Machine Learning
Supplementary Material of Lecture 2

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Aside - finding maxima and minima

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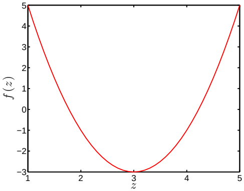

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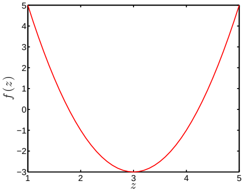

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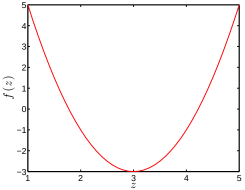

At a minimum (or a maximum), the gradient must be zero.

The gradient is given by the first derivative of the function:

$$\frac{df(z)}{dz} = 4z - 12$$

Setting to zero and solving for z

$$4z - 12 = 0,\ \ z = 12/4 = 3$$

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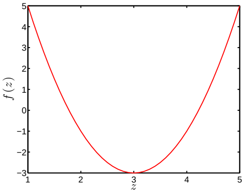

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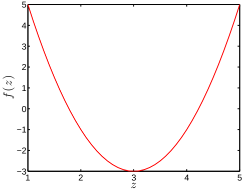


At a minimum, the gradient must be increasing.

Taking the second derivative:

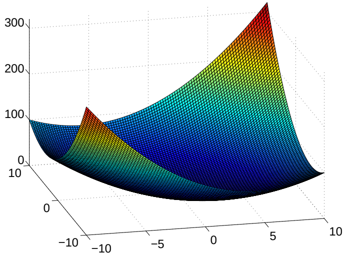
$$\frac{df(z)}{dz} = 4z - 12$$
$$\frac{d^2 z}{dz^2} = 4$$

The gradient is always increasing. Therefore, we have found a minimum and it is the only minumum.

Finding maxima and minima

What about functions of more than one variable?

$$\underset{y,z}{\operatorname{argmin}}\ f(y,z), \ f(y,z) = y^2 + z^2 + y + z + yz$$



We now use *partial derivatives*, $\frac{\partial f}{\partial z}$ and $\frac{\partial f}{\partial y}$

When calculating the partial derivative with respect to y we assume everything else (including z) is a constant.

$$\frac{\partial f}{\partial y} = 2y + 1 + z, \quad \frac{\partial f}{\partial z} = 2z + 1 + y$$

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To find a potential minimum, set both to zero and solve for y and z:

$$\begin{aligned} y &= -\frac{1}{3} \\ z &= -\frac{1}{3}. \end{aligned}$$

To make sure its a minimum, check second derivatives:

$$\frac{\partial^2 f}{\partial y^2} = 2, \quad \frac{\partial^2 f}{\partial z^2} = 2.$$

Both are positive so we have a minimum.

Back to our function

$$\mathcal{L} = \frac{1}{N}\sum_{n=1}^{N}(t_n - f(x_n; w_0, w_1))^2.$$

Now, recall that:

$$f(x_n; w_0, w_1) = w_0 + w_1 x$$

So:

$$\underset{w_0, w_1}{\text{argmin}}\ \mathcal{L} = \underset{w_0, w_1}{\text{argmin}}\ \frac{1}{N}\sum_{n=1}^{N}(t_n - w_0 - w_1 x_n)^2$$

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We need to find $\frac{\partial \mathcal{L}}{\partial w_0}$ and $\frac{\partial \mathcal{L}}{\partial w_1}$, do some algebra, and we'll have expressions for the *best* values!

Differentiating the loss

- Taking partial derivatives with respect to w_0 and w_1:

$$\begin{aligned}
\mathcal{L} &= \frac{1}{N}\sum_{n=1}^{N}(t_n - w_0 - w_1 x_n)^2 \\
\frac{\partial \mathcal{L}}{\partial w_0} &= -\frac{2}{N}\sum_{n=1}^{N}(t_n - w_0 - w_1 x_n) \\
\frac{\partial \mathcal{L}}{\partial w_1} &= -\frac{2}{N}\sum_{n=1}^{N}x_n(t_n - w_0 - w_1 x_n)
\end{aligned}$$

Two useful differentiation identities

$$\begin{aligned}
\frac{\partial}{\partial w_0}\left(\sum_{n=1}^{N} f_n(w_0)\right) &= \sum_{n=1}^{N}\frac{\partial f_n(w_0)}{\partial w_0} \\
\frac{\partial}{\partial w_0}\left(f(w_0)^2\right) &= 2f(w_0)\frac{\partial f(w_0)}{\partial w_0}
\end{aligned}$$

Finding w_0:

$$\frac{\partial \mathcal{L}}{\partial w_0} = -\frac{2}{N}\sum_{n=1}^{N}(t_n - w_0 - w_1 x_n)$$

$$0 = -\frac{2}{N}\sum_{n=1}^{N}(t_n - w_0 - w_1 x_n)$$

$$\frac{2}{N}\sum_{n=1}^{N} w_0 = \frac{2}{N}\sum_{n=1}^{N} t_n - \frac{2}{N}\sum_{n=1}^{N} w_1 x_n$$

$$w_0 = \bar{t} - w_1 \bar{x}$$

Where

$$\bar{t} = \frac{1}{N}\sum_{n=1}^{N} t_n, \ \bar{x} = \frac{1}{N}\sum_{n=1}^{N} x_n$$

Finding w_1:

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial w_1} &= -\frac{2}{N}\sum_{n=1}^{N} x_n(t_n - w_0 - w_1 x_n) \\
0 &= -\frac{2}{N}\sum_{n=1}^{N} x_n(t_n - w_0 - w_1 x_n) \\
w_1 \frac{1}{N}\sum_{n=1}^{N} x_n^2 &= \frac{1}{N}\sum_{n=1}^{N} x_n t_n - w_0 \frac{1}{N}\sum_{n=1}^{N} x_n \\
w_1 \overline{x^2} &= \overline{xt} - w_0 \overline{x}
\end{aligned}
$$

Where

$$
\overline{x^2} = \frac{1}{N}\sum_{n=1}^{N} x_n^2, \;\; \overline{xt} = \frac{1}{N}\sum_{n=1}^{N} x_n t_n
$$

Substituting:

Substituting our expression for w_0 into that for w_1:

$$\begin{aligned} w_0 &= \bar{t} - w_1\bar{x} \\ w_1\overline{x^2} &= \overline{xt} - w_0\bar{x} \\ w_1\overline{x^2} &= \overline{xt} - \bar{x}(\bar{t} - w_1\bar{x}) \\ w_1 &= \frac{\overline{xt} - \bar{x}\bar{t}}{\overline{x^2} - (\bar{x})^2} \end{aligned}$$

So, to summarise:

$$w_1 = \frac{\overline{xt} - \bar{x}\bar{t}}{\overline{x^2} - (\bar{x})^2}, \quad w_0 = \bar{t} - w_1\bar{x}$$

Note that $\overline{xt} \neq \bar{x}\bar{t}$ and $\overline{x^2} \neq (\bar{x})^2$.

Olympic data

n	x_n	t_n	$x_n t_n$	x_n^2
1	1896	12.00	22752.0	3.5948e+06
2	1900	11.00	20900.0	3.6100e+06
3	1904	11.00	20944.0	3.6252e+06
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
26	2004	9.85	19739.4	4.0160e+06
27	2008	9.69	19457.5	4.0321e+06
$(1/N)\sum_{n=1}^{N}$	1952.37	10.39	20268.1	3.8130e+06
	$\overline{x}$	$\overline{t}$	$\overline{xt}$	$\overline{x^2}$

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	$\overline{x}$	$\overline{t}$	$\overline{xt}$	$\overline{x^2}$

Substituting these values into our expressions gives:

$$w_1 = -0.0133, \;\; w_0 = 36.416$$