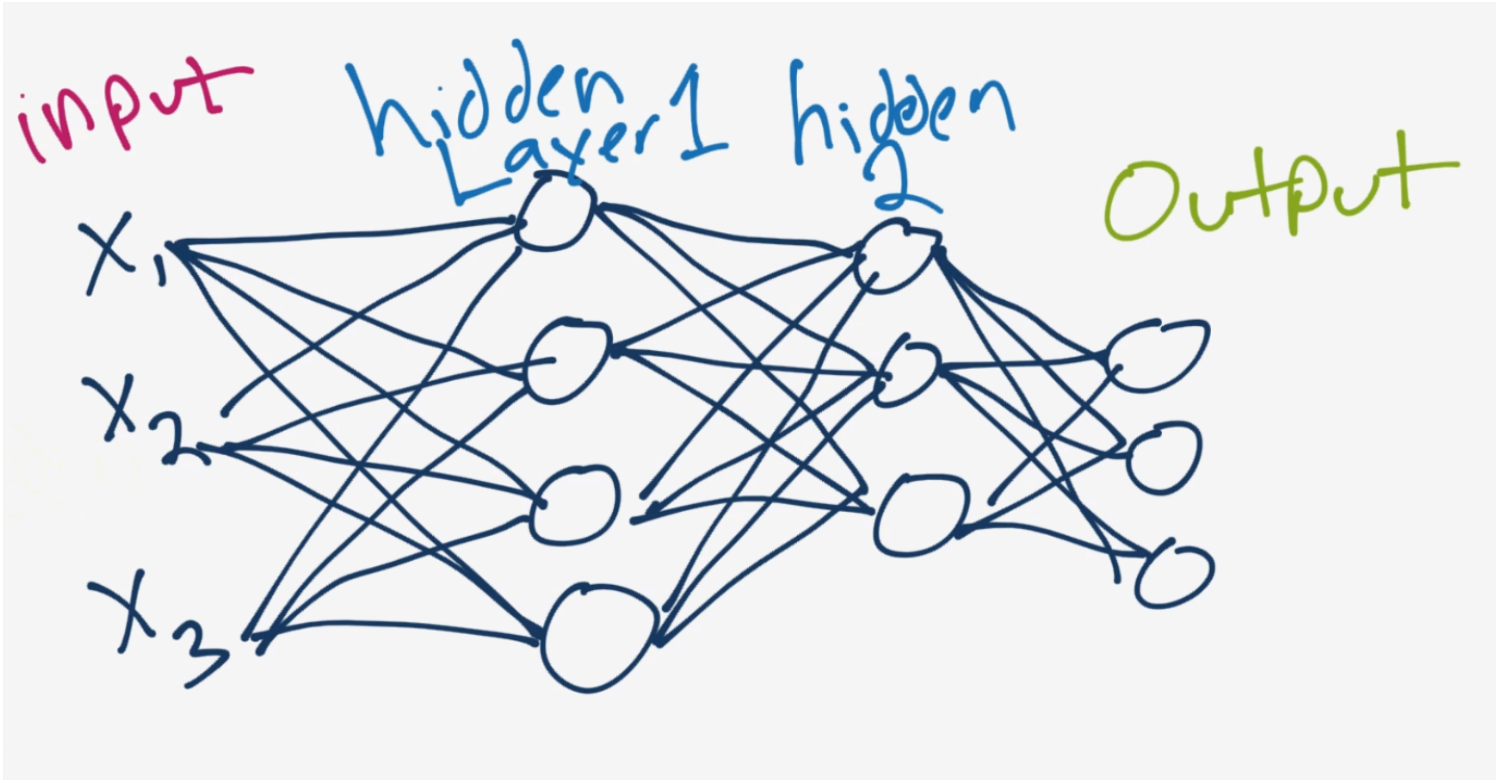
Deep Learning

Deep Networks

In the last lecture we have mentioned that:



- A NN with more than one hidden layer is called deep
- Deep networks can encode more complex relations than shallow ones
- I.e. they can have higher variance

So why has Deep Learning become a thing only in the last decade?

Enablers for Deep Learning

There are three main reasons:

1. Learning complex relations is viable only with abundant data

- With small datasets, high variance models risk overfitting
- ...And for complex relations low-variance models are enough
- Only recently larger data collection have become widely available

2. Handling abundant data may require considerable computational power

- Deep nets for many industrial problems are actually not too hard to train
- ...At least with modern hardware
- ...But the "famous" models take up to millions of $ to train!

3. Historically, there was no good training algorithm for deep nets

- This is worth explaining mode in detail...

Vanishing Gradient Problem

A network with n hidden layers can be seen as something like:

$$f(x, w) = g(w_g \cdot h(w_n \cdot h(w_{n-1} \cdot h(\ldots))))$$

- Where h_k is the activation function for k-th hidden layer
- And g is the activation function for the output layer.

When we apply gradient computation to the formula

...With some abuse of notation we get:

$$f'(x, w) = g' \, w_n^T h' \, w_{n-1}^T h' \ldots$$

- Historically, sigmoid activation functions were used in all hidden layers
- ...And for a sigmoid we have $|h'| < 1$

Therefore, the more layers we have, the weaker the gradient becomes!

Vanishing Gradient Problem

This problem is now usually solved with a very simple trick

I.e. by always using ReLUs in the hidden layers

- ReLUs are almost everywhere differentiable
- When they are inactive, their derivative is 0
  - ...Which kill the gradient completely
- ...But when they are active, their derivative is 1
  - ...Which does not dampen the gradient at all!

There are cases when other activation functions are used

...But there must be a good reason for doing that

- In most cases, sticking to ReLU is fine

Loading the Data

We will now see how to use deep networks in practice

Let's start by loading the housing dataset (again):

In [2]:
```
data = pd.read_csv('data/real_estate.csv', sep=',')
in_cols = [c for c in data.columns if c != 'price per area']
X = data[in_cols]
y = np.log(data[['price per area']])
X_tr, X_ts, y_tr, y_ts = train_test_split(X, y, test_size=0.34, random_state=42)

data.head()
```

Out[2]:

	house age	dist to MRT	#stores	latitude	longitude	price per area
0	14.8	393.2606	6	24.96172	121.53812	7.6
1	17.4	6488.0210	1	24.95719	121.47353	11.2
2	16.0	4066.5870	0	24.94297	121.50342	11.6
3	30.9	6396.2830	1	24.94375	121.47883	12.2
4	16.5	4082.0150	0	24.94155	121.50381	12.8

- The task is still estimating "price per area"
- It's boring, but it will make for an easier comparison w.r.t. other approaches

Standardization

Then we standardize the data

Once more: never forget this step unless you know your input is already fine

In [3]:

```
x_scaler, y_scaler = StandardScaler(), StandardScaler()
X_tr_s = pd.DataFrame(data=x_scaler.fit_transform(X_tr), columns=X_tr.columns)
X_ts_s = pd.DataFrame(data=x_scaler.transform(X_ts), columns=X_ts.columns)
y_tr_s = pd.DataFrame(data=y_scaler.fit_transform(y_tr), columns=y_tr.columns)
y_ts_s = pd.DataFrame(data=y_scaler.transform(y_ts), columns=y_ts.columns)
X_tr_s.describe()
```

Out[3]:

	house age	dist to MRT	#stores	latitude	longitude
count	2.730000e+02	2.730000e+02	2.730000e+02	2.730000e+02	2.730000e+02
mean	1.236292e-16	6.100127e-17	-1.187491e-16	1.263361e-13	-5.604015e-13
std	1.001837e+00	1.001837e+00	1.001837e+00	1.001837e+00	1.001837e+00
min	-1.539647e+00	-8.473385e-01	-1.391448e+00	-3.039301e+00	-4.045428e+00
25%	-7.664720e-01	-6.297593e-01	-1.054688e+00	-4.965293e-01	-4.071818e-01
50%	-1.479322e-01	-4.600779e-01	-4.440791e-02	1.446702e-01	3.410575e-01
75%	9.774665e-01	3.180448e-01	6.291121e-01	6.316881e-01	6.357777e-01
max	2.016957e+00	4.476150e+00	1.976152e+00	3.692478e+00	2.194834e+00

Building a Network

Now, we can build a deep network by simply stacking more layers

```
In [4]: def build_nn(input_shape, hidden):
            mdl = keras.Sequential()
            mdl.add(keras.Input(shape=input_shape))
            for k, h in enumerate(hidden):
                mdl.add(Dense(h, activation='relu'))
            mdl.add(Dense(1, activation='linear'))
            return mdl
```

We will build several networks, so we are using a function

- We explicitly build an `Input` layer
  - ...So that we don't have to worry about that in the rest of the code
- We can control the size and number of layers with the `hidden` parameters
  - E.g. with `hidden = [16, 8]`
  - ...We get one hidden layer with 16 neurons, then one with 8

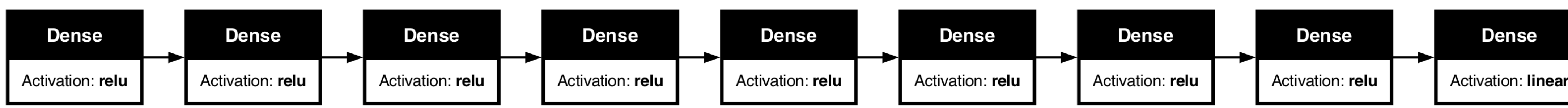
Building a Network

Let's try to build a few networks

A deeper network:

In [5]:
```
nns = {}
nns['8l'] = build_nn(input_shape=(len(in_cols), ), hidden=[16] * 8)
keras.utils.plot_model(nns['8l'], rankdir='LR', show_layer_activations=True, dpi=150)
```

Out[5]:



And a few less deep network for comparison:

In [6]:
```
nns['4l'] = build_nn(input_shape=(len(in_cols), ), hidden=[16] * 4)
nns['2l'] = build_nn(input_shape=(len(in_cols), ), hidden=[16] * 2)
nns['1l'] = build_nn(input_shape=(len(in_cols), ), hidden=[16])
nns['0l'] = build_nn(input_shape=(len(in_cols), ), hidden=[])
```

- `nn1` is shallow and `nn0` is just a linear regressor!

Training the Networks

Now, let's prepare the code to train the networks

In [7]:
```
def train_nn(nn, X_tr, y_tr, batch_size, epochs, verbose=1):
    nn.compile(loss='mse', optimizer='adam')
    history = nn.fit(X_tr, y_tr, batch_size=batch_size, epochs=epochs, verbose=verbose)
    cols = [k for k in history.history.keys()]
    vals = np.array([history.history[c] for c in cols]).T
    return pd.DataFrame(data=vals, columns=cols)
```

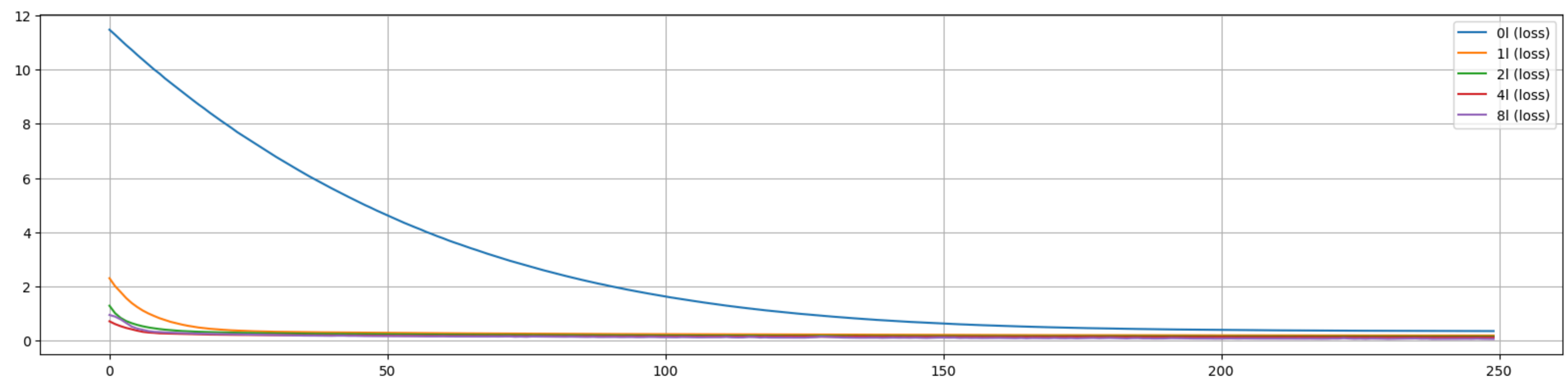
...And let's train all of them:

In [8]:
```
histories = []
for l, nn in sorted(nns.items()):
    history = train_nn(nn, X_tr_s, y_tr_s, batch_size=32, epochs=250, verbose=0)
    histories.append(history.rename(columns={c:f'{l} ({c})' for c in history.columns}))
histories = pd.concat(histories, axis=1)
```

Training Histories

Let's have a look at the training history

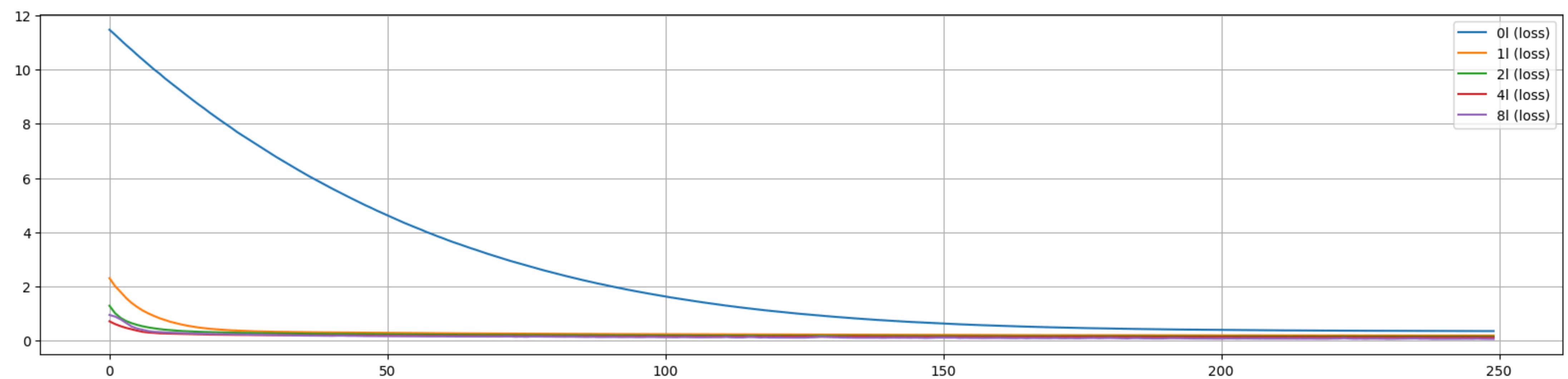
In [9]:
```
histories.plot(figsize=figsize, grid=':');
```



Training Histories

Let's have a look at the training history

```
In [9]: histories.plot(figsize=figsize, grid=':');
```



- Deeper networks tend to converge faster and to lower loss values
- ...But they also often start from a lower value (right after random initialization)
- This behavior is even now not completely understood

Evaluation

Let's have a look at the prediction quality

```
In [10]: pred_tr = {k: y_scaler.inverse_transform(nn.predict(X_tr_s, verbose=0)) for k, nn in sorted
         pred_ts = {k: y_scaler.inverse_transform(nn.predict(X_ts_s, verbose=0)) for k, nn in sorted

         r2_tr = {k: r2_score(y_tr, preds) for k, preds in sorted(pred_tr.items())}
         r2_ts = {k: r2_score(y_ts, preds) for k, preds in sorted(pred_ts.items())}

         for k in sorted(r2_tr.keys()):
             print(f'r2 score for {k}: {r2_tr[k]:.3f} (training), {r2_ts[k]:.3f} (test)')

         r2 score for 0l: 0.643 (training), 0.621 (test)
         r2 score for 1l: 0.806 (training), 0.708 (test)
         r2 score for 2l: 0.844 (training), 0.697 (test)
         r2 score for 4l: 0.878 (training), 0.727 (test)
         r2 score for 8l: 0.935 (training), 0.655 (test)
```

- Adding layers improves the behavior on the training set
- Too many layers may lead to overfitting

This is actually expected, since deeper networks have higher variance

Keeping Overfitting at Bay

How do we reduce overfitting for deep networks?

- We can of course tune the number of layers (and that's a good solution)
- ...But we loose some of the advantage of depth by doing that

...So what else can we do?

The first ingredient is Stochastic Gradient Descent

Let's see what happens if we switch to classical Gradient Descent

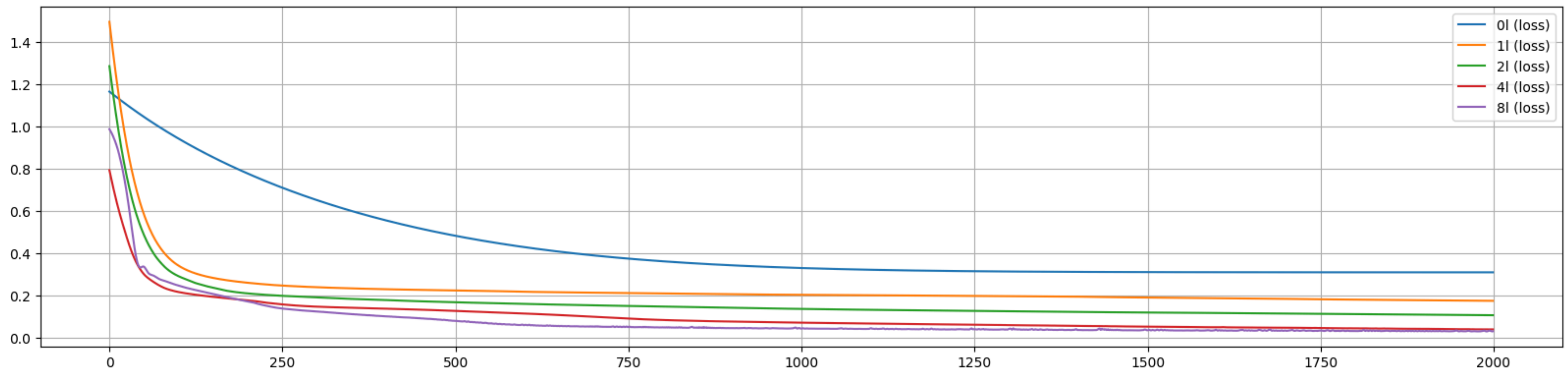
```
In [11]: nns_gd = {f'{k}l': build_nn(input_shape=(len(in_cols), ), hidden=[16] * k) for k in (8, 4, 
         histories_gd = []
         for l, nn in sorted(nns_gd.items()):
             history = train_nn(nn, X_tr_s, y_tr_s, batch_size=len(X_tr), epochs=250*8, verbose=0)
             histories_gd.append(history.rename(columns={c:f'{l} ({c})' for c in history.columns}))
         histories_gd = pd.concat(histories_gd, axis=1)
```

- We need to rebuild the networks since keras does not reset weights
- Since we are making fewer iterations per epoch, we need to use more epochs

Training Histories wit Classical GD

Let's have a look at the new training histories

In [12]:
```
histories_gd.plot(figsize=figsize, grid=':');
```



- These are not unlike the previous ones
- ...And in all cases we are reasonably close to convergence

Quality Evaluation with Classical GD

...But the prediction quality is considerably worse on unseen data!

In [13]:
```python
pred_tr_gd = {k: y_scaler.inverse_transform(nn.predict(X_tr_s, verbose=0)) for k, nn in sor
pred_ts_gd = {k: y_scaler.inverse_transform(nn.predict(X_ts_s, verbose=0)) for k, nn in sor
r2_tr_gd = {k: r2_score(y_tr, preds) for k, preds in sorted(pred_tr_gd.items())}
r2_ts_gd = {k: r2_score(y_ts, preds) for k, preds in sorted(pred_ts_gd.items())}
for k in sorted(r2_tr_gd.keys()):
    print(f'r2 score for {k}: {r2_tr_gd[k]:.3f} (training), {r2_ts_gd[k]:.3f} (test)')
```

```
r2 score for 0l: 0.691 (training), 0.644 (test)
r2 score for 1l: 0.826 (training), 0.698 (test)
r2 score for 2l: 0.894 (training), 0.703 (test)
r2 score for 4l: 0.961 (training), 0.493 (test)
r2 score for 8l: 0.969 (training), 0.561 (test)
```

Quality Evaluation with Classical GD

...But the prediction quality is considerably worse on unseen data!

```
In [13]: pred_tr_gd = {k: y_scaler.inverse_transform(nn.predict(X_tr_s, verbose=0)) for k, nn in sor
         pred_ts_gd = {k: y_scaler.inverse_transform(nn.predict(X_ts_s, verbose=0)) for k, nn in sor
         r2_tr_gd = {k: r2_score(y_tr, preds) for k, preds in sorted(pred_tr_gd.items())}
         r2_ts_gd = {k: r2_score(y_ts, preds) for k, preds in sorted(pred_ts_gd.items())}
         for k in sorted(r2_tr_gd.keys()):
             print(f'r2 score for {k}: {r2_tr_gd[k]:.3f} (training), {r2_ts_gd[k]:.3f} (test)')

         r2 score for 0l: 0.691 (training), 0.644 (test)
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         r2 score for 8l: 0.969 (training), 0.561 (test)
```

Deep networks have many local optima

- Using randomize mini-batches tends to lead the training process
- ...Toward local optima that are robust to perturbations

Early Stopping

A simple, but effective, option consists in using an early stopping callback

- At training time, we monitor the performance on a validation set
- ...And we stop training if we don't improve enough on that one

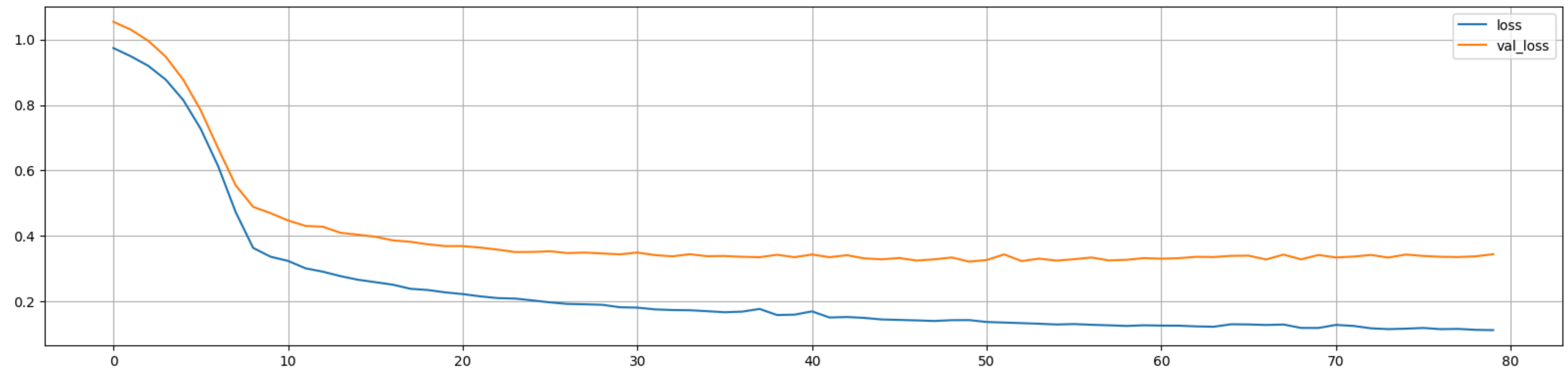
```
In [14]: def train_nn_es(nn, X_tr, y_tr, batch_size, epochs, verbose=1, patience=30):
             nn.compile(loss='mse', optimizer='adam')
             cb = [keras.callbacks.EarlyStopping(monitor='val_loss', patience=patience, restore_best_
             history = nn.fit(X_tr, y_tr, batch_size=batch_size, epochs=epochs, verbose=verbose,
                              callbacks=cb, validation_split=0.2)
             cols = [k for k in history.history.keys()]
             vals = np.array([history.history[c] for c in cols]).T
             return pd.DataFrame(data=vals, columns=cols)

         nn8_es = build_nn(input_shape=(len(in_cols), ), hidden=[16] * 8)
         history8_es = train_nn_es(nn8_es, X_tr_s, y_tr_s, batch_size=32, epochs=250, verbose=0)
```

- Typically, the callback waits for a number of epochs (patience)
- If no improvement is achieved within that time frame, training is stopped

Training History with Early Stopping

Let's have a look at the training for the 8-level network

```
In [15]: history8_es.plot(figsize=figsize, grid=':');
```



- We stopped far earlier than the 250 epochs limit

Prediction Quality with Early Stopping

Let's check the prediction quality

```
In [16]: pred_tr_nn8_es = y_scaler.inverse_transform(nn8_es.predict(X_tr_s, verbose=0))
         pred_ts_nn8_es = y_scaler.inverse_transform(nn8_es.predict(X_ts_s, verbose=0))

         r2_tr_nn8_es = r2_score(y_tr, pred_tr_nn8_es)
         r2_ts_nn8_es = r2_score(y_ts, pred_ts_nn8_es)

         print(f'r2 score for 8l (original): {r2_tr["8l"]:.3f} (training), {r2_ts["8l"]:.3f} (test)'
         print(f'r2 score for 8l (es): {r2_tr_nn8_es:.3f} (training), {r2_ts_nn8_es:.3f} (test)')
```

```
r2 score for 8l (original): 0.935 (training), 0.655 (test)
r2 score for 8l (es): 0.827 (training), 0.713 (test)
```

- We are doing worse on the training data
- ...But a bit better on unseen examples!

Dropout

Another consists in using the dropout regularization technique

Dropout consists in removing network nodes at random a training time

- At each gradient descent iteration, nodes are removed with a rate p
- Once the iteration is over, everything is restored

The approach forces the network to develop some redundancy

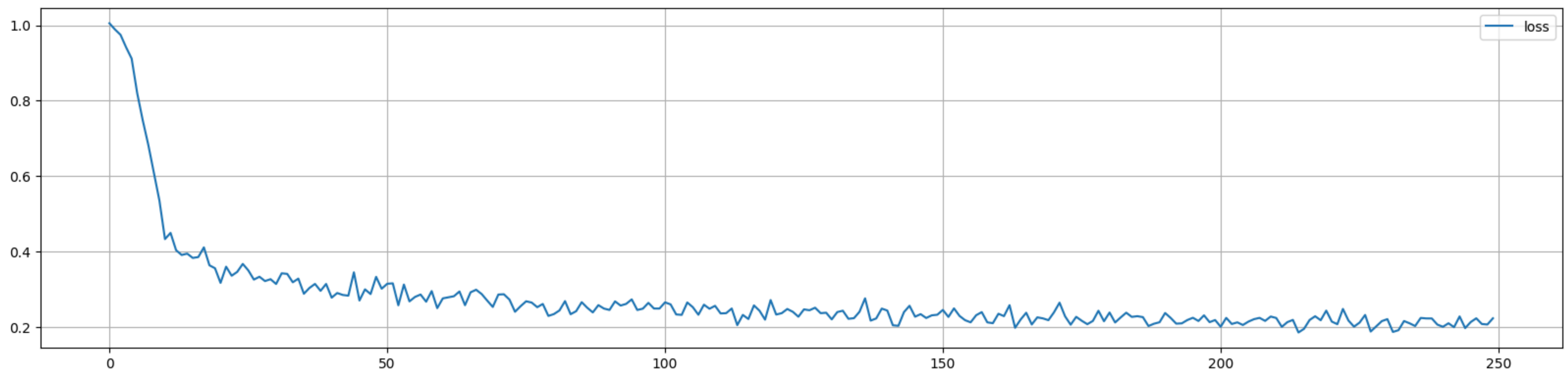
In Keras, dropout is implemented as a special layer:

In [17]:
```
def build_nn_do(input_shape, hidden, rate=0.05):
    mdl = keras.Sequential()
    mdl.add(keras.Input(shape=input_shape))
    for k, h in enumerate(hidden):
        mdl.add(Dense(h, activation='relu'))
        mdl.add(keras.layers.Dropout(rate))
    mdl.add(Dense(1, activation='linear'))
    return mdl
```

Training a Network with Dropout

Let's train our deeper network with dropout

In [18]:
```
nn8_do = build_nn_do(input_shape=(len(in_cols), ), hidden=[16] * 8)
history8_do = train_nn(nn8_do, X_tr_s, y_tr_s, batch_size=32, epochs=250, verbose=0)
history8_do.plot(figsize=figsize, grid=':');
```



- We will not use an early stopping callback in this case
- ...So preventing overfitting is totally up to the dropout layer

Quality Evaluation with Dropout

Let's check (one last time) the prediction quality

```
In [19]: pred_tr_nn8_do = y_scaler.inverse_transform(nn8_do.predict(X_tr_s, verbose=0))
         pred_ts_nn8_do = y_scaler.inverse_transform(nn8_do.predict(X_ts_s, verbose=0))

         r2_tr_nn8_do = r2_score(y_tr, pred_tr_nn8_do)
         r2_ts_nn8_do = r2_score(y_ts, pred_ts_nn8_do)

         print(f'r2 score for 8l (original): {r2_tr["8l"]:.3f} (training), {r2_ts["8l"]:.3f} (test)'
         print(f'r2 score for 8l (es): {r2_tr_nn8_es:.3f} (training), {r2_ts_nn8_es:.3f} (test)')
         print(f'r2 score for 8l (dropout): {r2_tr_nn8_do:.3f} (training), {r2_ts_nn8_do:.3f} (test)

r2 score for 8l (original): 0.935 (training), 0.655 (test)
r2 score for 8l (es): 0.827 (training), 0.713 (test)
r2 score for 8l (dropout): 0.828 (training), 0.690 (test)
```

- Dropout is considerably improving our test score
- Even without any access to unseen examples at training time
- ...Since we are not using a validation set!

Considerations and Take Home Messages

Deep network are a powerful tool

- They dramatically improve the variance of NN models
- ...And allow to tweak the bias/variance trade off by adjusting the depth

DNs should use ReLUs in the hidden layers

...Due to the vanishing gradient problem

- Unless of course there a very good reason to do otherwise

DNs should always be trained with stochastic gradient descent

...Since that helps reducing overfitting

- There are of course exceptions
- ...But those need to be well motivated

Other techniques to control overfitting include

...Early stopping callbacks and dropout