0. Diagrams for SGD Test Loss

We use diagrams for book-keeping of the Taylor terms (of test loss at a fixed initial weight). Each color in a diagram represents a data value and thus selects a particular loss function from the data-parameterized distribution of loss functions. Each node in a diagram represents a tensor obtained from derivatives of the loss function corresponding to that node's color. It is a diagram's edges in a diagram that specify those derivative tensors. We understand the edges as directed from left to right, with the source acting on the target by differentiation. Finally, a diagram's value is the expectation over all iid assignments of data to the colors. Thus,

$$\begin{split} & = \mathbb{E}_{\mathrm{red,green}} \nabla^a(l_{\mathrm{red}}) \nabla^a(l_{\mathrm{green}}) & \quad \bullet := \mathbb{E}_{\mathrm{red}} \nabla^a(l_{\mathrm{red}}) \nabla^a(l_{\mathrm{red}}) \\ & \quad \bullet := \mathbb{E}_{\mathrm{red,green,blue}} \nabla^a(l_{\mathrm{red}}) \nabla^a \nabla^b(l_{\mathrm{green}}) \nabla^b(l_{\mathrm{blue}}) \\ & \quad \bullet := \mathbb{E}_{\mathrm{red,green,blue}} \nabla^a(l_{\mathrm{red}}) \nabla^b(l_{\mathrm{green}}) \nabla^a \nabla^b(l_{\mathrm{blue}}) \end{split}$$

We see that $\bullet - \bullet \bullet$ gives the trace of the covariance of gradients. Moreover, $\bullet \bullet \bullet \bullet \bullet \bullet \bullet$, illustrating how diagram notation can streamline computation by helping to group terms. However, we caution that a diagram's value generally depends on a diagram's digraph structure, not just its undirected structure. For example:

Thus prepared, we may expand the test loss after T updates, each with batch-size 1 sampled without replacement. The recipe is to draw all the diagrams whose underlying poset has a unique rightmost element. Each node in the diagram contributes a symmetry factor 1/i! where i is the node's in-degree. On top of that, a diagram with a edges and v vertices has an overall combinatorial weight of $(-\eta)^a {T \choose v-1}$. We obtain:

$$\mathbb{E}\left(\text{SGD Test Loss}\right) = \bullet - \eta \binom{T}{1} \left(\bullet - \bullet\right) \\ + \eta^2 \binom{T}{2} \left(\bullet - \bullet\right) + \frac{1}{2} \bullet - \bullet\right) + \eta^2 \binom{T}{1} \left(\frac{1}{2} \bullet - \bullet\right) \\ - \eta^3 \binom{T}{3} \left(\bullet - \bullet\right) + \frac{1}{2} \bullet - \bullet + \frac{1}{6} \bullet - \bullet\right) \\ - \eta^3 \binom{T}{2} \left(\frac{1}{2} \bullet - \bullet\right) + \frac{1}{2} \bullet - \bullet + \frac{1}{6} \bullet - \bullet\right) \\ - \eta^3 \binom{T}{1} \left(\frac{1}{6} \bullet - \bullet\right) + o(\eta^3)$$

And a routine grouping of terms yields:

$$\cdots = \bullet - \eta \binom{T}{1} \left(\bullet - \bullet \right)$$

$$+ \eta^2 \binom{T}{2} \left(\frac{3}{2} \bullet - \bullet \right) + \eta^2 \binom{T}{1} \left(\frac{1}{2} \bullet - \bullet \right)$$

$$- \eta^3 \binom{T}{3} \left(\frac{5}{2} \bullet - \bullet - + \frac{1}{2} \bullet - \bullet - \frac{1}{6} \bullet - \bullet \right)$$

$$- \eta^3 \binom{T}{2} \left(\bullet - \bullet - + \frac{5}{6} \bullet - \bullet - \bullet \right)$$

$$- \eta^3 \binom{T}{1} \left(\frac{1}{6} \bullet - \bullet - \bullet \right) + o(\eta^3)$$