Derivative of scalar function w.r.t. arguments of BatchNorm operation

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Let $Y = \gamma \hat{X} + \beta$, where $\hat{X} \in \mathbb{R}^{N \times D}$, $\gamma \in \mathbb{R}^D$, $\beta \in \mathbb{R}^D$, $\hat{X} = \frac{X - \mu}{\sigma}$, $\mu = \frac{1}{N} \sum_{i=1}^{N} x_i$, $v = \frac{1}{N} \sum_{i=1}^{N} (x_i - \mu)^2$, $\sigma = \sqrt{v + \epsilon}$, $\epsilon \in \mathbb{R}$ is a small scalar to omit zero division.

Let $f : \mathbb{R}^{N \times D} \to \mathbb{R}$ is a differentiable scalar function. We also know $\frac{\partial f}{\partial Y}$. Derive $\frac{\partial f}{\partial X}$, $\frac{\partial f}{\partial \gamma}$, $\frac{\partial f}{\partial \beta}$.

Notice that

- y_i depends on x_j, where $1 \leq j \leq N$
- there is only per-column dependency: y_{ij} depends on x_{kj}, where $1 \leq k \leq N$
- γ_j and β_j is the same for all y_{ij}, $1 \leq i \leq N$, $1 \leq j \leq D$.

Because columns are independent, consider j-th column of X as x. Hence,

$$y = \gamma \hat{x} + \beta$$
$$y, x, \hat{x} \in \mathbb{R}^N$$
$$\gamma, \beta, \mu, v, \sigma \in \mathbb{R}$$

$\frac{\partial f}{\partial x_j} = \sum_{i=1}^{N} \frac{\partial f}{\partial y_i} \frac{\partial y_i}{\partial \hat{x}_i} \frac{\partial \hat{x}_i}{\partial x_j}$, where x_j is the j-th element of x.
$\frac{\partial f}{\partial \gamma} = \sum_{i=1}^{N} \frac{\partial f}{\partial y_i} \frac{\partial y_i}{\partial \gamma} = \sum_{i=1}^{N} \frac{\partial f}{\partial y_i} \hat{x}_i$
$\frac{\partial f}{\partial \beta} = \sum_{i=1}^{N} \frac{\partial f}{\partial y_i} \frac{\partial y_i}{\partial \beta} = \sum_{i=1}^{N} \frac{\partial f}{\partial y_i}$

Tricky part here is $\frac{\partial f}{\partial x_j}$. Let's derive it with two approaches: forward-mode differentiation (deriving $\frac{\partial f}{\partial x_j}$ directly from $f(x_j)$) and backward-mode differentiation (through writing computation graph and traversing it in reverse mode: from f to x_j).

Knowing expression for $\frac{\partial f}{\partial x_j}$, expression for $\frac{\partial f}{\partial X}$ comes straightforwardly from it.

Forward-mode differentiation

Let's derive expressions for building blocks:

$\frac{\partial y}{\partial \hat{x_i}} = \gamma$

$\frac{\partial \hat{x_i}}{\partial x_j} = \frac{\partial (x_i - \mu)}{\partial x_j}(v+\epsilon)^{-\frac{1}{2}} + (x_i - \mu)(-\frac{1}{2})(v+\epsilon)^{-\frac{3}{2}}\frac{\partial (v+\epsilon)}{\partial x_j}$

$\frac{\partial \mu}{\partial x_j} = \frac{1}{N}$

$\frac{\partial x_i}{\partial x_j} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$

Let's derive $\frac{\partial v}{\partial x_j}$.

Consider i-th component of sum in v as y_i.

$\frac{\partial y_i}{\partial x_j} = \begin{cases} 2(x_i - \mu)(1 - \frac{1}{N}) = -\frac{2}{N}(x_i - \mu) + 2(x_i - \mu) & i = j \\ -\frac{2}{N}(x_i - \mu) & i \neq j \end{cases}$

So, $\frac{\partial v}{\partial x_j} = \frac{1}{N}(-\frac{2}{N}\sum_{i=1}^{N}(x_i - \mu) + 2(x_j - \mu))$.

Note, that $\sum_{i=1}^{N}(x_i - \mu) = \sum_{i=1}^{N} x_i - N\mu = N\mu - N\mu = 0$.

So, $\frac{\partial v}{\partial x_j} = \frac{2}{N}(x_j - \mu)$.

Now we can expand $\frac{\partial \hat{x_i}}{\partial x_j}$. Let's do it in case $i \neq j$:

$$\frac{\partial \hat{x}_i}{\partial x_j} = -\frac{1}{N}(v+\epsilon)^{-\frac{1}{2}} + (x_i - \mu)(-\frac{1}{2})(v+\epsilon)^{-\frac{3}{2}}\frac{2}{N}(x_j - \mu) = \\ -\frac{1}{N}(v+\epsilon)^{-\frac{1}{2}}(1 + (x_i - \mu)(x_j - \mu)(v+\epsilon)^{-1})$$

Note that the only difference of case $i = j$ is the first multiplier of the first term: it's $1 - \frac{1}{N}$ instead of $-\frac{1}{N}$.

Now we have all to derive $\frac{\partial f}{\partial x_j}$:

$$\frac{\partial f}{\partial x_j} = \sum_{i=1}^{N} \frac{\partial f}{\partial y_i} \frac{\partial y_i}{\partial \hat{x}_i} \frac{\partial \hat{x}_i}{\partial x_j} = \gamma \sum_{i=1}^{N} \frac{\partial f}{\partial y_i} \frac{\partial \hat{x}_i}{\partial x_j} =$$

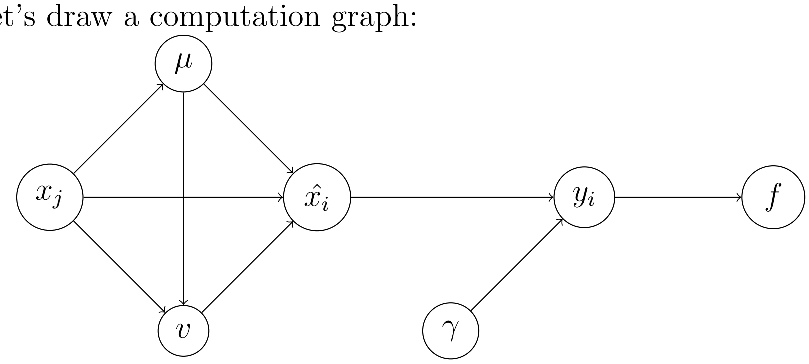
$$\gamma \left(\sum_{i=1}^{N} -\frac{1}{N} (v+\epsilon)^{-\frac{1}{2}} (1 + (x_i - \mu)(x_j - \mu)(v+\epsilon)^{-1}) \frac{\partial f}{\partial y_i} + (v+\epsilon)^{-\frac{1}{2}} \frac{\partial f}{\partial y_j} \right) =$$

$$\gamma (v+\epsilon)^{-\frac{1}{2}} \left(-\frac{1}{N} \sum_{i=1}^{N} (1 + (x_i - \mu)(x_j - \mu)(v+\epsilon)^{-1}) \frac{\partial f}{\partial y_i} + \frac{\partial f}{\partial y_j} \right) =$$

$$\gamma (v+\epsilon)^{-\frac{1}{2}} \left(-\frac{1}{N} \sum_{i=1}^{N} \frac{\partial f}{\partial y_i} - (x_j - \mu)(v+\epsilon)^{-1} \frac{1}{N} \sum_{i=1}^{N} (x_i - \mu) \frac{\partial f}{\partial y_i} + \frac{\partial f}{\partial y_j} \right)$$

Backward-mode differentiation

Let's draw a computation graph:



Note that there are three paths from x_j and two paths from μ. So, derivative expressions through these nodes will consist of three and two terms respectively:

$$\frac{\partial f}{\partial x_j} = \sum_{i=1}^{N} \frac{\partial f}{\partial y_i} \frac{\partial y_i}{\partial \hat{x}_i} \left(\frac{\partial \hat{x}_i}{\partial x_j} + \frac{\partial \hat{x}_i}{\partial v} \frac{\partial v}{\partial x_j} + \left(\frac{\partial \hat{x}_i}{\partial \mu} + \frac{\partial \hat{x}_i}{\partial v} \frac{\partial v}{\partial \mu} \right) \frac{\partial \mu}{\partial x_j} \right)$$

$\frac{\partial y_i}{\partial \hat{x}_i} = \gamma$

$\frac{\partial \hat{x}_i}{\partial x_j} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$

$\frac{\partial \hat{x}_i}{\partial v} = (x_i - \mu)(-\frac{1}{2})(v+\epsilon)^{-\frac{3}{2}}$

$\frac{\partial v}{\partial x_j} = \frac{2}{N}(x_j - \mu)$
$\frac{\partial \hat{x_i}}{\partial \mu} = -(v+\epsilon)^{-\frac{1}{2}}$
$\frac{\partial v}{\partial \mu} = -\frac{2}{N}\sum_{i=1}^{N}(x_i - \mu) = 0$
$\frac{\partial \mu}{\partial x_j} = \frac{1}{N}$
Now let's derive $\frac{\partial f}{\partial x_j}$:

$$\frac{\partial f}{\partial x_j} = \gamma \left(\sum_{i=1}^{N} \frac{\partial f}{\partial y_i} \left(-(x_i-\mu)(v+\epsilon)^{-\frac{3}{2}} \frac{1}{N}(x_j-\mu) - \frac{1}{N}(v+\epsilon)^{-\frac{1}{2}} \right) + (v+\epsilon)^{-\frac{1}{2}} \frac{\partial f}{\partial y_j} \right) =$$
$$\gamma(v+\epsilon)^{-\frac{1}{2}} \left(-\frac{1}{N}\sum_{i=1}^{N}\frac{\partial f}{\partial y_i} - (x_j-\mu)(v+\epsilon)^{-1}\frac{1}{N}\sum_{i=1}^{N}(x_i-\mu)\frac{\partial f}{\partial y_i} + \frac{\partial f}{\partial y_j} \right)$$

Note that result is the same as in previous approach.
Knowing $\frac{\partial f}{\partial x_j}$, it's easy to write $\frac{\partial f}{\partial X}$:

$$\frac{\partial f}{\partial X} = \gamma(v+\epsilon)^{-\frac{1}{2}} \left(-\frac{1}{N}\sum_{i=1}^{N}\frac{\partial f}{\partial y_i} - (X-\mu)(v+\epsilon)^{-1}\frac{1}{N}\sum_{i=1}^{N}(x_i-\mu)\frac{\partial f}{\partial y_i} + \frac{\partial f}{\partial Y} \right)$$

Here $x, y, v, \mu, \gamma \in \mathbb{R}^D$.