

Insight into the Gradient Formula

The second formula in Taylor's Theorem (Theorem 1) can seem puzzling. Let's see where it comes from.

$$\nabla f(x + p) = \nabla f(x) + \int_0^1 \nabla^2 f(x + tp)p dt$$

This is just the Fundamental Theorem of Calculus, $g(1) - g(0) = \int_0^1 g'(t)dt$, applied to a vector function.

1. Define $g(t) = \nabla f(x + tp)$ for $t \in [0, 1]$.
2. Apply the theorem: $g(1) = \nabla f(x + p)$ and $g(0) = \nabla f(x)$

$$\text{So, } \nabla f(x + p) - \nabla f(x) = \int_0^1 g'(t)dt.$$

Let's differentiate $g(t) = \nabla f(x + tp)$ with respect to t : $g'(t) = \frac{d}{dt} \nabla f(x + tp)$. Using the multivariate chain rule:

$$g'(t) = \underbrace{\nabla^2 f(x + tp)}_{\substack{\text{Derivative of } \nabla f \\ \text{Derivative of } x+tp}} \cdot \overbrace{p}^{\substack{\text{Derivative of } x+tp}}$$

Substituting this back into the integral gives the final result.



Comments

Let's break down the second formula from the Theorem 1, as its origin is not immediately obvious. The formula is a beautiful application of single-variable calculus to a multivariate setting.

The key is to reduce the problem to one dimension. We are interested in the change of the gradient, ∇f , as we move from point x to point $x + p$ along a straight line. We can parameterize this path using a variable $t \in [0, 1]$, where our position is $x + tp$.

We define a new vector function of a single variable, $g(t) = \nabla f(x + tp)$. This function simply tells us the gradient of f at a point t -fraction of the way along the vector p .

Now, we can apply the Fundamental Theorem of Calculus to $g(t)$, which states that the total change in g from $t = 0$ to $t = 1$ is the integral of its rate of change, $g'(t)$. In other words, $g(1) - g(0) = \int_0^1 g'(t)dt$.

Substituting our definitions back in, $g(1) = \nabla f(x + p)$ and $g(0) = \nabla f(x)$. The final piece is to find $g'(t)$. Using the chain rule, the derivative of $\nabla f(x + tp)$ with respect to t is the derivative of the outer function (∇f) evaluated at the inner function ($x + tp$), multiplied by the derivative of the inner function. The derivative of the gradient vector ∇f is the Hessian matrix $\nabla^2 f$, and the derivative of $x + tp$ with respect to t is simply the vector p .

Thus, the rate of change of the gradient along the path is $\nabla^2 f(x + tp)p$. Integrating this rate of change from the start to the end gives the total change in the gradient. The formula simply states:

Final Gradient = Initial Gradient + Total Accumulated Change.