Tim Albrecht Q+A - 16/12/2020

This Q+A is from the following AI3SD Video:

- **Series:** AI3SD Winter Seminar Series 2020
- **Title:** When charge transport data are a worm – a transfer learning approach for unsupervised data classification

Q1: Is it practical to use quantum chemistry methods to complete the current that you measured? If so, what method is needed?

TA: You can do that, and this has been done by the Group of Jenna Solomon, for example, in Copenhagen, and the level of theory that's a bit difficult to say. They used a relatively simple DfT implementation, and then basically simulated different scenarios for example, depending on where atoms sit in the junction, for example how the junction evolves and then select the particular scenarios that would then inform the training of their network, and the network that would then search data to identify these different classes. Therefore you could then make a connection between the experimentally observed trays and the model data. Of course, that then it really does depend then on what you similar, what you choose to simulate, which types of traces. While that can be very useful, there is a potential than that you introduce a certain bias in the way you select these. Again, that sort of level of theory required is that's difficult to say or in general terms.

Q2: When you use the autoencoder, how do you make a decision about the dimensionality of the bottleneck?

TA: We just keep it simple so in this case it was just 2 neurons, because it makes our life very easy in terms of visualizing the results.
Audience member: So, you get a nice two deep block?
TA: Actually that made me realize I didn't talk about the structure of the autoencoder, so that depended a little bit on the feature extractor that we used so far Alex net, that gives you a thing in 9216 component vector. That was then of course the input for the auto encoder and in total we have nine layers, so it went then down to 1024 down to 2 and then up again.
Audience member: This is a straight autoencoder as opposed to variational?
TA: Yeah, that's a straight.
Audience member: I think a variational it could be really, really interesting because then in that case you could kind of do the thing of moving around in that latent space and use it to generate new examples which could be very interesting for seeing how movements in that reduced dimensionality latent space correspond to changes in in the input signal. That could be a lot of fun.