbf{X}\theta - \theta^\top \mathbf{X}^\top \mathbf{y} - \mathbf{y}^\top \mathbf{X}\theta + \mathbf{y}^\top \mathbf{y}).
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&= \tfrac{1}{2}\nabla_\theta \operatorname{tr}(\theta^\top \mathbf{X}^\top \mathbf{X}\theta - \theta^\top \mathbf{X}^\top \mathbf{y} - \mathbf{y}^\top \mathbf{X}\theta + \mathbf{y}^\top \mathbf{y}).
\end{aligned}
$$

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&= \tfrac{1}{2}\nabla_\theta(\theta^\top \mathbf{X}^\top \mathbf{X}\theta - \theta^\top \mathbf{X}^\top \mathbf{y} - \mathbf{y}^\top \mathbf{X}\theta + \mathbf{y}^\top \mathbf{y}). \\
&= \tfrac{1}{2}\nabla_\theta \operatorname{tr}(\theta^\top \mathbf{X}^\top \mathbf{X}\theta - \theta^\top \mathbf{X}^\top \mathbf{y} - \mathbf{y}^\top \mathbf{X}\theta + \mathbf{y}^\top \mathbf{y}). \\
&= \tfrac{1}{2}\nabla_\theta \operatorname{tr}\theta^\top \mathbf{X}^\top \mathbf{X}\theta - \operatorname{tr}\theta^\top \mathbf{X}^\top \mathbf{y} - \operatorname{tr}\mathbf{y}^\top \mathbf{X}\theta + \operatorname{tr}\mathbf{y}^\top \mathbf{y}.
\end{aligned}
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Computing Directly θ

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\begin{aligned}
\nabla_\theta J(\theta) &= \nabla_\theta \tfrac{1}{2}(\mathbf{X}\theta - \mathbf{y})^\top(\mathbf{X}\theta - \mathbf{y}). \\
&= \nabla_\theta \tfrac{1}{2}(\theta^\top \mathbf{X}^\top - \mathbf{y}^\top)(\mathbf{X}\theta - \mathbf{y}). \\
&= \tfrac{1}{2}\nabla_\theta(\theta^\top \mathbf{X}^\top \mathbf{X}\theta - \theta^\top \mathbf{X}^\top \mathbf{y} - \mathbf{y}^\top \mathbf{X}\theta + \mathbf{y}^\top \mathbf{y}). \\
&= \tfrac{1}{2}\nabla_\theta \operatorname{tr}(\theta^\top \mathbf{X}^\top \mathbf{X}\theta - \theta^\top \mathbf{X}^\top \mathbf{y} - \mathbf{y}^\top \mathbf{X}\theta + \mathbf{y}^\top \mathbf{y}). \\
&= \tfrac{1}{2}\nabla_\theta \operatorname{tr}\theta^\top \mathbf{X}^\top \mathbf{X}\theta - \operatorname{tr}\theta^\top \mathbf{X}^\top \mathbf{y} - \operatorname{tr}\mathbf{y}^\top \mathbf{X}\theta + \operatorname{tr}\mathbf{y}^\top \mathbf{y}.
\end{aligned}
$$

Using $\operatorname{tr} A = \operatorname{tr} A^\top$ and $(ABC)^\top = C^\top B^\top A^\top$,

we have $\operatorname{tr}\theta^\top \mathbf{X}^\top \mathbf{y} = \operatorname{tr}(\theta^\top \mathbf{X}^\top \mathbf{y})^\top = \operatorname{tr}\mathbf{y}^\top \mathbf{X}\theta$.

Computing Directly θ

$$
\begin{aligned}
\nabla_\theta J(\theta) &= \nabla_\theta \tfrac{1}{2}(\mathbf{X}\theta - \mathbf{y})^\top(\mathbf{X}\theta - \mathbf{y}). \\
&= \nabla_\theta \tfrac{1}{2}(\theta^\top \mathbf{X}^\top - \mathbf{y}^\top)(\mathbf{X}\theta - \mathbf{y}). \\
&= \tfrac{1}{2}\nabla_\theta(\theta^\top \mathbf{X}^\top \mathbf{X}\theta - \theta^\top \mathbf{X}^\top \mathbf{y} - \mathbf{y}^\top \mathbf{X}\theta + \mathbf{y}^\top \mathbf{y}). \\
&= \tfrac{1}{2}\nabla_\theta \operatorname{tr}(\theta^\top \mathbf{X}^\top \mathbf{X}\theta - \theta^\top \mathbf{X}^\top \mathbf{y} - \mathbf{y}^\top \mathbf{X}\theta + \mathbf{y}^\top \mathbf{y}). \\
&= \tfrac{1}{2}\nabla_\theta \operatorname{tr}\theta^\top \mathbf{X}^\top \mathbf{X}\theta - \operatorname{tr}\theta^\top \mathbf{X}^\top \mathbf{y} - \operatorname{tr}\mathbf{y}^\top \mathbf{X}\theta + \operatorname{tr}\mathbf{y}^\top \mathbf{y}.
\end{aligned}
$$

Using $\operatorname{tr} A = \operatorname{tr} A^\top$ and $(ABC)^\top = C^\top B^\top A^\top$,

we have $\operatorname{tr}\theta^\top \mathbf{X}^\top \mathbf{y} = \operatorname{tr}(\theta^\top \mathbf{X}^\top \mathbf{y})^\top = \operatorname{tr}\mathbf{y}^\top \mathbf{X}\theta$.

$$
= \tfrac{1}{2}\nabla_\theta \operatorname{tr}\theta^\top \mathbf{X}^\top \mathbf{X}\theta - 2\operatorname{tr}\mathbf{y}^\top \mathbf{X}\theta.
$$

Computing Directly θ

$$\nabla_\theta J(\theta) = \frac{1}{2}\nabla_\theta \operatorname{tr} \theta^\top \mathbf{X}^\top \mathbf{X}\theta - 2 \operatorname{tr} \mathbf{y}^\top \mathbf{X}\theta.$$

Computing Directly θ

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Computing Directly θ

$$\begin{aligned}\nabla_\theta J(\theta) \quad &= \quad \tfrac{1}{2}\nabla_\theta \text{ tr } \theta^\top \mathbf{X}^\top \mathbf{X}\theta - 2 \text{ tr } \mathbf{y}^\top \mathbf{X}\theta. \\ &\quad\ \ \tfrac{1}{2}\nabla_\theta \text{ tr } \theta^\top \mathbf{X}^\top \mathbf{X}\theta - 2\nabla_\theta \text{ tr } \mathbf{y}^\top \mathbf{X}\theta.\end{aligned}$$

Using tr $AB =$ tr BA, with $A = \mathbf{y}^\top \mathbf{X}$, $B = \theta$.

$$\tfrac{1}{2}\nabla_\theta \text{ tr } \theta^\top \mathbf{X}^\top \mathbf{X}\theta - 2\nabla_\theta \text{ tr } \theta\mathbf{y}^\top \mathbf{X}.$$

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Using $\nabla_{A^\top} \text{ tr } ABA^\top C = B^\top A^\top C^\top + BA^\top C$,

with $A^\top = \theta, B = \mathbf{X}^\top \mathbf{X}, C = I$,

Computing Directly θ

$$\nabla_\theta J(\theta) \quad = \quad \frac{1}{2}\nabla_\theta \text{ tr } \theta^\top \mathbf{X}^\top \mathbf{X}\theta - 2 \text{ tr } \mathbf{y}^\top \mathbf{X}\theta.$$

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and using $\nabla_A \text{ tr } AB = B^\top$, with $A = \theta$, $B = \mathbf{y}^\top \mathbf{X}$.

Computing Directly θ

$$\begin{aligned}
\nabla_\theta J(\theta) &= \tfrac{1}{2}\nabla_\theta \operatorname{tr} \theta^\top \mathbf{X}^\top \mathbf{X}\theta - 2 \operatorname{tr} \mathbf{y}^\top \mathbf{X}\theta. \\
& \tfrac{1}{2}\nabla_\theta \operatorname{tr} \theta^\top \mathbf{X}^\top \mathbf{X}\theta - 2\nabla_\theta \operatorname{tr} \mathbf{y}^\top \mathbf{X}\theta. \\
& \text{Using } \operatorname{tr} AB = \operatorname{tr} BA, \text{ with } A = \mathbf{y}^\top \mathbf{X}, B = \theta. \\
& \tfrac{1}{2}\nabla_\theta \operatorname{tr} \theta^\top \mathbf{X}^\top \mathbf{X}\theta - 2\nabla_\theta \operatorname{tr} \theta\mathbf{y}^\top \mathbf{X}. \\
& \text{Using } \nabla_{A^\top} \operatorname{tr} ABA^\top C = B^\top A^\top C^\top + BA^\top C, \\
& \text{with } A^\top = \theta, B = \mathbf{X}^\top \mathbf{X}, C = I, \\
& \text{and using } \nabla_A \operatorname{tr} AB = B^\top, \text{ with } A = \theta, B = \mathbf{y}^\top \mathbf{X}. \\
&= \tfrac{1}{2}(\mathbf{X}^\top \mathbf{X}\theta + \mathbf{X}^\top \mathbf{X}\theta - 2\mathbf{X}^\top \mathbf{y}).
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$$
\begin{aligned}
&= \tfrac{1}{2}(\mathbf{X}^\top \mathbf{X}\theta + \mathbf{X}^\top \mathbf{X}\theta - 2\mathbf{X}^\top \mathbf{y}). \\
&= \mathbf{X}^\top \mathbf{X}\theta - \mathbf{X}^\top \mathbf{y}.
\end{aligned}
$$

Why the Cost Function J is Reasonable?

Given a training example i, we may write

$$y^{(i)} = \theta^\top \mathbf{x}^{(i)} + \epsilon^{(i)},$$

with the assumption

$$\epsilon^{(i)} \sim \mathcal{N}(0, \sigma^2).$$

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This implies

$$p(y^{(i)} | \mathbf{x}^{(i)}; \theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(- \frac{(y^{(i)} - \theta^\top \mathbf{x}^{(i)})^2}{2\sigma^2} \right).$$

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The likelihood of θ is:

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$$\begin{aligned} L(\theta) &= \prod_{i=1}^{m} p(y^{(i)}|\mathbf{x}^{(i)}; \theta) \\ &= \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(- \frac{(y^{(i)} - \theta^\top \mathbf{x}^{(i)})^2}{2\sigma^2} \right). \end{aligned}$$

Maximum Likelihood of θ

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$$
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&= \sum_{i=1}^{m} \log \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^\top \mathbf{x}^{(i)})^2}{2\sigma^2} \right)
\end{aligned}
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&= \sum_{i=1}^{m} \log \frac{1}{\sqrt{2\pi}\sigma} \exp\left(- \frac{(y^{(i)} - \theta^\top \mathbf{x}^{(i)})^2}{2\sigma^2} \right) \\
&= m \log \tfrac{1}{\sqrt{2\pi}\sigma} - \tfrac{1}{\sigma^2} \cdot \tfrac{1}{2} \sum_{i=1}^{m} (y^{(i)} - \theta^\top \mathbf{x}^{(i)})^2
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$$

Maximum Likelihood of θ

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&= m \log \frac{1}{\sqrt{2\pi}\sigma} - \frac{1}{\sigma^2} \cdot \frac{1}{2} \sum_{i=1}^{m} (y^{(i)} - \theta^\top \mathbf{x}^{(i)})^2
\end{aligned}$$

Hence, maximizing $\ell(\theta)$ gives the same answer as minimizing

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

Locally Adjusting the Model

The algorithm works as follows:

1. Fit θ to minimize $\sum_i w^{(i)}(y^{(i)} - \theta^\top x^{(i)})^2$.
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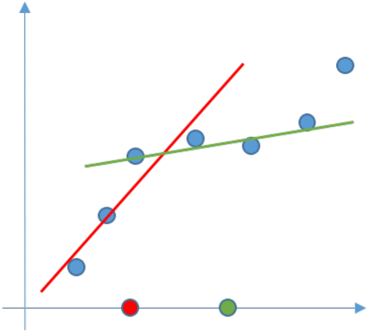
Where $w^{(i)}$'s are non-negative valued weights.

A good choice for the weights is:

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

Locally Adjusting the Model



Thank you!

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