Constrained ML via Inference-Time Projection

It's never too late to quit violating constraints

From Data Projection

Let's consider again our data projection approach

First we project the training data:

$$z^* = \operatorname*{argmin}_z \{ L(z, y) \mid g(z) \leq 0 \}$$

...Then we train a supervised learning model as usual:

$$\theta^* = \operatorname*{argmin}_\theta \{ L(\hat{y}, z^*) \mid \hat{y} = f(x; \theta) \}$$

By doing this, we push the model towards learning the constraints

...But we do it by decomposing the original problem

- This leads to some significant advantages (mainly flexibility)
- ...And a few disadvantages (e.g. less precise approximation)

...To Inference-Time Projection

What if we swapped the two steps?

We could start by trainingn a model as usual:

$$\theta^* = \operatorname*{argmin}_{\theta} \{ L(\hat{y}, y) \mid \hat{y} = f(x; \theta) \}$$

...And then projecting the predictions:

$$\hat{z} = \operatorname*{argmin}_{z} \{ L(z, f(x; \theta^*)) \mid g(z) \leq 0 \}$$

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- We still perform projetion in the output space
- ...But in this case we do it at inference-time

For this reason, we'll call this approach inference-time projection

Probabilistic Semantic

As for data projection, when L represents a likelihood

...We can see the projection process process as MAP computation:

$$\hat{z} = \underset{z}{\operatorname{argmin}} \{ L(z, f(x; \theta^*)) \mid g(z) \leq 0 \}$$

- We seek a feasible vector $\hat{z}$
- ...That has the largest estimated probability w.r.t. the predictions

This trick is extensively used in ML!

- Rounding in binary classification is a form of projection
- ...And the same goes for the argmax used in multiclass classification

Let's start to study in detail this approach

Two is Complicated, Three is a Crisis

To begin with, our original does not really work

$$\hat{z} = \underset{z}{\operatorname{argmin}}\{L(z, f(x; \theta^*)) \mid g(z) \leq 0\}$$

This projection problem is well defined for the training data

- However, since we are projecting at inference time
- ...We'll need to do it for unseen examples as well

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Unseen examples might not come in batches

...And even when they do, they may not be representative samples

- So, it's hard to deal with relational constraints and distribution constraints
- In most cases, we'll be projecting one example at a time

...Though there are exceptions to this rule

Where did the Input Go?

All our constraint formulations so far make no mention of the input

For example, in our projection problem

$$\hat{z} = \underset{z}{\operatorname{argmin}} \{ L(z, f(x; \theta^*)) \mid g(z) \leq 0 \}$$

...The constraint function $g(x)$ is defined on the output space alone

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When working with the training data, this is totally fine

- It's quite frequent for the input to have an impact on the constraint
- ...But the input is fixed at training time
- ...And therefore we can include its effect in the definition of g

Where did the Input Go?

On unseen examples, this is no longer the case

...And we need to account for the input explicitly:

$$\hat{z}(x) = \underset{z}{\operatorname{argmin}} \{ L(z, f(x; \theta^*)) \mid g(x, z) \leq 0 \}$$

Formally:

- The projection $\hat{z}$ will be always input-dependent
- The constraint function $g(x, y)$ will be input-depended in general

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In practice, this isn't a big change

- We'll need to build our constraints based on the value of x
- ...And then we can solve the projection problem as usual

Computational Effort

The computational effort for our projection operator

$$\hat{z}(x) = \operatorname*{argmin}_z \{ L(z, f(x; \theta^*)) \mid g(x, z) \leq 0 \}$$

...Is similar to the one we had for data-projection

- The fact that we typically project individual examples is good news
- ...Since it makes our problems smaller and simpler

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However, there are cases when even this can be an issue

Some applications (e.g. control systems) require very low latencey

- In this case, we might not have time enough to project

Some hardware has trouble with projection

- E.g. no optimization packages or not enough power on cyber-physical systems

The Bad, the Ugly, and the Good

So far, we've focused on the issues of this approach

- It's hard to deal with many examples, which is bad
- There's a non-trivial computation step at inference time, which is ugly

So, why should we use inference-time projection at all?

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So, why should we use inference-time projection at all?

Three words.
Guaranteed Constraint Satisfaction

...And it holds also out-of-distribution!

- In some cases this can be a massive advantage
- Inference time projection is the simplest method to achieve it

Let's consider a simple case study for inference-time projection

Mutually Exclusive Classes

Let's consider a multilabel classification problem

- Given an input sample
- ...We need to assign to it zero-to-k classes

The problem arises in a number of settings

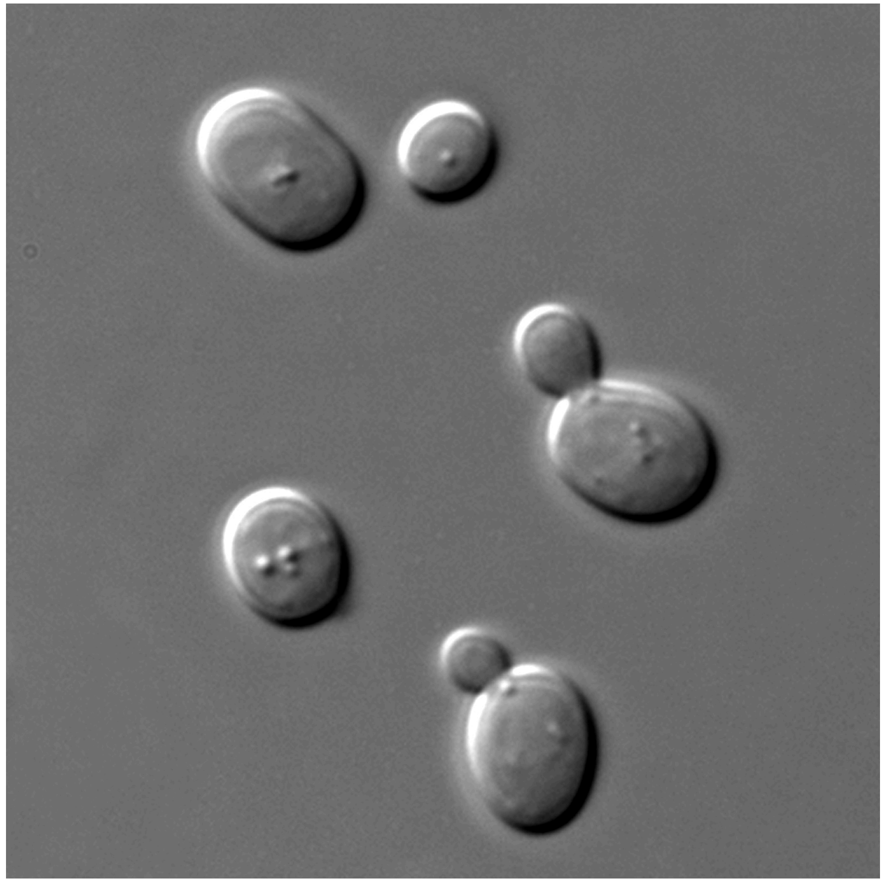
- Assigning tags to posts, or items in a marketplace
- Estimating properties of materials
- Identifying the favorite music/movie genres for a user
- ...

We can build individual classifiers for each class

...But using a single model for them all allows to exploit correlations

Yeast Traits

We'll focus on estimating genetic traits of yeast cells



- Given numeric data from a micro-array analysis
- ...We want to estimate the characteristic of a given yeast

Loading the Data

Let's load our dataset

...Which comes fom the Multi-label Classification Dataset Repository

In [85]:
```
fname = os.path.join('..', 'data', 'Yeast.arff')
X_tr, X_ts, y_tr, y_ts = util.load_multilabel_dataset(fname, label_num=14, standardize=True,
display(y_tr.head())
```

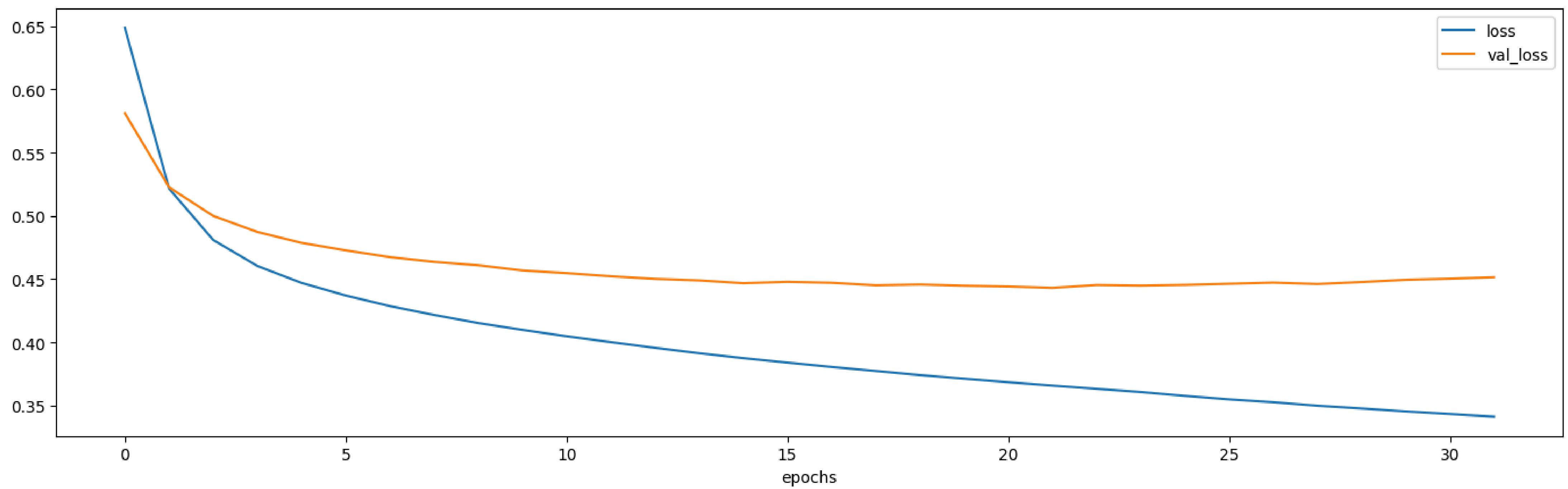
	Class1	Class2	Class3	Class4	Class5	Class6	Class7	Class8	Class9	Class10	Class11	Class12	Class13	Class14
1681	0	1	1	1	0	0	0	0	0	1	1	1	1	0
1565	1	1	0	0	0	1	1	0	0	0	0	1	1	0
544	0	1	1	1	1	1	0	0	0	0	0	0	0	0
1517	0	0	0	0	0	0	1	1	0	0	0	1	1	0
821	1	1	0	0	0	0	0	0	0	0	0	1	1	0

- All inputs are numeric
- ...And we have 14 possible classes

Unconstrained Model

We'll start by training an unconstrained model

In [86]:
```
nn0 = util.build_ml_model(input_size=X_tr.shape[1], output_size=y_tr.shape[1], hidden=[32],
history = util.train_ml_model(nn0, X_tr, y_tr, epochs=200, validation_split=0.1, loss='bina
util.plot_training_history(history, figsize=figsize)
```



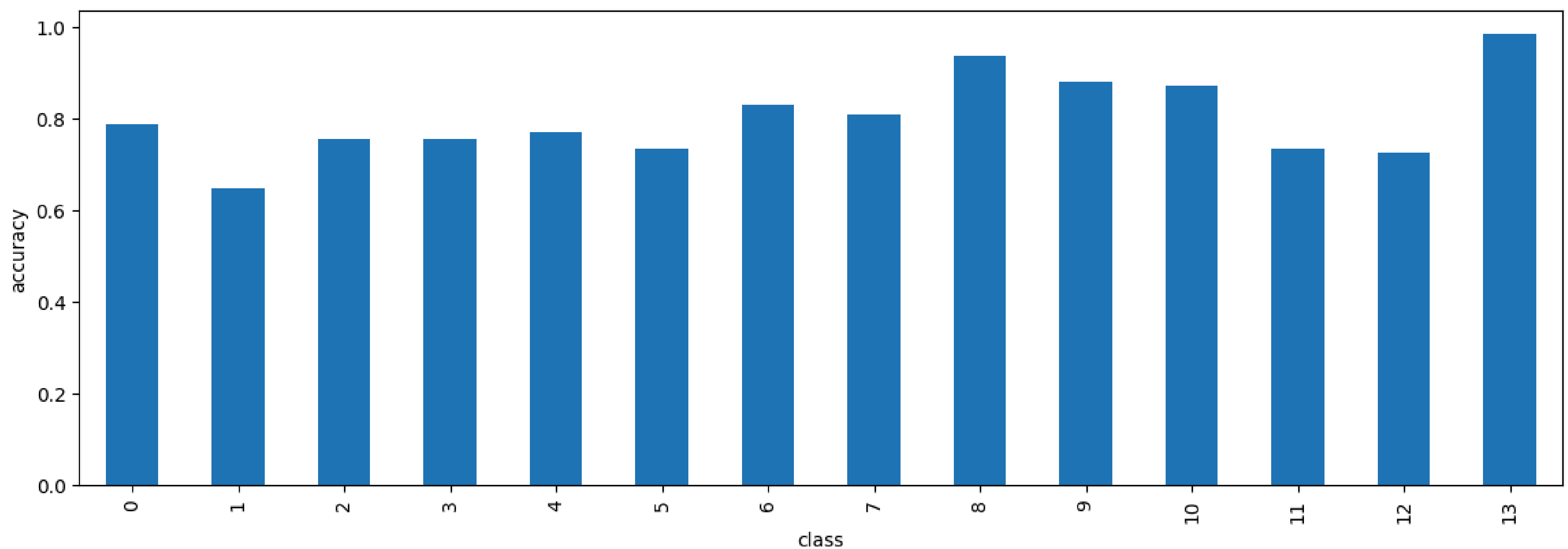

```
Model loss: 0.3658 (training) 0.4431 (validation)
```

Accuracy Evaluation

We can evaluated the model in terms of per-class accuracy

In [87]:
```
p_ts = nn0.predict(X_ts, verbose=0)
c_ts = np.round(p_ts)
ts_acc = util.get_multi_label_accuracy(y_ts, c_ts, series_name='original')
ts_acc.plot.bar(figsize=figsize, xlabel='class', ylabel='accuracy');
print(f'Average class accuracy: {ts_acc.mean():.3f} (test)')
```

```
Average class accuracy: 0.802 (test)
```



Mutually Exclusive Classes

We will assume that certaint traits cannot occur together

...Meaning that certain classes are mutually exclusive

- In this case, the constraint is just a purely synthetic example
- In the real world, contraints may come from regulation, domain knowledge, etc.

We will treat as mutually exclusive all pairs of classes

...That have a low-enough rate of co-occurrence in the entire dataset

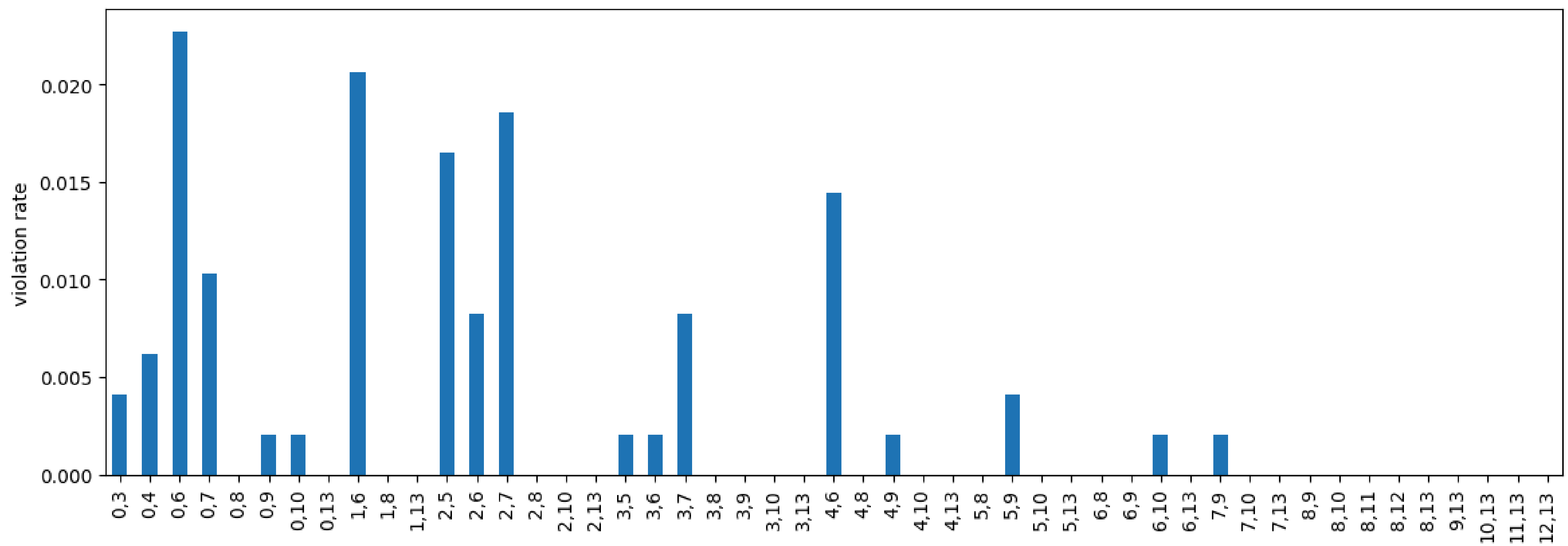
In [88]:
```
all_y = pd.concat((y_tr, y_ts))
forbidden = util.get_forbidden_pairs(all_y, cutoff_quantile=0.5)
print(forbidden)
```

```
{(4, 9), (3, 7), (4, 6), (12, 13), (3, 10), (5, 13), (3, 13), (5, 10), (8, 9), (8, 12),
(1, 6), (0, 8), (2, 5), (2, 8), (7, 10), (6, 8), (7, 13), (3, 9), (4, 8), (3, 6), (5, 9),
(8, 11), (0, 7), (0, 4), (0, 10), (2, 7), (9, 13), (0, 13), (2, 10), (1, 8), (11, 13), (2,
13), (7, 9), (6, 13), (6, 10), (3, 5), (4, 10), (3, 8), (4, 13), (5, 8), (0, 3), (0, 9),
(8, 10), (10, 13), (0, 6), (8, 13), (1, 13), (2, 6), (6, 9)}
```

Checking Violations

We can check how often our constraints are violated on the test data

In [100]:
```
util.forbidden_pair_violation(c_ts, forbidden).plot.bar(figsize=figsize, ylabel='violation
```



There some violation, though not many

Projection Model

We now need to define out projection problem:

$$\hat{z}(x) = \operatorname*{argmin}_{z} \{ L(z, \hat{y}) \mid g(x, z) \leq 0 \} \qquad \text{with: } \hat{y} = f(x; \theta^*)$$

For pre-computed $\hat{y}$, we'll need to obtain a declarative model of:

- The decision variables z
- The loss function $L(z, \hat{y})$
- The constraints $g(x, z) \leq 0$

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The decision variables represent a vector of classes

$$z_i \in \{0, 1\} \qquad \text{with } z_i = 1 \text{ iff we predict class } i$$

Projection Model

We'l use the binary cross entropy as our loss function

- The decision variables represent actual classes
- ...While the $\hat{y}$ contains estimated probabilities

Hence, we can model the loss function as:

$$L(z, \hat{y}) = -\sum_{i=1}^{k} z_i \log(\hat{y}_i + \varepsilon) + (1 - z_i) \log(1 - \hat{y}_i + \varepsilon)$$

- Since the cross-entropy is not well defined for $\hat{y}$ equal to 0 or 1
- ...We add a small constant to the logarithm

Overall, we have a liner expression defined on z

Projection Model

The constraints state that certaint pairs of classes cannot occur together

...Which can be modeled as:

$$z_i + z_j \leq 1 \quad \forall (i, j) \in F$$

- We consider all pairs of mutually exclusive classes
- ...And we allow at most one of the associated z variables to be 1

Overall, we have the following Mixed Integer Linear Program

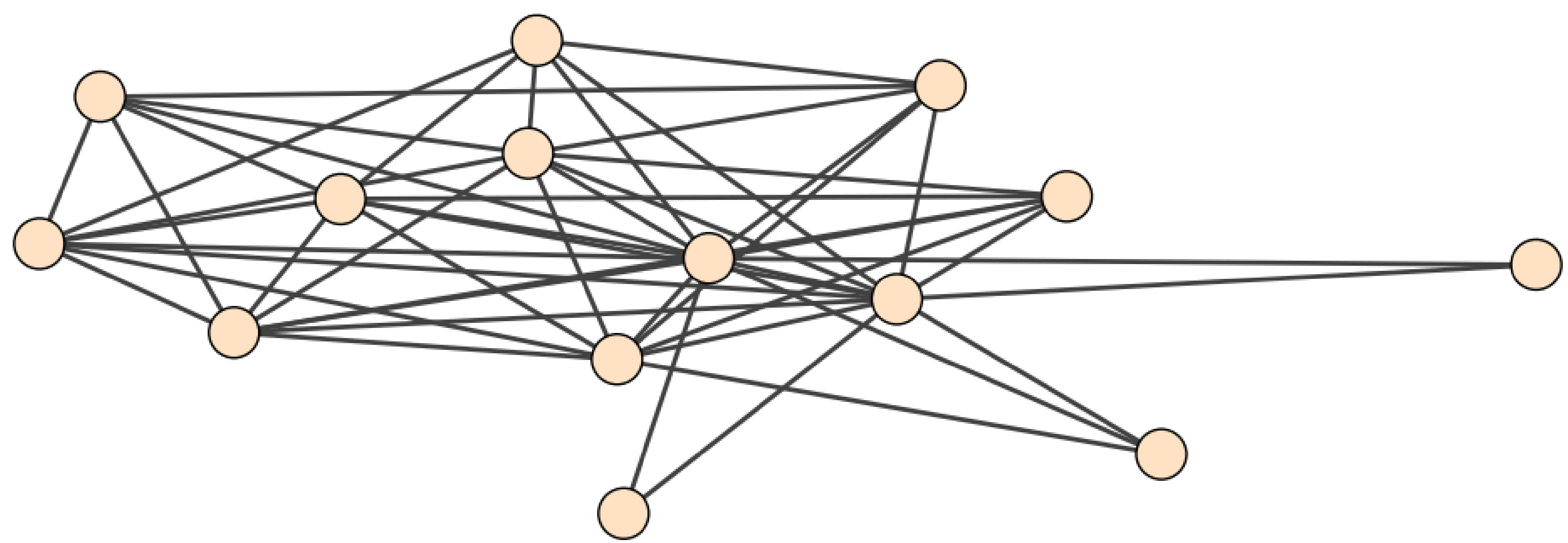
$$\begin{aligned} &\operatorname*{argmin}_z z^T \log(\hat{y} + \varepsilon) + (1 - z)^T \log(1 - \hat{y} + \varepsilon) \\ &\text{subject to: } z_i + z_j \leq 1 && \forall (j, j) \in F \\ &\qquad\qquad\quad z_i \in \{0, 1\} && \forall i = 1..n_c \end{aligned}$$

Maximum Weight Indedendent Set

What we are looking for is a maximum weight independent set

...On the graph defined by the mutually exclusive classes

In [101]:
```
util.plot_forbidden_pairs(nclasses=y_tr.shape[1], forbidden=forbidden, figsize=figsize)
```



- This is an NP-hard problem, but not a very difficult one!

Implementation

An implementation of the model is available in the `util` module

```
def project_multilabel_classification(p, forbidden, solver='CBC', tlim=10):
    ...
    z = [slv.IntVar(0, 1, 'z_{c}') for c in range(label_num)]
    for c0, c1 in forbidden: # constraintes
        slv.Add(z[c0] + z[c1] <= 1)
    for ii in range(p.shape[0]):
        # Define the objective
        obj = - sum([z[c] * np.log(p[ii, c] + 1e-4) +
                     (1 - z[c])*np.log(1 - p[ii, c] + 1e-4)
                     for c in range(label_num)])
        slv.Minimize(obj)
        status = slv.Solve()
        ...
```

- For improved efficiency, we build a single model to project multiple examples
- On each example, we just change the objective function

Computing the Projections

We can now compute the inference-time projections for the test set

```
In [104]: %time pc_ts = util.project_multilabel_classification(p_ts, forbidden=forbidden, tlim=10, so
          print(f'For {len(p_ts)} test examples')
```

```
CPU times: user 194 ms, sys: 31.6 ms, total: 225 ms
Wall time: 225 ms
For 484 test examples
```

- Even if the problem is technically intractable (NP-hard)
- ...The run time is very low!

For roughly 10% of the example the projection results in a change:

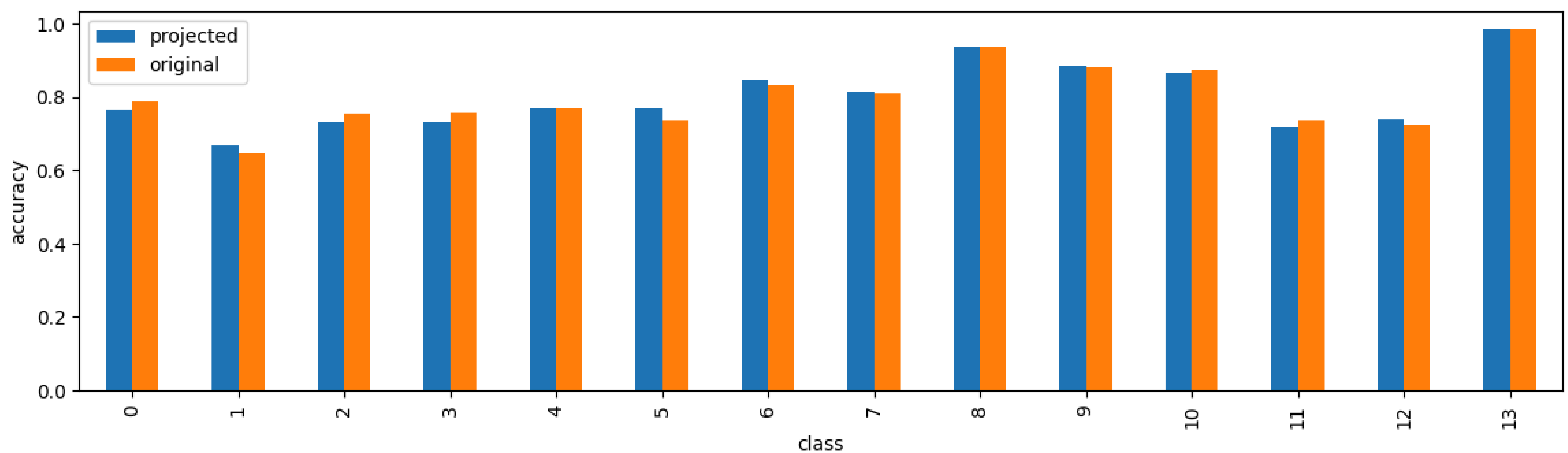
```
In [105]: nc_ts = np.any(np.abs(pc_ts - c_ts) > 0, axis=1).sum()
          print(f'Non-trivial projections: {nc_ts} (test)')
```

```
Non-trivial projections: 44 (test)
```

Accuracy Evaluation

We can compare the accuracy of the constrained model with the original one

```
In [109]: tmp = pd.concat([ts_acc_p, ts_acc], axis=1)
          tmp.plot.bar(figsize=(figsize[0], figsize[1]*0.8), xlabel='class', ylabel='accuracy');
```



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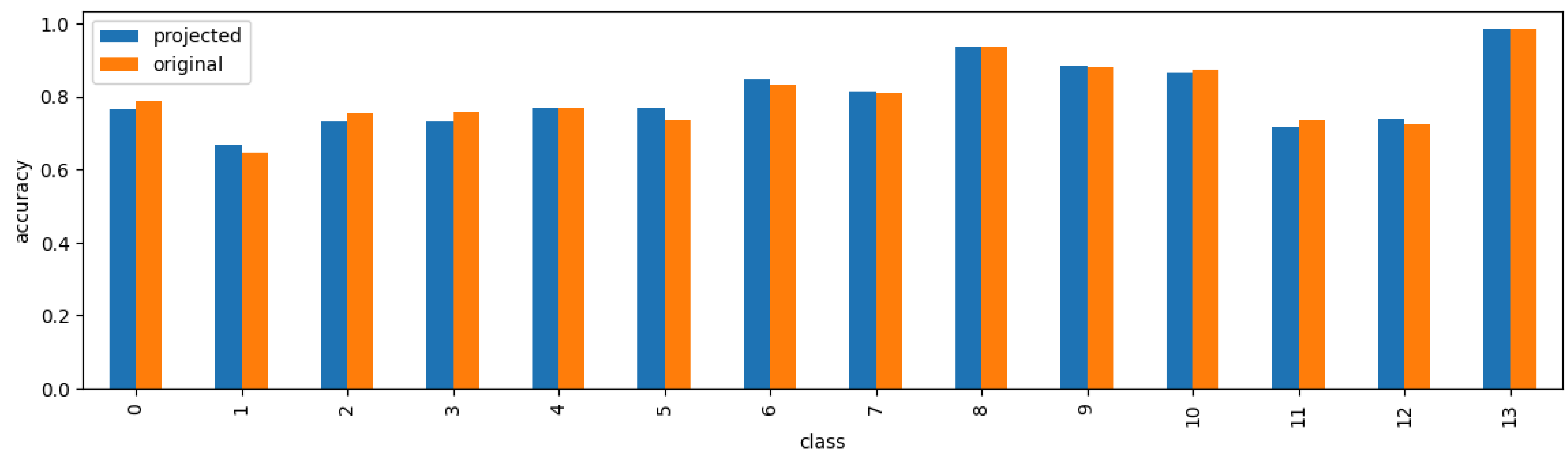


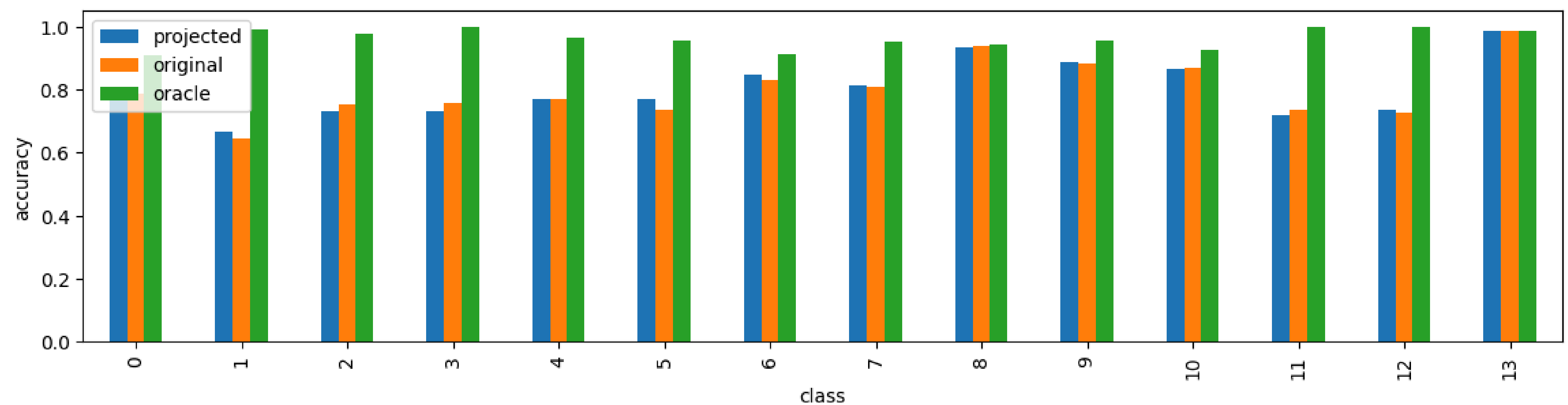
- For some classes, the constrained model works even better!
- This happens since the constraint encode some information about unseen examples

Accuracy Evaluation

Projection methods enable also a comparison against an oracle

Which can be obtained by projecting the ground truth labels

```
In [112]: ts_acc_o = util.get_multi_label_accuracy(y_ts, oc_ts, series_name='oracle')
          tmp = pd.concat([ts_acc_p, ts_acc, ts_acc_o], axis=1)
          tmp.plot.bar(figsize=(figsize[0], figsize[1]*0.7), xlabel='class', ylabel='accuracy');
```



Doing this tells us the best we can do, accounting for the constraints