Click-Through Rate Prediction

Click-Through Rate Prediction

Let's consider an automatic recommendation problem

- Given a set of restaurant indexed on a a web platform (think Tripadvisor)
- ...We want to estimate how likely a user is to actually open the restaurant card

This is know as click-through rate

This example (and the approach) is based on this TensorFlow Lattice Tutorail

Loading the Data

Let's start by loading the dataset

In [2]:
```
tr, val, ts = util.load_restaurant_data()
tr.iloc[:3]
```

Out[2]:

	avg_rating	num_reviews	dollar_rating	clicked
0	3.927976	122.0	DDDD	1
1	3.927976	122.0	DDDD	0
2	3.927976	122.0	DDDD	0

- There are two numeric attributes, a categorical one, and a target
- Each row represents one visualization event, hence there are duplicates

In [3]:
```
dt_in = ['avg_rating', 'num_reviews', 'dollar_rating']
ndup = np.sum(tr.duplicated(dt_in))
print(f'#examples: {len(tr)}, #duplicated inputs {ndup}')
```

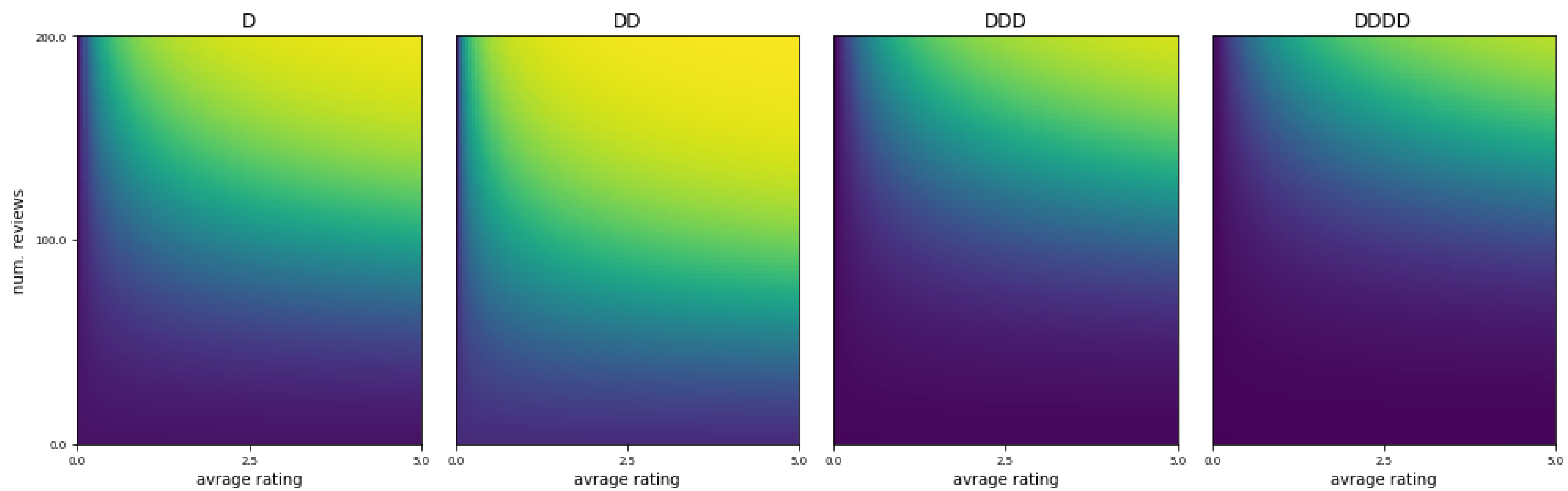
```
#examples: 835, #duplicated inputs 395
```

- The click rate can be inferred by number of clicks for each restaurant

Target Function

This is a synthetic dataset, for which we know the target function

```
In [4]: util.plot_ctr_truth(figsize=figsize)
```

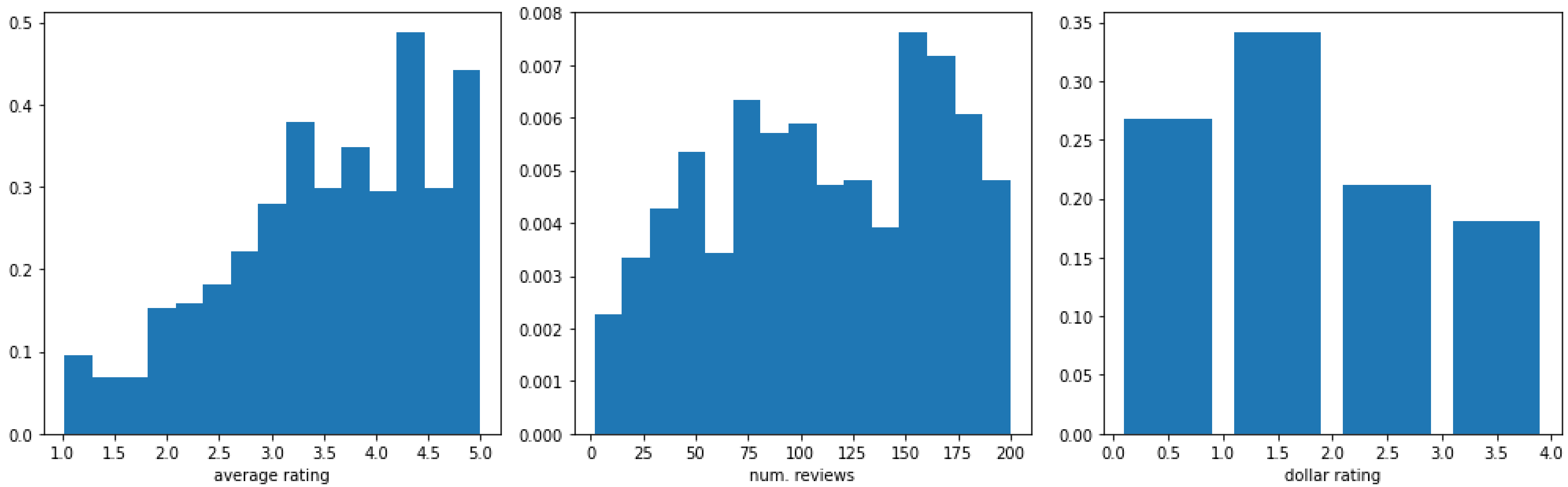


- The click rate grows with the average rating and the number of reviews
- Average priced restaurant are clicked the most

Data Distribution

Let's check the attribute distribution on the training set

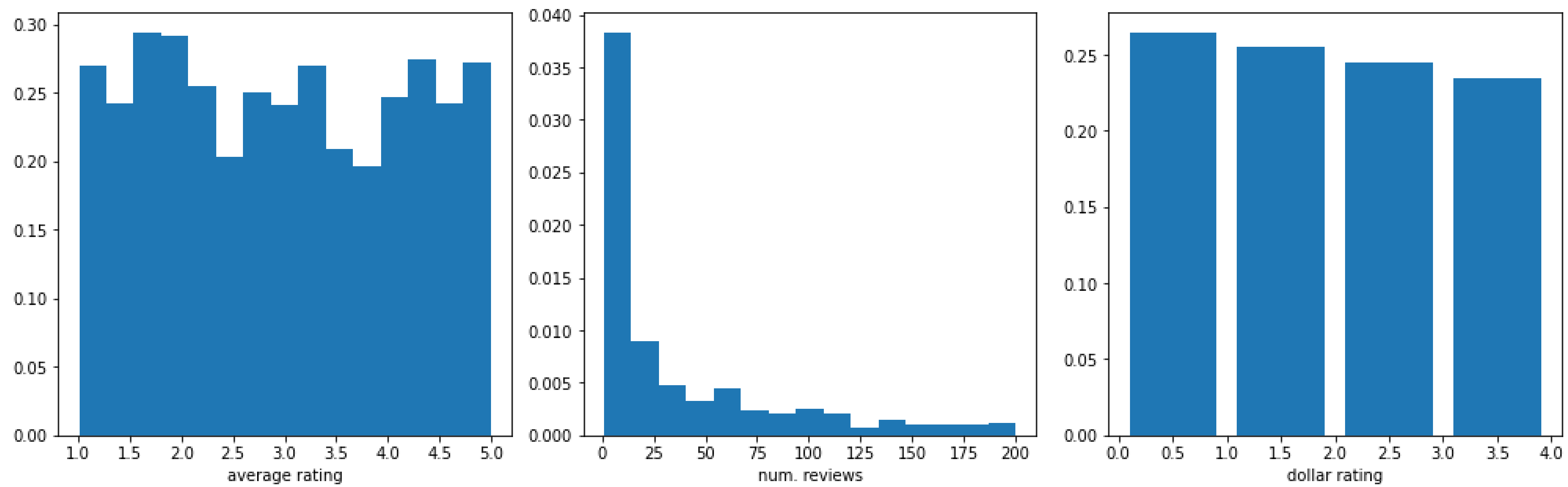
In [5]:
```
util.plot_ctr_distribution(tr, figsize=figsize)
```



Data Distribution

...And on the test set

In [6]:
```
util.plot_ctr_distribution(ts, figsize=figsize)
```



Here there is a strong discrepancy w.r.t. the training set

Distribution Discrepancy

What is the reason for the discrepancy?

A training set for this kind of problem will come from app usage data

- Users seldom scroll through all search results
- ...So their clicks will be biased toward high ranked restaurant

Any training set obtained in this fashion will be strongly biased

However, click rate prediction is typically use for ranking search results

...Meaning that we will need to evaluate also less viewed restaurants

- In a practical problem, the test set would not even be available
- We have it just as a mean for validating our results

A bias in the training can be problematic: we will try to see that in action

A Baseline Approach

Preparing the Data

We will start by tackling the problem using a Multi Layer Perceptron

We normalize the numeric data:

In [7]:
```
nf = ['avg_rating', 'num_reviews']
scale = tr[nf].max()

tr_s = tr.copy()
tr_s[nf] = tr_s[nf] / scale
val_s = val.copy()
val_s[nf] = val_s[nf] / scale
ts_s = ts.copy()
ts_s[nf] = ts_s[nf] / scale
```

We also adopt a one-hot encoding for the categorical data:

In [8]:
```
tr_sc = pd.get_dummies(tr_s).astype(np.float32)
val_sc = pd.get_dummies(val_s).astype(np.float32)
ts_sc = pd.get_dummies(ts_s).astype(np.float32)
dt_in_c = [c for c in tr_sc.columns if c != 'clicked']
```

Preparing the Data

Here is the result of our preparation

In [9]:
```
tr_sc
```

Out[9]:

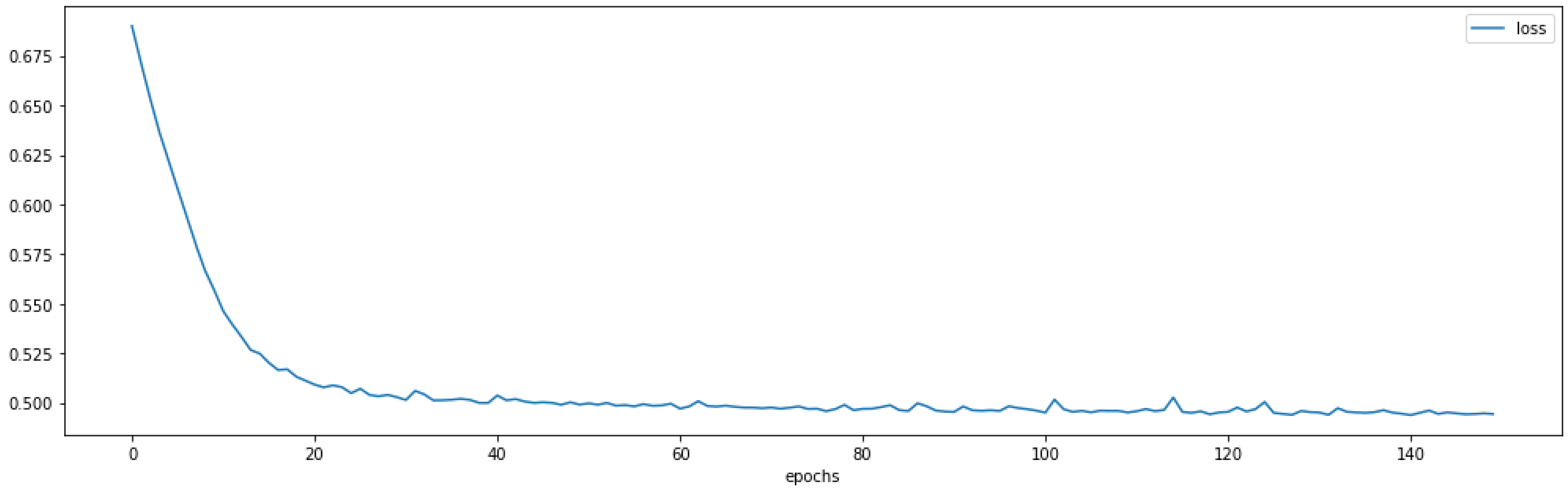
	avg_rating	num_reviews	clicked	dollar_rating_D	dollar_rating_DD	dollar_rating_DDD	dollar_rating_DDDD
0	0.785773	0.610	1.0	0.0	0.0	0.0	1.0
1	0.785773	0.610	0.0	0.0	0.0	0.0	1.0
2	0.785773	0.610	0.0	0.0	0.0	0.0	1.0
3	0.866150	0.610	1.0	0.0	0.0	0.0	1.0
4	0.619945	0.590	0.0	0.0	1.0	0.0	0.0
...	...	...	...	...	...	...	...
830	0.597304	0.055	1.0	0.0	1.0	0.0	0.0
831	0.783784	0.505	1.0	1.0	0.0	0.0	0.0
832	0.783784	0.505	1.0	1.0	0.0	0.0	0.0
833	0.688336	0.270	1.0	0.0	1.0	0.0	0.0
834	0.688336	0.270	0.0	0.0	1.0	0.0	0.0

835 rows × 7 columns

Training the MLP

We can now train the MLP model

```
In [11]: nn = util.build_ml_model(input_size=len(dt_in_c), output_size=1, hidden=[16, 16],
                              output_activation='sigmoid')
         history = util.train_ml_model(nn, tr_sc[dt_in_c], tr_sc['clicked'], batch_size=32, epochs=150,
                                  validation_split=0.0, loss='binary_crossentropy')
         util.plot_training_history(history, figsize=figsize)
```




```
Model loss: 0.4943 (training)
```

Evaluating the Predictions

This is not a classification problem, so the accuracy is not a good metric

- The output of our system is meant to be interpreted as a probability
- ...So, rounding to obtain a deterministic prediction may be too restrictive

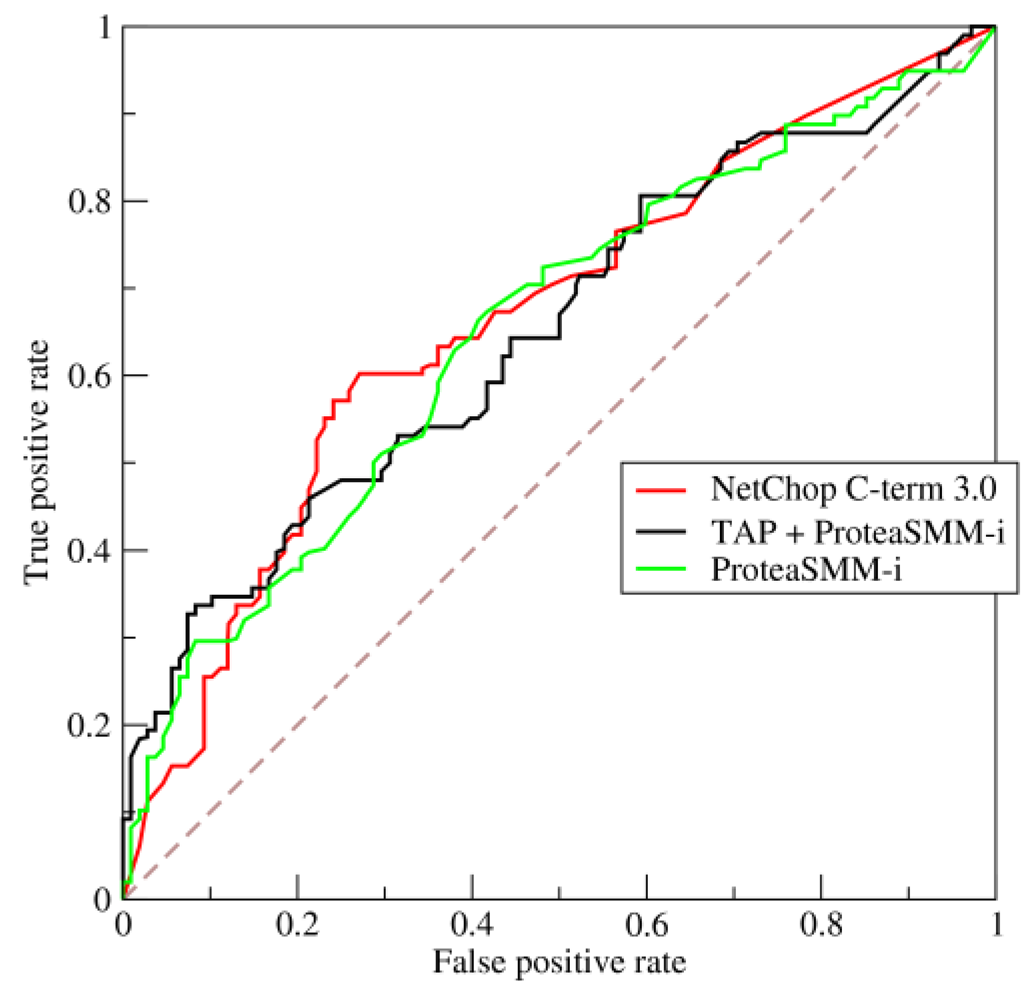
Instead, we will make a first evaluation using a ROC curve

A Receiver Operating Characteristic curve is a type of plot

- We consider multiple threshold values
  - Each threshold is meant to be used for discriminating between classes
  - The usual rounding approach is equivalent to a 0.5 threshold
- On the x axis, we report the false positive rate for each threshold
- On the y axis, we report the true positive rate for each threshold

Evaluating the Predictions

A ROC curve looks like this (image from wikipedia)



- The large the Area Under Curve (AUC), the better the performance
- The AUC value is guaranteed to be in the $[0, 1]$ interval

Evaluating the Predictions

Let's compute the AUC values for all sets

In [12]:
```
pred_tr = nn.predict(tr_sc[dt_in_c])
pred_val = nn.predict(val_sc[dt_in_c])
pred_ts = nn.predict(ts_sc[dt_in_c])
auc_tr = roc_auc_score(tr_sc['clicked'], pred_tr)
auc_val = roc_auc_score(val_sc['clicked'], pred_val)
auc_ts = roc_auc_score(ts_sc['clicked'], pred_ts)
print(f'AUC score: {auc_tr:.2f} (training), {auc_val:.2f} (validation), {auc_ts:.2f} (test)')
```

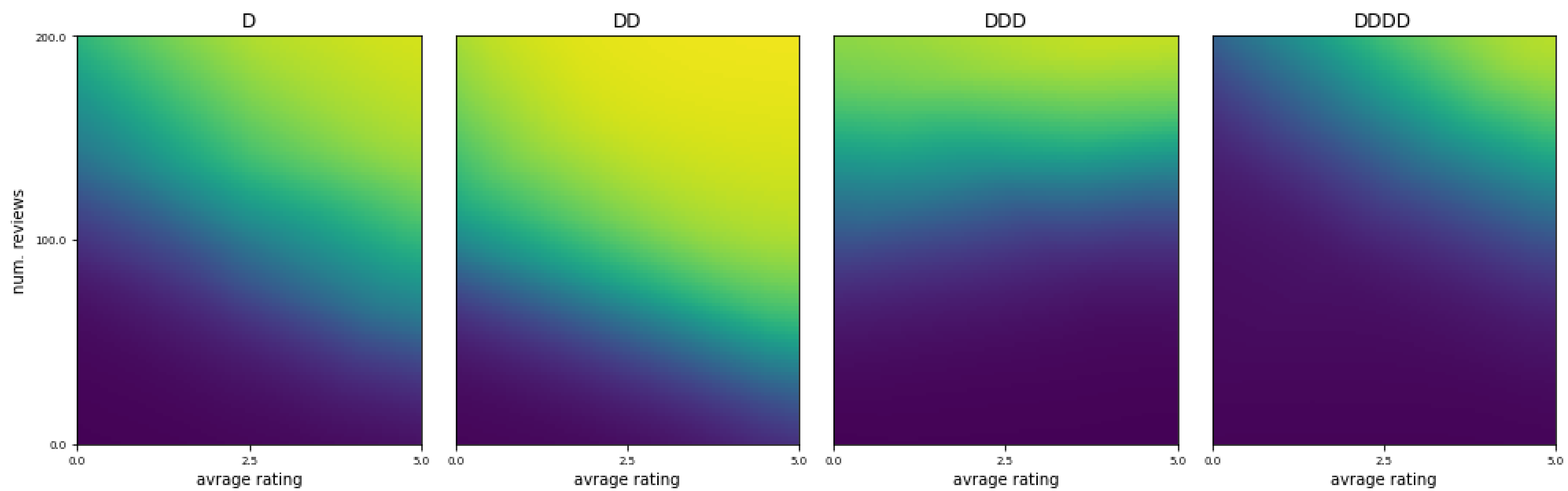
```
AUC score: 0.81 (training), 0.80 (validation), 0.76 (test)
```

- The model works well on the training distribution
- ...But a little worse on the testing data

Issues with the MLP

Let's check the full (prediction) output space for the MLP

In [13]:
```
util.plot_ctr_estimation(nn, scale, figsize=figsize)
```



- Some of the expected monotonicities may not respected
- ...And this is a critical problem in some cases!

Projected Gradient Method

Shape Constraints

Monotonicity are an example of shape constraints

Shape constraints are restrictions on the shape of the input-output function, e.g.:

- 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:

- Opening a valve is going to increase the power output (monotonicity)
- Reducing the price will raise the sales volume (monotonicity)
- Too low/high temperatures will lead to worse bakery products (convexity)
- Massive price reductions will be less effective (monotonicity + convexity)

How can they be implemented?

Implementing Shape Constraints

In some cases, shape constraints translate onto the model parameters

Consider a linear regressor:

$$f(x, \omega) = \omega_{1..n}^T x + \omega_0$$

- Where $\omega_0, \ldots \omega_n$ is the weight vector (ω_0 is the intercept)

In this context

- An increasing monotoniticiy w.r.t. all attributes x_j with $j \in J$
- ...Is equivalent to the constraints $\omega_j \geq 0 \; \forall j \in J$

In other words:

- We started from a constraints in the shape of the input-output functions
- ...And we transformed it into a constraints on the model parameters

Implementing Shape Constraints

Then, training consists in solving:

$$\text{argmin}_\omega \{ L(f(\hat{x}, \omega)) \mid \omega_j \geq 0 \ \forall j \in J \}$$

Where:

- $\{\hat{x}, \hat{y}\}$ is the training set
- $L(y)$ is the MSE loss, i.e. $L(y) = 1/n \|y - \hat{y}\|_2^2$

This is a constrained optimization problem

- It cannot be solved via the Linear Least Squares method
- ...And neither via gradient descent

So, what can we use instead?

Projected Gradient Method

A potential approach is the projected gradient method

We will explain how to use the method to tackle ML problems in the form:

$$\text{argmin}_\omega \left\{ L(f(\hat{x}, \omega)) \mid \omega \in C \right\}$$

Here C is a generic feasible set

- In our case, $C = \{\omega \mid \omega_j \geq 0 \ \forall j \in J\}$
- ...But in much more general constraints could be captured in principle

There are some assumptions:

- L needs to be differentiable (we will use a gradient)
- If both L and C are convex, we converge to a global optimum
- ...Otherwise we can still find a local optimum (in some cases)

Projected Gradient Method

The projected gradient method is an iterative process

Each iteration is defined by the equations:

$$\omega^{(k+1)} = \mathbf{proj}_C \left(\omega^{(k)} - \eta^{(k)} \nabla_\omega L \left(f\left(\hat{x}, \omega^{(k)}\right)\right)\right)$$

$$\mathbf{proj}_C(\omega) = \mathrm{argmin}_{\omega'} \left\{ \frac{1}{2} \|\omega' - \omega\|_2^2 \mid \omega \in C \right\}$$

Intuitively:

- First we perform a gradient descent step
- Then we project the parameter vector on the feasible space
- Projection = the feasible point with smallest L_2 distance

Projected Gradient Method in Our Example

In our case, given the current weight vector $\omega^{(k)}

First we perform a gradient descent step to obtain:

$$\tilde{\omega}^{(k+1)} = \omega^{(k)} - \eta^{(k)} \nabla_{\omega} L\left(f\left(\hat{x}, \omega^{(k)}\right)\right)$$

Then we need to solve the projection step:

$$\omega^{(k+1)} = \operatorname{argmin}_{\omega'} \left\{ \frac{1}{2} \|\omega' - \tilde{\omega}^{(k+1)}\|_2^2 \mid \omega_j \geq 0 \; \forall j \in J \right\}$$

- In practice we need to clip at 0 every $\tilde{\omega}_j^{(k)}$ with $j \in J$

This case is simple and useful enough to be implemented in many libraries

Limitations of the Approach

Could we use this for Deep Learning?

- Convexity does not hold for deep networks
- ...But that's not a critical issues (local optima may be nice enough)

The real issue is the lack of interpretability

- Since NN (and deep nets in particular) are opaque
- ...It's very difficult to define meaningful constraints on their weights

In the cases where this can be done, the PG method is viable

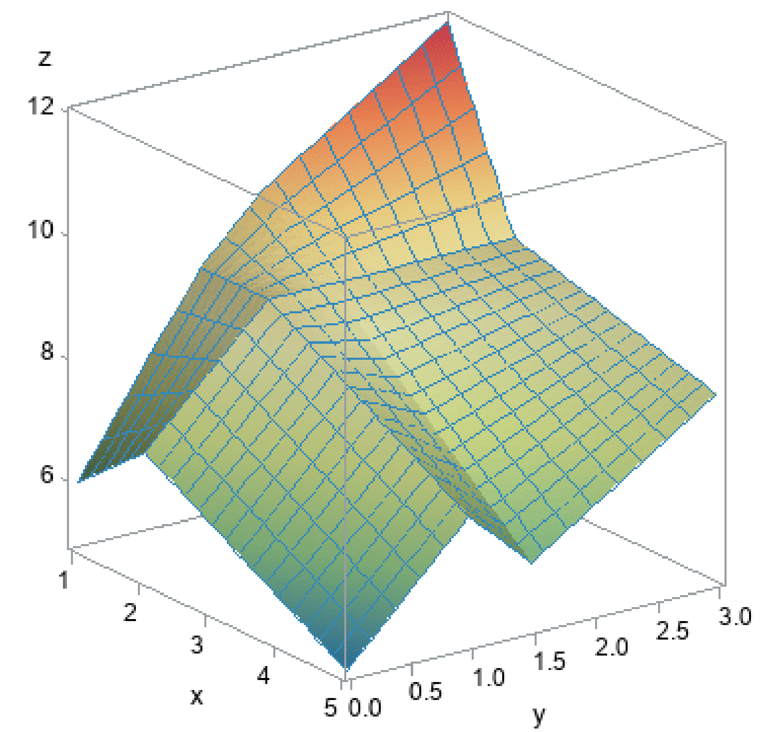
...But in general we need a more interpretable model type

We'll see an example now

Lattice Models

Lattice Models

Lattice models are a form of piecewise linear interpolated model



- They are defined over a grid on their input variables
- Their parameters are the output values at each grid points
- The remaining output values are linearly interpolated

They are available in tensorflow via the tensorflow-lattice module

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"
- The input variables have bounded domains (namely $[0, n_i - 1]$)
- ...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 very 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

Implementing a Lattice Model

The first step for implementing a lattice model is choosing the lattice size

```
In [14]: lattice_sizes = [4] * 2 + [2] * 4
```

- We are using 4 knots for numeric inputs and 2 knots for the boolean inputs

Next, we need to split the individual input columns

```
In [15]: tr_ls = [tr_sc[c] * (s-1) for c, s in zip(dt_in_c, lattice_sizes)]
         val_ls = [val_sc[c] * (s-1) for c, s in zip(dt_in_c, lattice_sizes)]
         ts_ls = [ts_sc[c] * (s-1) for c, s in zip(dt_in_c, lattice_sizes)]
```

- This step is required by the tensorflow-lattice API
- We also scale the input to the range expected by the lattice

Implementing a Lattice Model

The we build the symbolic tensors for the model input

In [16]:
```
mdl_inputs = []
for cname in dt_in_c:
    cname_in = layers.Input(shape=[1], name=cname)
    mdl_inputs.append(cname_in)
```

- We have one tensor per input column

Finally we can build our lattice model

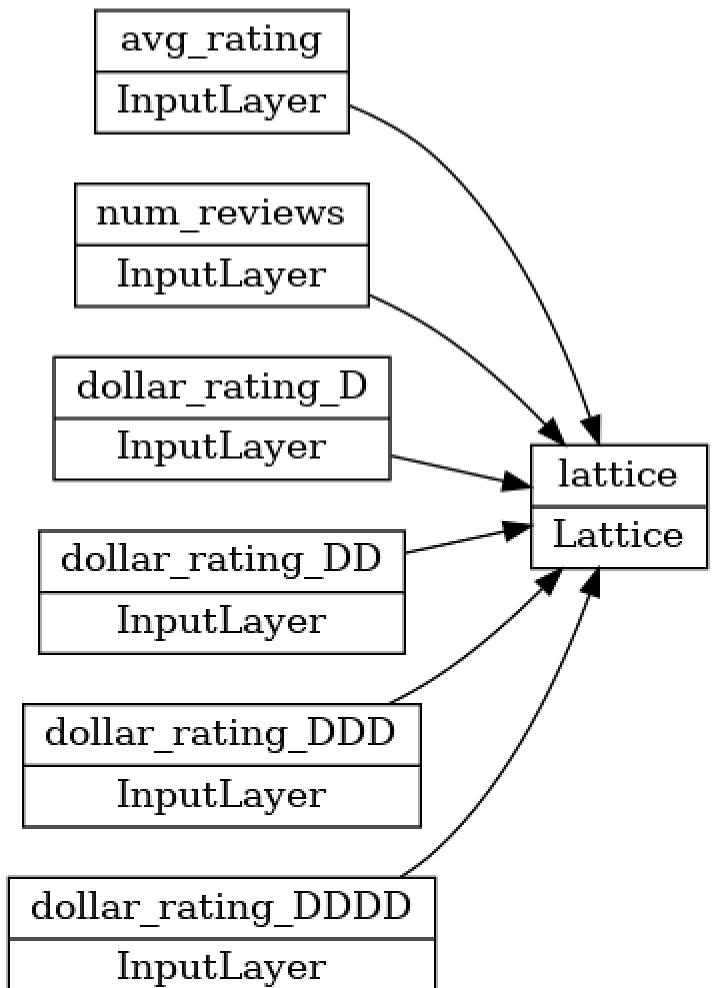
In [17]:
```
import tensorflow_lattice as tfl

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

lm = keras.Model(mdl_inputs, mdl_out)
```

Implementing a Lattice Model

We can plot the model structure

In [18]:
```
keras.utils.plot_model(lm, rankdir='LR')
```

Out[18]:

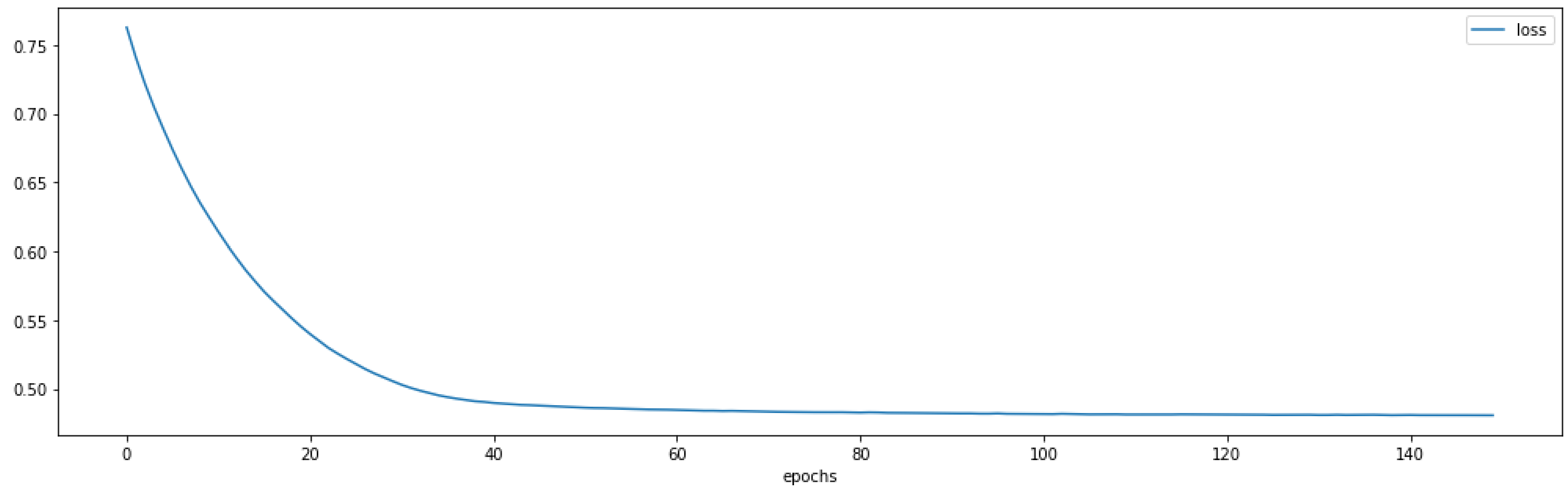


Implementing a Lattice Model

We can train the model as usual

In [19]:

```
history = util.train_ml_model(lm, tr_ls, tr_sc['clicked'], batch_size=32, epochs=150,
                              validation_split=0.0, loss='binary_crossentropy')
util.plot_training_history(history, figsize=figsize)
```




```
Model loss: 0.4808 (training)
```

Lattice Model Evaluation

A large enough lattice model can peform as well as a Deep Network

Let's see the performance in terms of AUC

In [20]:
```
pred_tr2 = lm.predict(tr_ls)
pred_val2 = lm.predict(val_ls)
pred_ts2 = lm.predict(ts_ls)
auc_tr2 = roc_auc_score(tr_sc['clicked'], pred_tr2)
auc_val2 = roc_auc_score(val_sc['clicked'], pred_val2)
auc_ts2 = roc_auc_score(ts_sc['clicked'], pred_ts2)
print(f'AUC score: {auc_tr2:.2f} (training), {auc_val2:.2f} (validation), {auc_ts2:.2f} (test)')
```

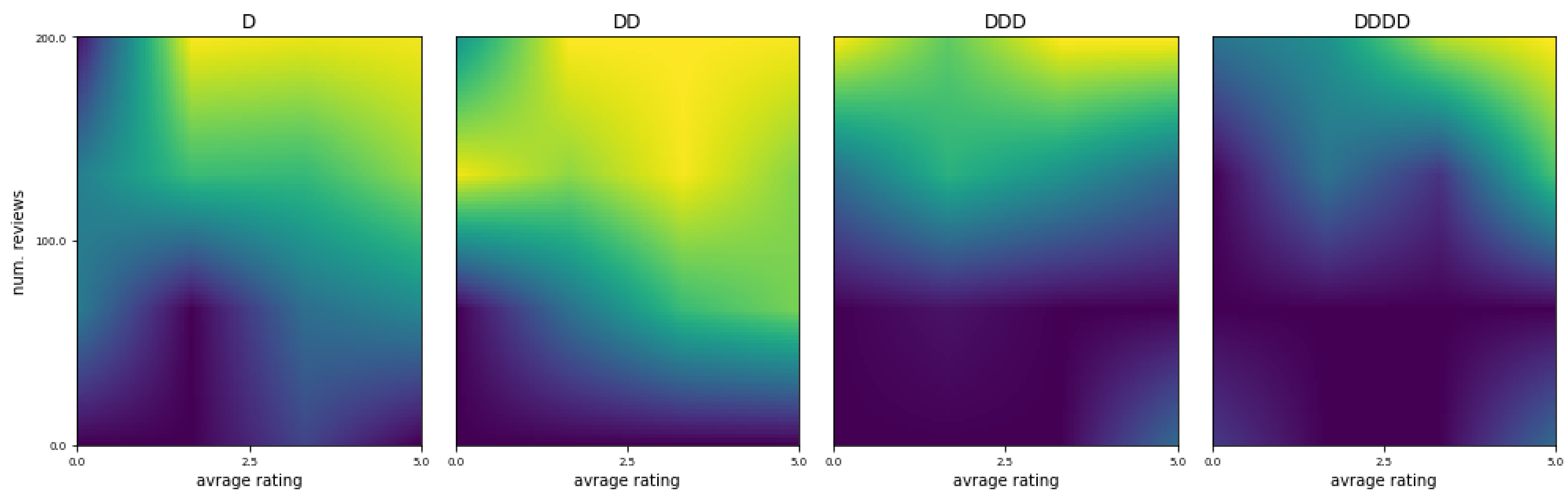
```
AUC score: 0.82 (training), 0.79 (validation), 0.76 (test)
```

- It is indeed comparable to that of the deep MLP
- ...Also in the fact that it works poorly on the test distribution

Lattice Model Evaluation

...But it can behave also just as poorly (or even worse)

In [21]:
```
lscale = scale / [s-1 for s in lattice_sizes[:2]]
util.plot_ctr_estimation(lm, lscale, split_input=True, figsize=figsize)
```



- The expected monotonicity constraints are still violated
- There are still many mistakes for less represented areas of the input space

Calibration

Calibration

Let's start fixing some of the outstanding issues

In a lattice model, the number of grid points if 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

In tensorflow-lattice, scalability issues are mitigated via two approaches:

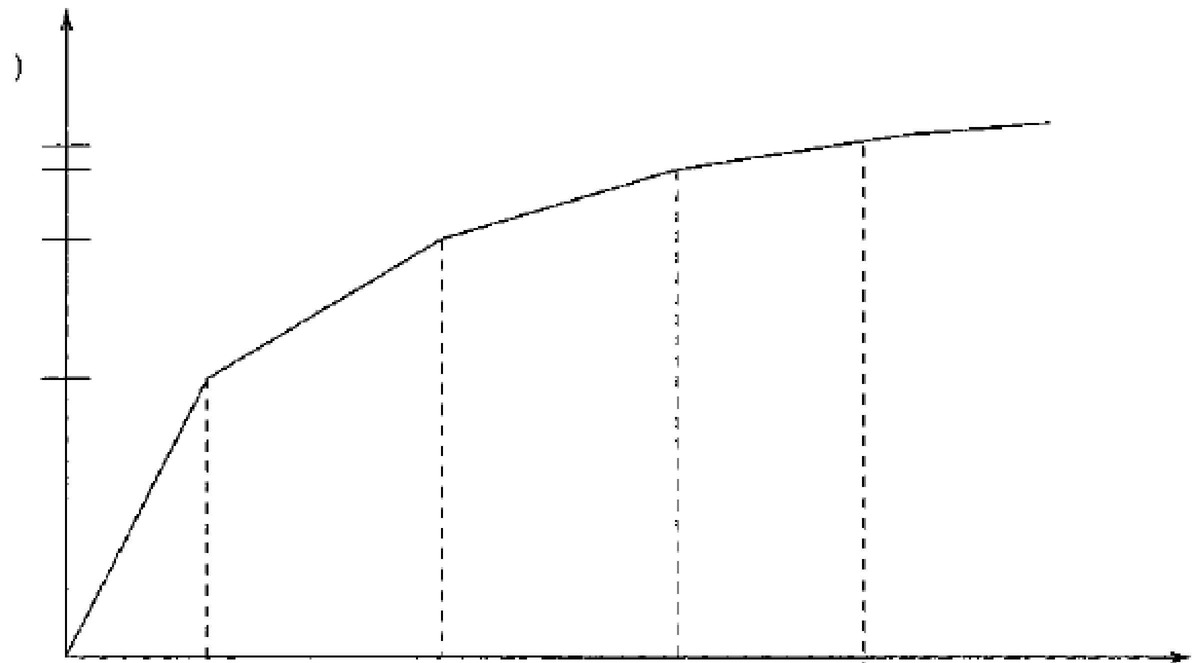
- Ensembles of small lattices (we will not cover this one)
- Applying a calibration step to each input variables

We will focus on this latter approach

Calibration for Numeric Inputs

Calibration for numeric attributes...

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

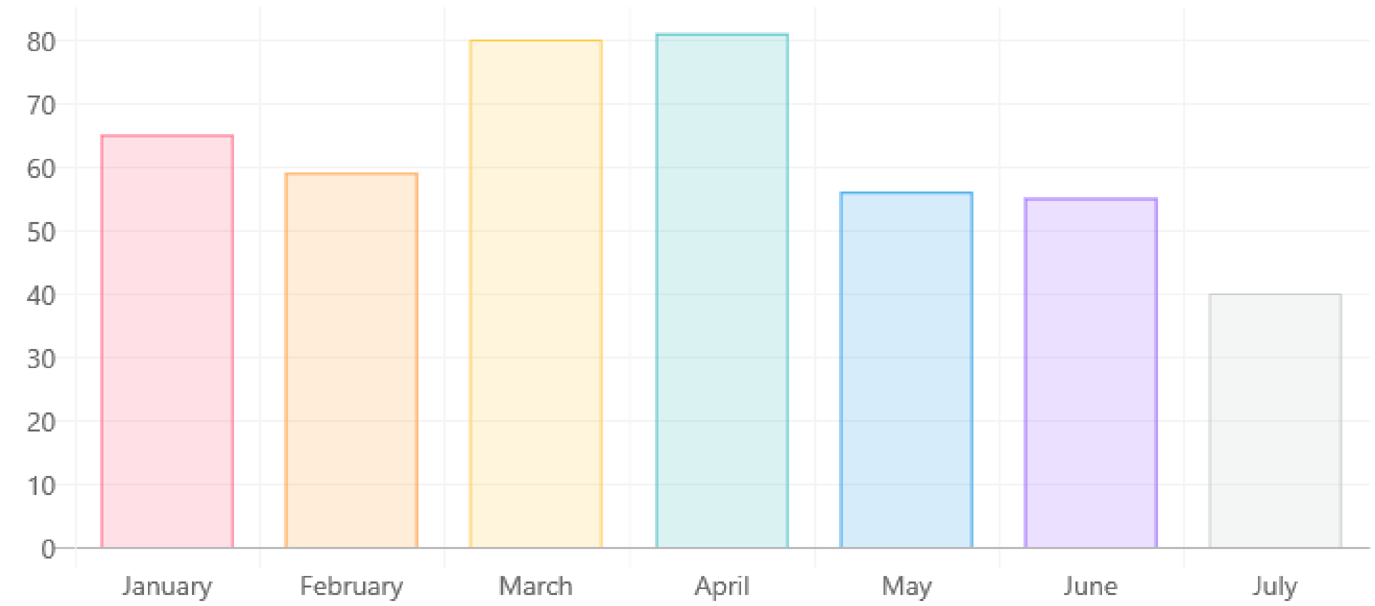


- This is essentially a 1-D lattice
- Calibration parameters are the function value at all knots
- Calibration allows to introduce complexity, without increasing the lattice size

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 value
- There is one parameter for each possible input value

Calibration

Calibration allows enables the use of fewer knots in the lattice

- E.g. 5 knots per layer, single lattice: $5 \times 5 = 25$ parameters
- Wherease 5 calibration knots + 2 lattice knots: $5 \times 2 + 2 \times 2 = 14$
- Additionally, we tend to get more regular results

Calibration enables using categorical inputs without a one-hot encoding

...Since the calibration map is almost equivalent

- E.g. 5 categories, no calibration: $2 \times 5 = 10$ parameters
- Whereas with calibration: $5 + 2 = 7$ parameters

We can therefore adjust our lattice sizes accordingly

We will use just two knots per dimension

In [22]:
```
lattice_sizes2 = [2] * 3
```

Preparing the Input

First, we need to encode out categorical input using integers

We start by converting our string data input pandas categories

In [23]:
```
tr_sc2 = tr_s.copy()
tr_sc2['dollar_rating'] = tr_sc2['dollar_rating'].astype('category')
tr_sc2[:3]
```

Out[23]:

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

We can check how the categories are mapped into integer codes:

In [24]:
```
tr_sc2['dollar_rating'].cat.categories
```

Out[24]:
```
Index(['D', 'DD', 'DDD', 'DDDD'], dtype='object')
```

- The codes are are the positional indexes of the strings

Preparing the Input

Now we replace the category data with the codes themselves

In [25]:
```
tr_sc2['dollar_rating'] = tr_sc2['dollar_rating'].cat.codes
tr_sc2['dollar_rating'][:3]
```

Out[25]:
```
0    3
1    3
2    3
Name: dollar_rating, dtype: int8
```

...And we apply the same treatment to the validation and test set:

In [26]:
```
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
```

Piecewise Linear Calibration

We use `PWLCalibration` objects for all numeric inputs

In [27]:
```
avg_rating = layers.Input(shape=[1], name='avg_rating')
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_sizes2[0] - 1.0,
    name='avg_rating_cal'
)(avg_rating)

num_reviews = layers.Input(shape=[1], name='num_reviews')
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_sizes2[1] - 1.0,
    name='num_reviews_cal'
)(num_reviews)
```

- The knot position must be a-priori defined
- ...And we use the training distribution quantiles

Categorical Calibration

We use `CategoricalCalibration` objects for the categorical input

```
In [28]: dollar_rating = layers.Input(shape=[1], name='dollar_rating')
         dollar_rating_cal = tfl.layers.CategoricalCalibration(
             num_buckets=4,
             output_min=0.0, output_max=lattice_sizes2[2] - 1.0,
             name='dollar_rating_cal'
         )(dollar_rating)
```

- We use one "bucket" for each possible category

We should also remember to split the training data

Building the Calibrated Lattice Model

We can now build the lattice model

In [29]:
```
lt_inputs2 = [avg_rating_cal, num_reviews_cal, dollar_rating_cal]

mdl_out2 = tfl.layers.Lattice(
    lattice_sizes=lattice_sizes2,
    output_min=0, output_max=1,
    name='lattice',
)(lt_inputs2)

mdl_inputs2 = [avg_rating, num_reviews, dollar_rating]
lm2 = keras.Model(mdl_inputs2, mdl_out2)
```

We can compare the number of parameters

In [30]:
```
print(f'#Parameters in the original lattice: {sum(len(w) for w in lm.get_weights())}')
print(f'#Parameters in the new lattice: {sum(len(w) for w in lm2.get_weights())}')
```

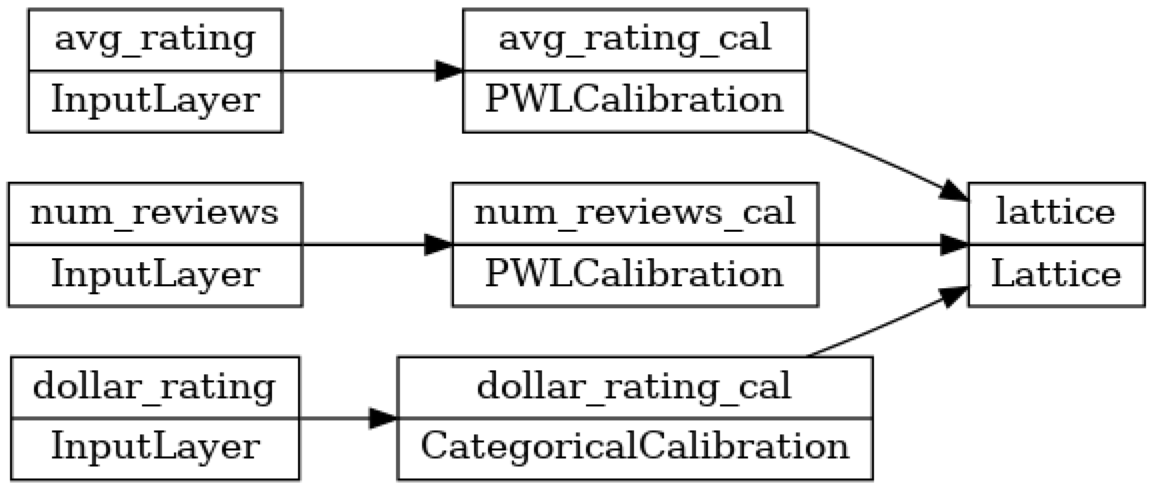
```
#Parameters in the original lattice: 256
#Parameters in the new lattice: 52
```

Building the Calibrated Lattice Model

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

In [31]:
```
keras.utils.plot_model(lm2, rankdir='LR')
```

Out[31]:



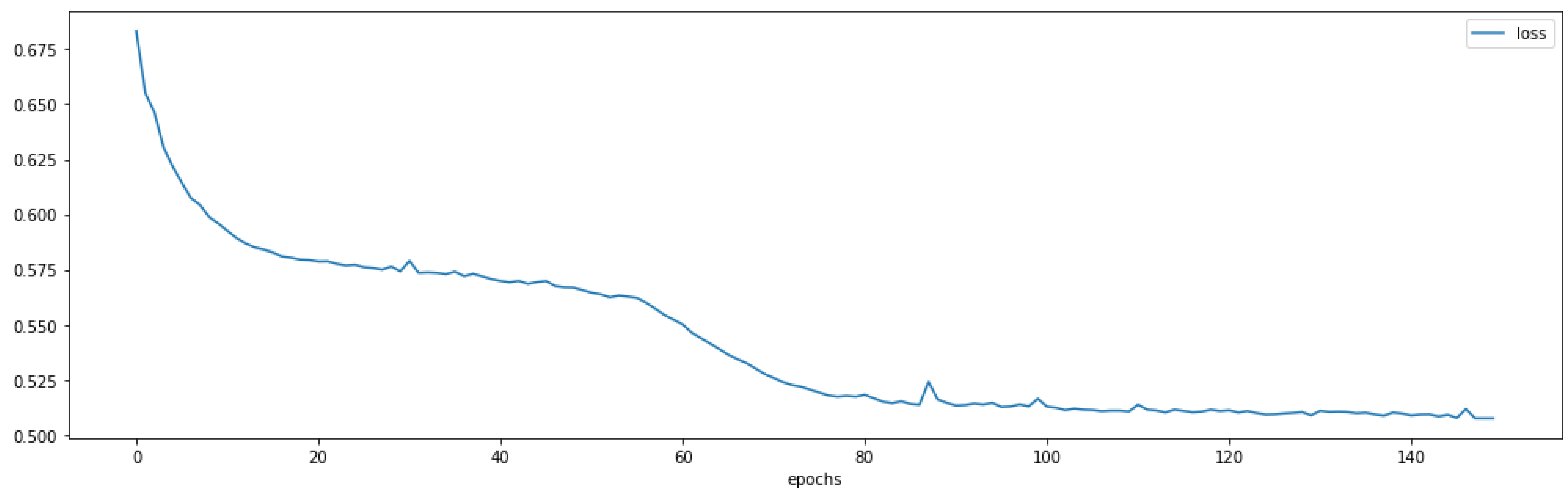
Now we need to split the training data to enable training

In [32]:
```
tr_ls2 = [tr_sc2[c] for c in dt_in]
val_ls2 = [val_sc2[c] for c in dt_in]
ts_ls2 = [ts_sc2[c] for c in dt_in]
```

Training the Calibrated Lattice

We can train the new model as usual

In [33]:
```
history = util.train_ml_model(lm2, tr_ls2, tr_sc['clicked'], batch_size=32, epochs=150,
                              validation_split=0.0, loss='binary_crossentropy')
util.plot_training_history(history, figsize=figsize)

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

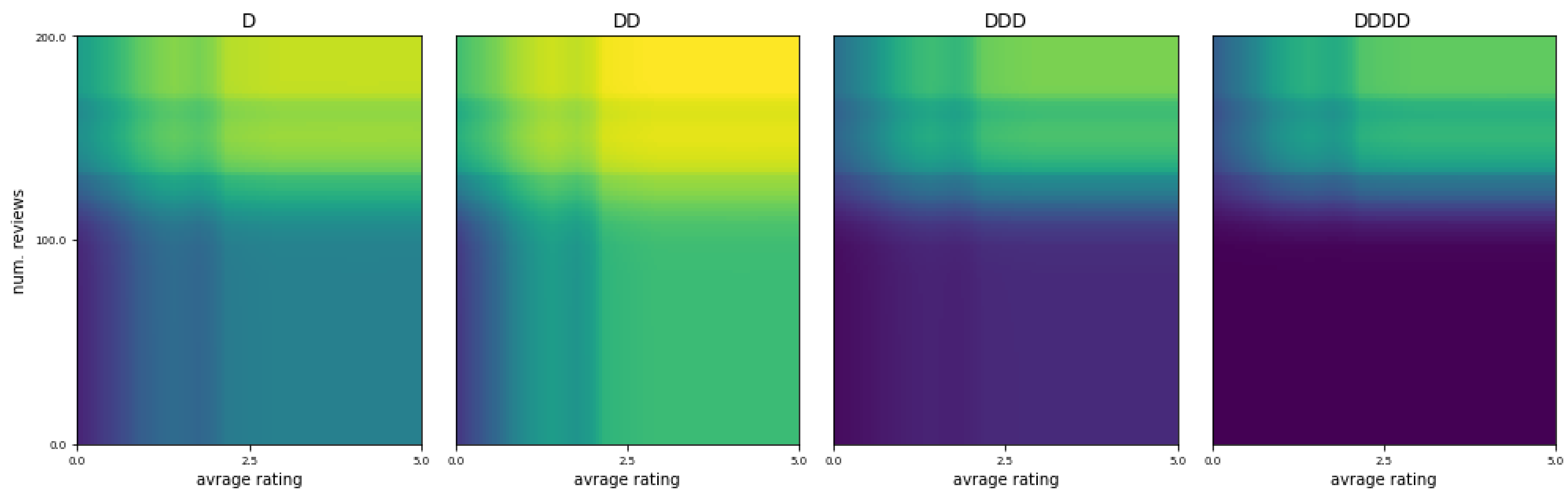



```
Model loss: 0.5075 (training)
```

Inspecting the Calibrated Lattice

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

```
In [34]: util.plot_ctr_estimation(lm2, scale, split_input=True, one_hot_categorical=False, figsize=figsi
```

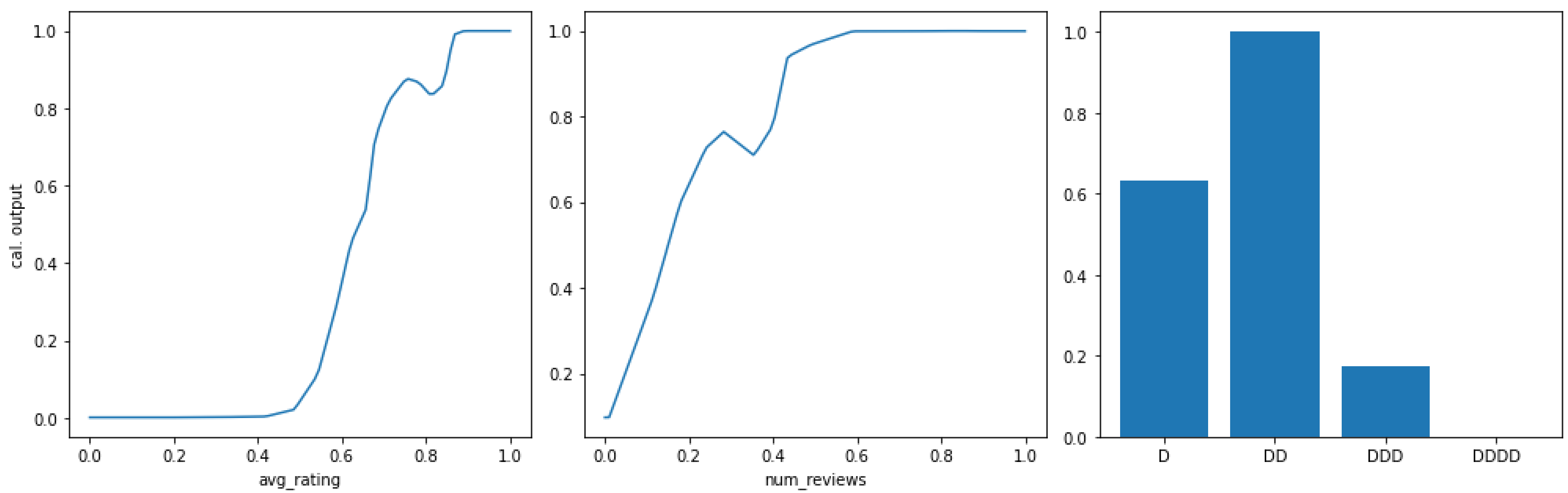


- The structure follows a (piecewise linear) "tartan pattern"
- This is particularly evident now, since we use just two knots per dimension

Inspecting the Calibrated Lattice

It is useful to inspect the calibration layers

In [35]:
```
calibrators = [keras.Model(mdl_inputs2[i], lt_inputs2[i]) for i in range(3)]
util.plot_ctr_calibration(calibrators, scale, figsize=figsize)
```



- The learned calibration functions violate the expected monotonicities

We cannot confidently show results like this to a customer

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:

- Opening a valve is going to increase the power output (monotonicity)
- 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 shape constraints (and regularizers) 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 note of input i...
- ...While all the remaining attributes and knots (i.e. $\bar{i}$ and $\bar{k}$) are fixed

Then (increasing) monotonicity translates to:

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

- 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:

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

- 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 [36]: 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_sizes2[0] - 1.0,
             monotonicity='increasing',
             kernel_regularizer=('hessian', 0, 1),
             name='avg_rating_cal'
         )(avg_rating2)
```

- The "hessian" regularizer 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. a restaurant with 200 reviews will be clicked much more than one with 10
- ...But not much more than one with 150

In [37]:
```
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_sizes2[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
- The "wrinkle" regularizer penalizes the third derivative
    - ...Thus making the regularizer 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 [38]:
```
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_sizes2[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

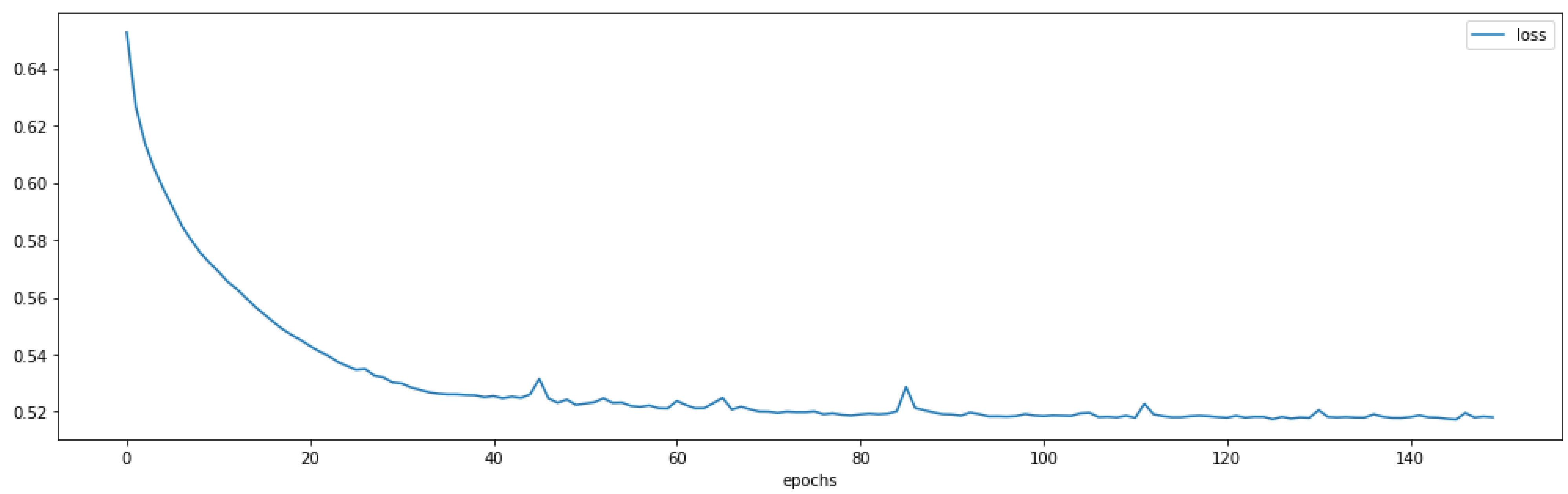
In [39]:
```
lt_inputs3 = [avg_rating_cal2, num_reviews_cal2, dollar_rating_cal2]

mdl_out3 = tfl.layers.Lattice(
    lattice_sizes=lattice_sizes2,
    output_min=0, output_max=1,
    monotonicities=['increasing'] * 3,
    name='lattice',
)(lt_inputs3)

mdl_inputs3 = [avg_rating2, num_reviews2, dollar_rating2]
lm3 = keras.Model(mdl_inputs3, mdl_out3)
```

- If we specify monotonicities in the calibration layers, the lattice must be monotone, too
- In this case the lattice monotonicities should always be "increasing"
  - ...Since two "decreasing" monotonicies would lead to an "increasing" one

Lattice Model with Shape Constraints

Let's train the constrained model

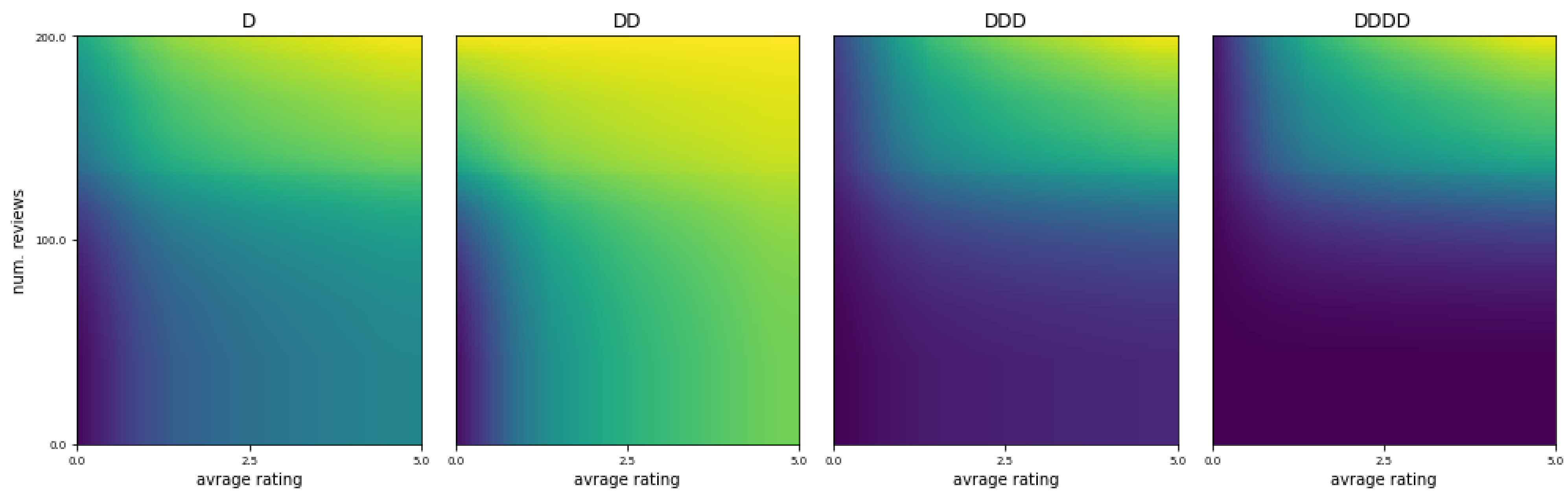
In [40]:
```
history = util.train_ml_model(lm3, tr_ls2, tr_sc['clicked'], batch_size=32, epochs=150,
                              validation_split=0.0, loss='binary_crossentropy')
util.plot_training_history(history, figsize=figsize)

pred_tr4 = lm3.predict(tr_ls2)
pred_val4 = lm3.predict(val_ls2)
pred_ts4 = lm3.predict(ts_ls2)
auc_tr4 = roc_auc_score(tr_s['clicked'], pred_tr3)
auc_val4 = roc_auc_score(val_s['clicked'], pred_val3)
auc_ts4 = roc_auc_score(ts_s['clicked'], pred_ts3)
print(f'AUC score: {auc_tr4:.2f} (training), {auc_val4:.2f} (validation), {auc_ts4:.2f} (test)')
```



Inspecting the Calibrated Lattice

Let's inspect the learned function

In [41]:
```
util.plot_ctr_estimation(lm3, scale, split_input=True, one_hot_categorical=False, figsize=figsi
```

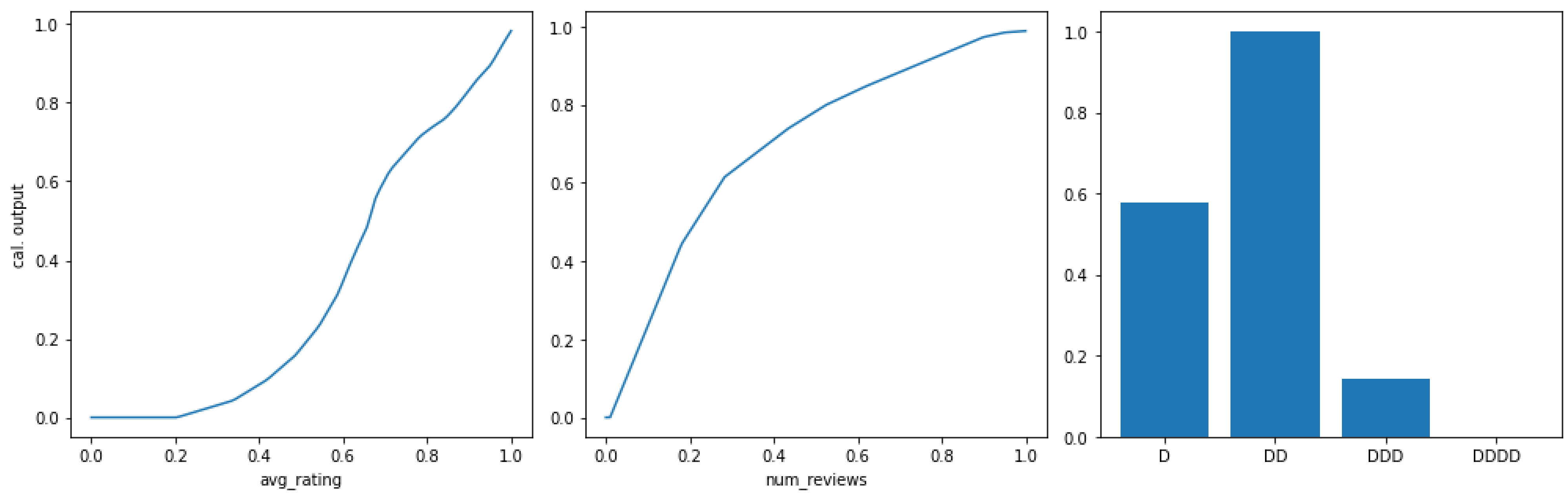


- All monotonicities are respected, the functions are much more regular
- Tartan-pattern apart, they closely match our ground truth

Inspecting the Calibrated Lattice

The most interesting changes will be in the calibration functions

In [42]:
```
calibrators = [keras.Model(mdl_inputs3[i], lt_inputs3[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

Some References

- Parikh, Neal, and Stephen Boyd. "Proximal algorithms." Foundations and trends® in Optimization 1.3 (2014): 127-239.
- Seungil You, David Ding, Kevin Robert Canini, Jan Pfeifer, Maya R. Gupta: Deep Lattice Networks and Partial Monotonic Functions. NIPS 2017: 2981-2989
- Maya R. Gupta, Andrew Cotter, Jan Pfeifer, Konstantin Voevodski, Kevin Robert Canini, Alexander Mangylov, Wojtek Moczydlowski, Alexander Van Esbroeck: Monotonic Calibrated Interpolated Look-Up Tables. J. Mach. Learn. Res. 17: 109:1-109:47 (2016)
- Maya R. Gupta, Dara Bahri, Andrew Cotter, Kevin Robert Canini: Diminishing Returns Shape Constraints for Interpretability and Regularization. NeurIPS 2018: 6835-6845