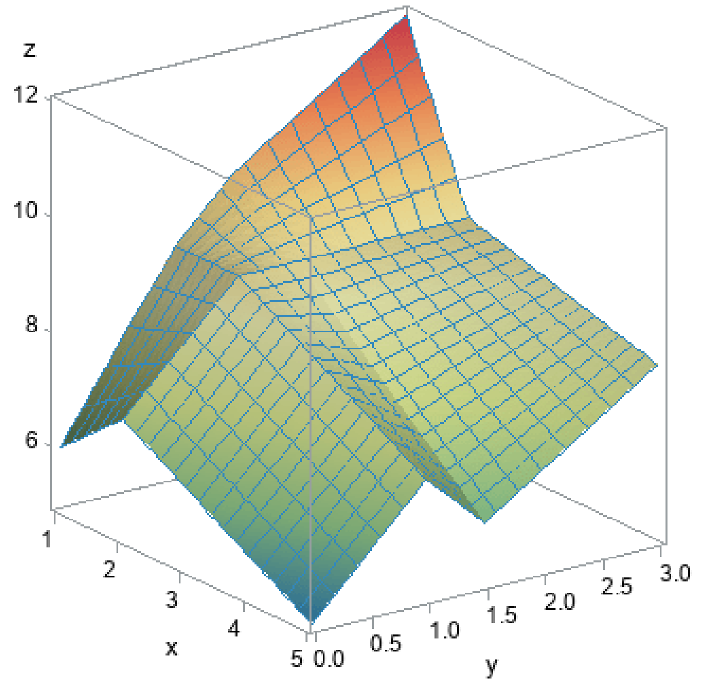
Lattice Models to Support Constraints

Lattice Models

We will deal with the constraint by relying on a Lattice model

Lattice models are a form of piecewise linear interpolated model



- They are defined via a grid over their input variables
- Their parameters are the output values at each grid point
- Other output values are obtained via linear interpolation

Lattice Models

Lattice models:

- Can represent non-linear multivariate functions
- Can be trained by (e.g.) gradient descent

The grid is defined by splitting each input domain into intervals

- The domain of variable x_i is split by choosing a fixed set of n_i "knots"
- ...Of course this leads to scalability issues: we will discuss them later

The lattice parameters are interpretable

They simply represent output values for certain input vectors

- They can be changed with predictable effects
- They can be constrained so that the model behaves in a desired fashion
- If we use hard constraints, we get a guaranteed behavior

Lattice Models and Interpretability

Interpretability is a major open issue in modern ML

It is often a key requirement in industrial applications

- Customers have trouble accepting models that they do not understand
- Sometimes you are legally bound to provide motivations

There are two main ways to achieve interpretability

The first is using a model that is inherently interpretable

- There are a few examples of this: linear regression, DTs, (some) SVMs, rules...
- Lattice models fall into this class

The second approach is computing a posteriori explanations

- E.g. approximate linear explanations
- ...Such as in the LIME or SHAP approaches

Combining Lattice Models

Combining Lattice Models

Using a single lattice model leads to scalability issues

In a lattice model, the number of grid points is given by:

$$n = \prod_{i=1}^{m} n_i$$

- ...Hence the parameter number scales exponentially with the number of inputs
- So that modeling complex non-linear function seems to come at a steep cost

Scalability issues can be mitigated via two approaches:

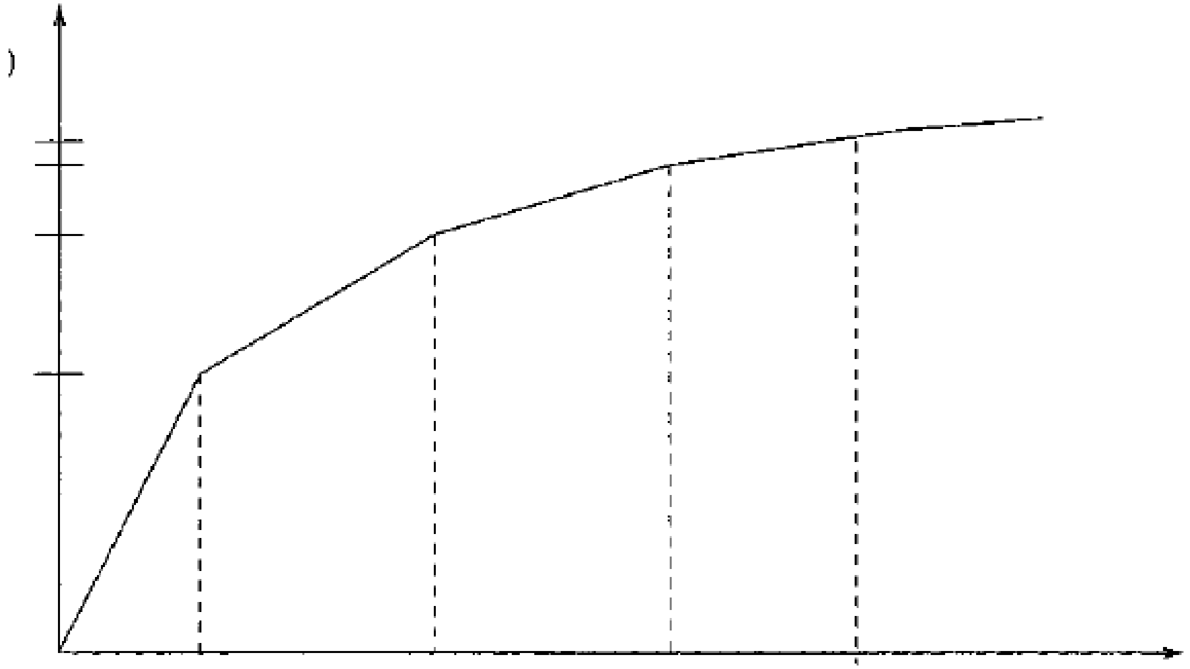
- Ensembles of small lattices (we will not cover this one)
- Processing each input variable individually using a smaller Lattice

We will focus on this latter approach, which is sometimes called "calibration"

Calibration for Numeric Inputs

Calibration for numeric attributes...

...Consists in applying a piecewise linear transformation to each input

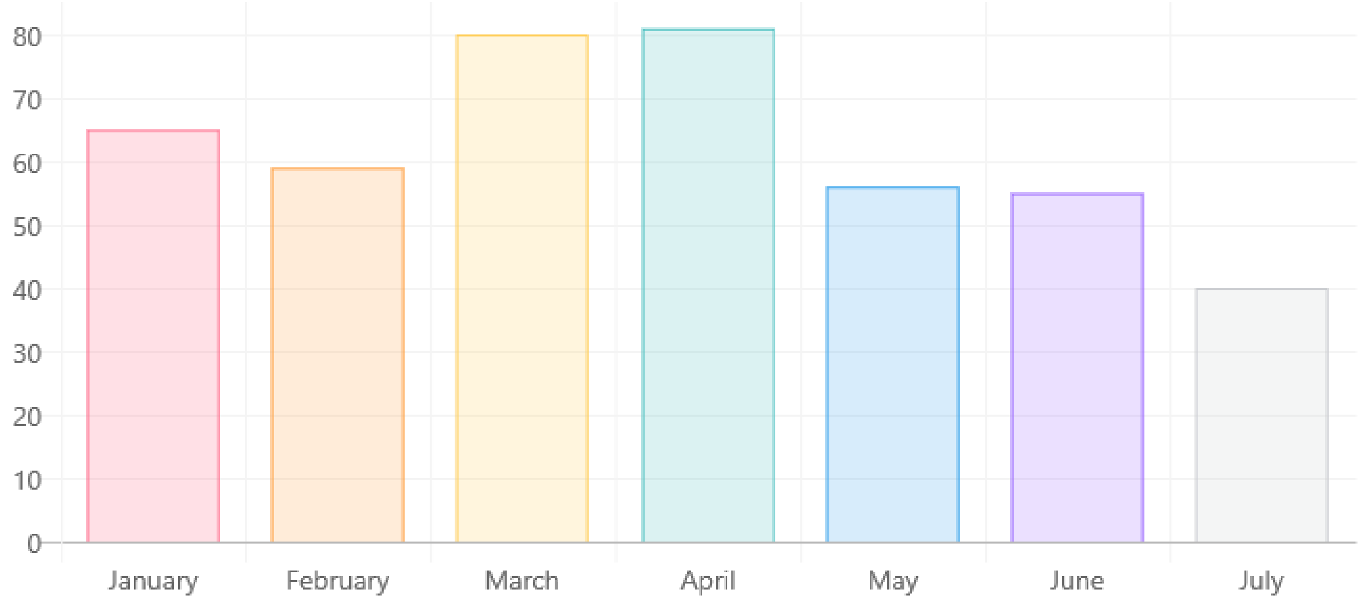


- This is in fact a 1-D lattice
- Calibration parameters are the function values at all knots

Calibration for Categorical Inputs

Calibration for categorical inputs...

...Consists in applying a map:



- Categorical inputs must be encoded as integers
- Each input value is mapped to an output value
- The parameters are the map output values

About Calibration

With this approach:

- We make each input more complicated
- ...Which allows us to make the lattice model simple

Calibration enables the use of fewer knots in the lattice

E.g. say we are aiming for 5 grid values per attribute, with 2 attributes

- With 5 knots per layer an single lattice: $5 \times 5 = 25$ parameters
- With 5 calibration knots + 2 lattice knots: $5 \times 2 + 2 \times 2 = 14$

We do not get the same level of flexibility, but we get close

- Additionally, we tend to get more regular results
- ...Since we have more bias and less variance

This might be an advantage for out-of-distribution generalization

Data Preprocessing

As usual, we need to start with some data pre-processing

We start by converting our string data into integers

In [2]:

```
tr_sc2 = tr_s.copy()
tr_sc2['dollar_rating'] = tr_sc2['dollar_rating'].astype('category')
tr_sc2['dollar_rating'] = tr_sc2['dollar_rating'].cat.codes
tr_sc2['dollar_rating'][:3]
val_sc2 = val_s.copy()
val_sc2['dollar_rating'] = val_sc2['dollar_rating'].astype('category').cat.codes
ts_sc2 = ts_s.copy()
ts_sc2['dollar_rating'] = ts_sc2['dollar_rating'].astype('category').cat.codes

tr_sc2[:3]
```

Out[2]:

	avg_rating	num_reviews	dollar_rating	clicked
0	0.785773	0.61	3	1
1	0.785773	0.61	3	0
2	0.785773	0.61	3	0

Implementing a Lattice Model

Now we need to choose the size for the main lattice

```
In [3]: lattice_sizes = [2] * 3
```

- We will use only two knots per dimension
- Since most of the complex processing will be done by calibration

Then we separate the features and we build individual input tensors

```
In [4]: tr_ls2 = [tr_sc2[c] * (s-1) for c, s in zip(dt_in, lattice_sizes)]
        val_ls2 = [val_sc2[c] * (s-1) for c, s in zip(dt_in, lattice_sizes)]
        ts_ls2 = [ts_sc2[c] * (s-1) for c, s in zip(dt_in, lattice_sizes)]

        avg_rating = layers.Input(shape=[1], name='avg_rating')
        num_reviews = layers.Input(shape=[1], name='num_reviews')
        dollar_rating = layers.Input(shape=[1], name='dollar_rating')
```

- This is needed for compatibility with the tensorflow-lattice implementation

Piecewise Linear Calibration

We use `PWLCalibration` objects for all numeric inputs

In [5]:
```
import tensorflow_lattice as tfl

avg_rating_cal = tfl.layers.PWLCalibration(
    input_keypoints=np.quantile(tr_sc2['avg_rating'], np.linspace(0, 1, num=20)),
    output_min=0.0, output_max=lattice_sizes[0] - 1.0, name='avg_rating_cal'
)(avg_rating)

num_reviews_cal = tfl.layers.PWLCalibration(
    input_keypoints=np.quantile(tr_sc['num_reviews'], np.linspace(0, 1, num=20)),
    output_min=0.0, output_max=lattice_sizes[1] - 1.0, name='num_reviews_cal'
)(num_reviews)
```

- The knot values are learnable parameters
- ...But their positions are fixed (in this case to specific quantiles)

Categorical Calibration

We use `CategoricalCalibration` objects for the categorical input

In [6]:
```
dollar_rating_cal = tfl.layers.CategoricalCalibration(
    num_buckets=4,
    output_min=0.0, output_max=lattice_sizes[2] - 1.0,
    name='dollar_rating_cal'
)(dollar_rating)
```

- We use one "bucket" for each possible category

Finally, we build the actual lattice

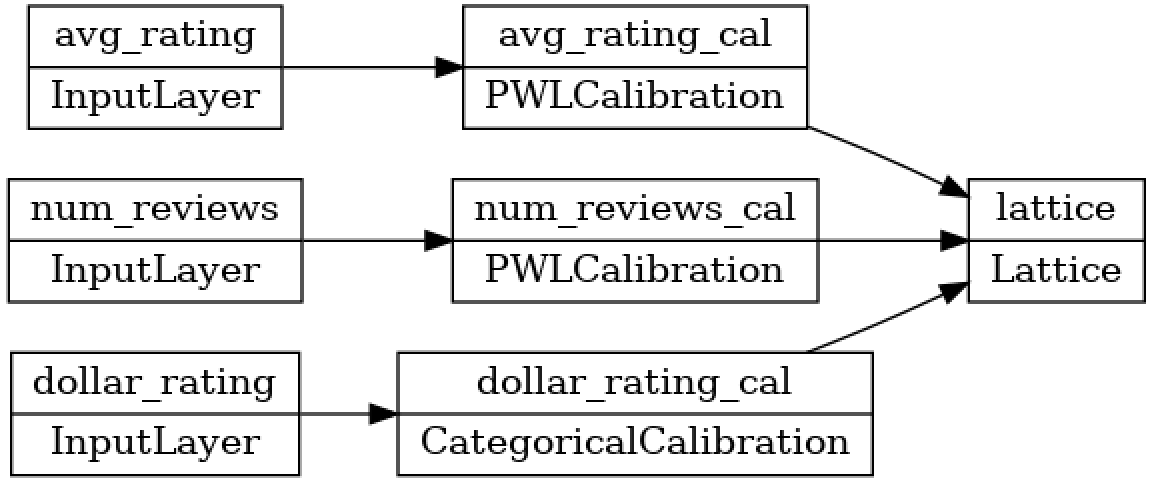
In [7]:
```
lt_inputs = [avg_rating_cal, num_reviews_cal, dollar_rating_cal]

mdl_out = tfl.layers.Lattice(
    lattice_sizes=lattice_sizes,
    output_min=0, output_max=1, name='lattice',
)(lt_inputs)

mdl_inputs = [avg_rating, num_reviews, dollar_rating]
lm = keras.Model(mdl_inputs, mdl_out)
```

Building the Calibrated Lattice Model

Let's see which kind of architecture we have now:

In [9]:
```
util.plot_nn_model(lm, show_layer_activations=True, show_layer_names=True, show_shapes=False)
```

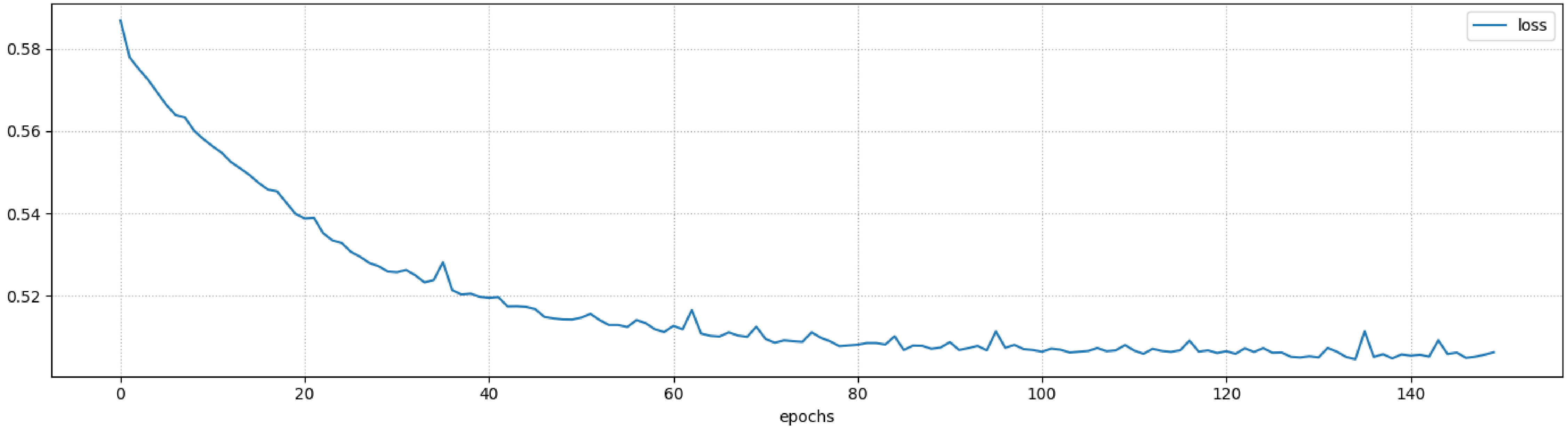
Out[9]:



Training the Calibrated Lattice

We can train the new model as usual

```
In [10]: history = util.train_nn_model(lm, tr_ls2, tr_sc['clicked'], loss='binary_crossentropy', batch_si
         util.plot_training_history(history, figsize=figsize)
```




```
Final loss: 0.5063 (training)
```

Evaluating the Calibrated Lattice

...And finally we can evaluate the results

In [11]:
```
pred_tr2 = lm.predict(tr_ls2, verbose=0)
pred_val2 = lm.predict(val_ls2, verbose=0)
pred_ts2 = lm.predict(ts_ls2, verbose=0)
auc_tr2 = roc_auc_score(tr_s['clicked'], pred_tr2)
auc_val2 = roc_auc_score(val_s['clicked'], pred_val2)
auc_ts2 = roc_auc_score(ts_s['clicked'], pred_ts2)
print(f'AUC score: {auc_tr2:.2f} (training), {auc_val2:.2f} (validation), {auc_ts2:.2f} (test)')
```

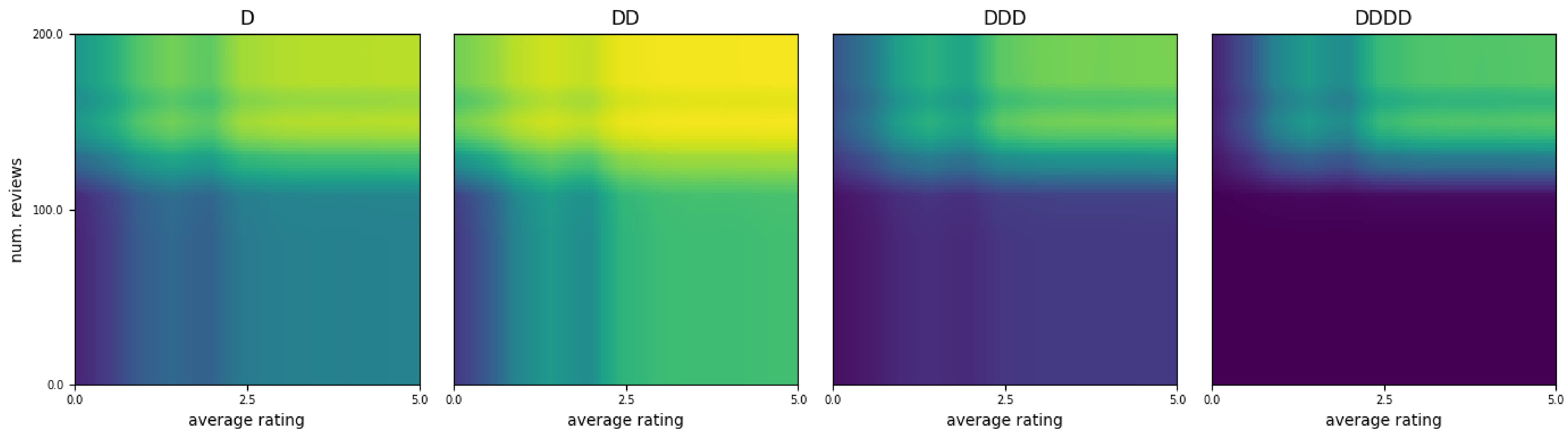
```
AUC score: 0.80 (training), 0.80 (validation), 0.80 (test)
```

- The performance is on par with the original one
- ...Except on the test set, where it works much better

Inspecting the Calibrated Lattice

We can inspect the learned function visually to get a better insight

```
In [12]: util.plot_ctr_estimation(lm, scale, split_input=True, one_hot_categorical=False, figsize=figsize
```

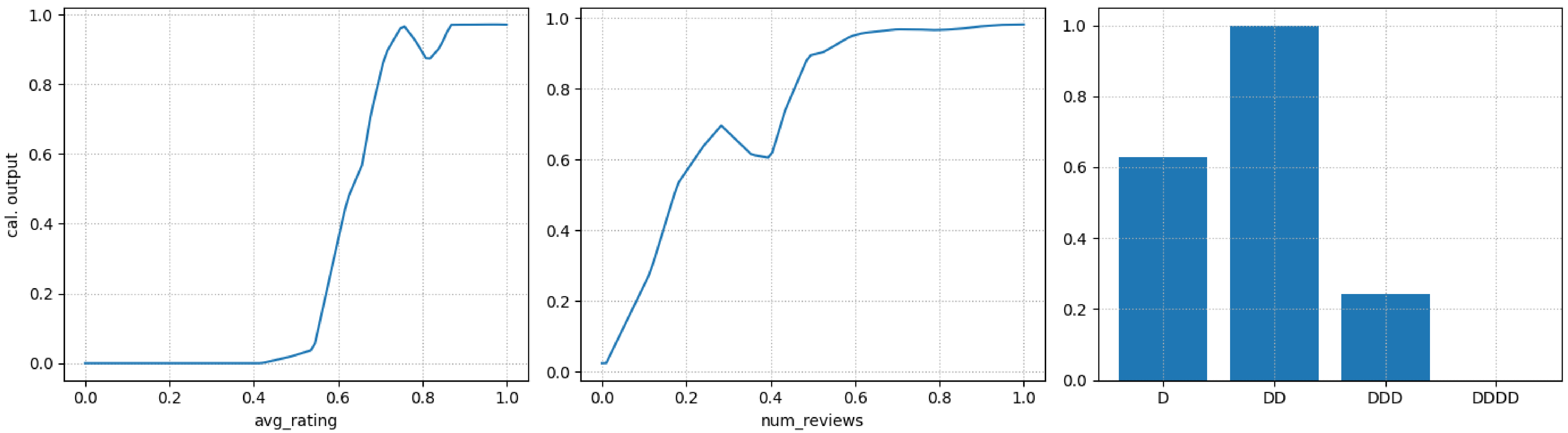


- The structure follows a (piecewise linear) "tartan pattern"
- This is particularly evident now, since we use just two knots per dimension

Inspecting the Calibrated Lattice

It is useful to inspect the calibration layers

In [14]:
```
calibrators = [keras.Model(mdl_inputs[i], lt_inputs[i]) for i in range(3)]
util.plot_ctr_calibration(calibrators, scale, figsize=figsize)
```



- The learned calibration functions violate the expected monotonicities
- ...Meaning that we still have one problem to solve

Shape Constraints

Shape Constraints

Lattice models are well suited to deal with shape constraints

Shape constraints are restrictions on the input-output function, such as:

- Monotonicity (e.g. "the output should grow when an input grows")
- Convexity/concavity (e.g. "the output should be convex w.r.t. an input")

Shape constraints are very common in industrial applications

Some examples:

- Reducing the price will raise the sales volume (monotonicity)
- Massive price reductions will be less effective (diminishing returns)
- Too low/high temperatures will lead to worse bakery products (convexity)

We can use them to fix our calibration issues

Shape Constraints

Shape constraints translate into constraints on the lattice parameters

- Let $\theta_{i,k,\bar{i},\bar{k}}$ be the parameter for the k-th knot of input i...
- ...While all the remaining attributes and knots (i.e. $\bar{i}$ and $\bar{k}$) are fixed

Then (increasing) monotonicity translates to:

$$\theta_{i,k,\bar{i},\bar{k}} \leq \theta_{i,k+1,\bar{i},\bar{k}}$$

- I.e. all else being equal, the lattice value at the grid points must be increasing
- Decreasing monotonicity is just the inverse

Then convexity translates to:

$$\left(\theta_{i,k+1,\bar{i},\bar{k}} - \theta_{i,k,\bar{i},\bar{k}}\right) \leq \left(\theta_{i,k+2,\bar{i},\bar{k}} - \theta_{i,k+1,\bar{i},\bar{k}}\right)$$

- I.e. all else being equal, the adjacent parameter differences should increase

Monotonicity and Smoothness

We can expect a monotonic effect of the average rating

I.e. Restaurants with a high rating will be clicked more often

In [16]:
```
avg_rating2 = layers.Input(shape=[1], name='avg_rating')
avg_rating_cal2 = tfl.layers.PWLCalibration(
    input_keypoints=np.quantile(tr_s['avg_rating'], np.linspace(0, 1, num=20)),
    output_min=0.0, output_max=lattice_sizes[0] - 1.0,
    monotonicity='increasing',
    kernel_regularizer=('hessian', 0, 1),
    name='avg_rating_cal'
)(avg_rating2)
```

In addition to monotonicity, we use a Hessian regularizer:

- This is a regularization term that penalizes the second derivative
- ...Thus making the calibrator more linear
- The two parameters are an L1 weight and L2 weights

Diminishing Returns

We can expect a diminishing returns from the number of reviews

- I.e. 200 reviews will be linked to much more clicks than 10 reviews
- ...But only a little more than 150 reviews

In [18]:
```
num_reviews2 = layers.Input(shape=[1], name='num_reviews')
num_reviews_cal2 = tfl.layers.PWLCalibration(
    input_keypoints=np.quantile(tr_s['num_reviews'], np.linspace(0, 1, num=20)),
    output_min=0.0, output_max=lattice_sizes[1] - 1.0,
    monotonicity='increasing',
    convexity='concave',
    kernel_regularizer=('wrinkle', 0, 1),
    name='num_reviews_cal'
)(num_reviews2)
```

By coupling monotonicity with concavity we enforce diminishing returns

- We also use the "wrinkle" reguralizer, which penalizes the third derivative
- ...Thus making the calibration function smoother

Partial Orders on Categories

We can expect more clicks for reasonably priced restaurants...

...At least compared to very cheap and very expensive ones

```
In [19]: dollar_rating2 = layers.Input(shape=[1], name='dollar_rating')
         dollar_rating_cal2 = tfl.layers.CategoricalCalibration(
             num_buckets=4,
             output_min=0.0, output_max=lattice_sizes[2] - 1.0,
             monotonicities=[(0, 1), (3, 1)],
             name='dollar_rating_cal'
         )(dollar_rating2)
```

On categorical attributes, we can enforce partial order constraints

- Each (i, j) pair translates into an inequality $\theta_i \leq \theta_j$
- Here we specify that "D" and "DDDD" will tend to have fewer clicks than "DD"

Lattice Model with Shape Constraints

Then we can build the actual lattice model

```
In [21]: lt_inputs2 = [avg_rating_cal2, num_reviews_cal2, dollar_rating_cal2]

         mdl_out2 = tfl.layers.Lattice(
             lattice_sizes=lattice_sizes,
             output_min=0, output_max=1,
             monotonicities=['increasing'] * 3, name='lattice',
         )(lt_inputs2)

         mdl_inputs2 = [avg_rating2, num_reviews2, dollar_rating2]
         lm2 = keras.Model(mdl_inputs2, mdl_out2)
```

If we specify monotonicities in the calibration layers

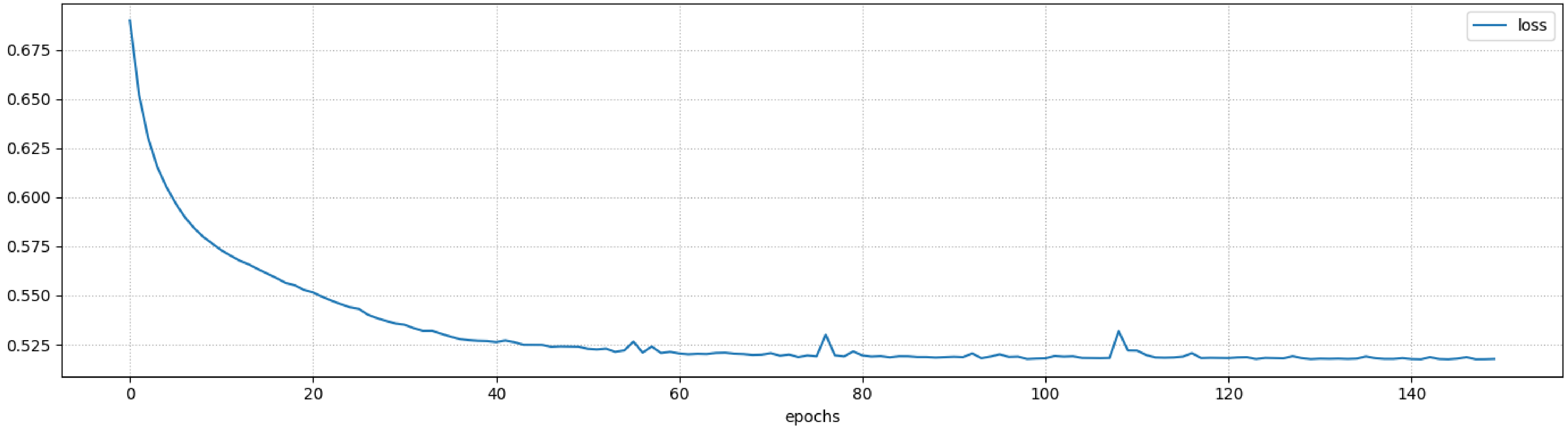
...Then the lattice must be monotone, too

- Otherwise, we risk loosing all our benefits
- Lattice monotonicities are always set to "increasing"
- ...Since we just want to preserve monotonicities from the calibration layers

Lattice Model with Shape Constraints

Let's train the constrained model

In [22]:
```
history = util.train_nn_model(lm2, tr_ls2, tr_sc['clicked'], loss='binary_crossentropy', batch_s
util.plot_training_history(history, figsize=figsize)
```




```
Final loss: 0.5177 (training)
```

Evaluating the Lattice Model with Shape Constraints

In [23]:
```
pred_tr3 = lm2.predict(tr_ls2, verbose=0)
pred_val3 = lm2.predict(val_ls2, verbose=0)
pred_ts3 = lm2.predict(ts_ls2, verbose=0)
auc_tr3 = roc_auc_score(tr_s['clicked'], pred_tr2)
auc_val3 = roc_auc_score(val_s['clicked'], pred_val2)
auc_ts3 = roc_auc_score(ts_s['clicked'], pred_ts2)
print(f'AUC score: {auc_tr3:.2f} (training), {auc_val3:.2f} (validation), {auc_ts3:.2f} (test)')
```

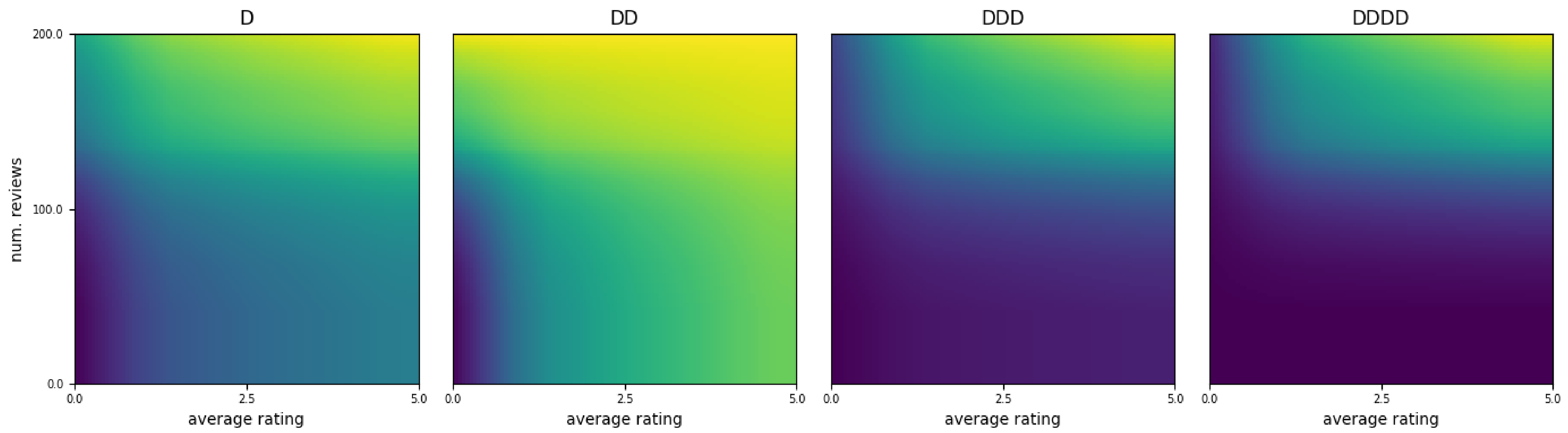
```
WARNING:tensorflow:5 out of the last 1262 calls to <function Model.make_predict_function.<loca
ls>.predict_function at 0x7f572c7ef880> triggered tf.function retracing. Tracing is expensive
and the excessive number of tracings could be due to (1) creating @tf.function repeatedly in a
loop, (2) passing tensors with different shapes, (3) passing Python objects instead of tensor
s. For (1), please define your @tf.function outside of the loop. For (2), @tf.function has red
uce_retracing=True option that can avoid unnecessary retracing. For (3), please refer to http
s://www.tensorflow.org/guide/function#controlling_retracing and https://www.tensorflow.org/api
_docs/python/tf/function for  more details.
AUC score: 0.80 (training), 0.80 (validation), 0.80 (test)
```

The results are on par with the previous ones

Inspecting the Calibrated Lattice

Let's inspect the learned function

In [24]:
```
util.plot_ctr_estimation(lm2, scale, split_input=True, one_hot_categorical=False, figsize=figsi
```

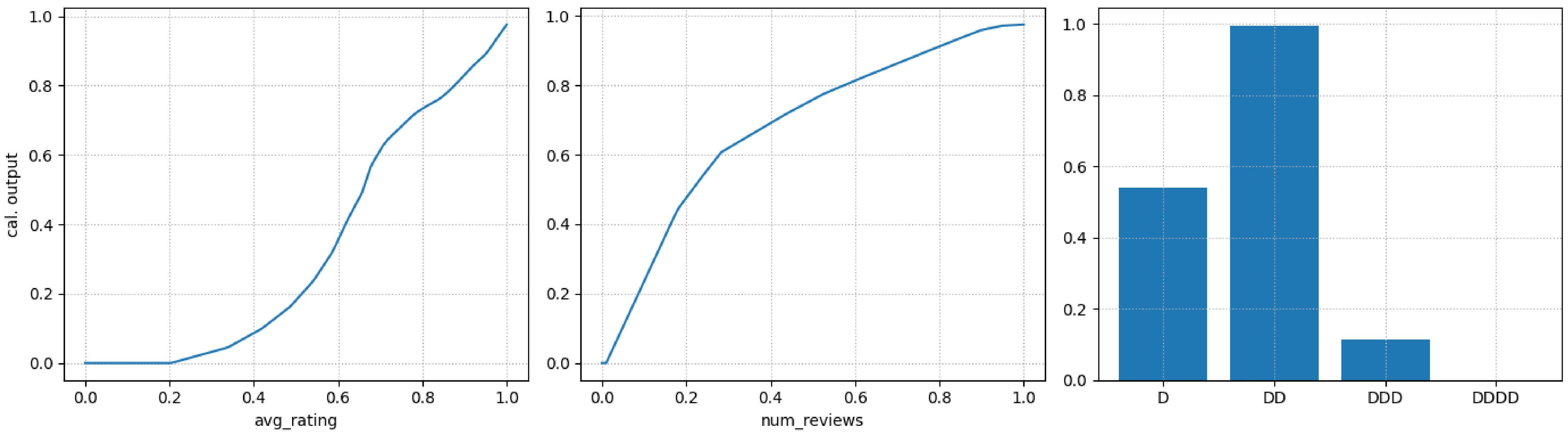


- All monotonicities are respected, the functions are much more regular
- Tartan-pattern apart, they closely match our ground truth

Inspecting the Calibrated Lattice

The most interesting changes will be in the calibration functions

```
In [25]: calibrators = [keras.Model(mdl_inputs2[i], lt_inputs2[i]) for i in range(3)]
         util.plot_ctr_calibration(calibrators, scale, figsize=figsize)
```



- Indeed, all monotonicities are respected
- The `avg_rating` regularizer is more linear
- The `num_reviews` one is convex and smooth

Considerations

Lattice models are little known, but they can be very useful

- They are interpretable
- Customer react (very) poorly to violation of known properties

In general, shape constraints are related to the topic of reliability

- I.e. the ability of a ML model to respect basic properties
- ...Especially in areas of the input space not well covered by the training set

Reliability is a very important topic for many applications of AI methods

Calibration is not restricted to the lattice input

- Indeed, we can add a calibration layer on the output as well
- ...So that we gain flexibility at a cost of a few more parameters