Iterated Projection

They say repetion is the mother of learning

A Simple Constraint

Let's consider a relatively simple constraint for binary classification

$$\sum_{i=1}^{m} \text{round}(\hat{y}_i) \leq (1 + \varepsilon)\frac{m}{2}$$

- $\hat{y}_i$ is the estimated probability of class $\boldsymbol{i}$
- $\text{round}(\hat{y}_i)$ is the corresponding rounded class
- The summation denotes the number of examples with class 1
- ...Which we require to be approximaly equal to 50%

The restricton is synthetic and we'll use it just as an example

- However, the example is stil practically relevant
- ...Since many fairness constraints in classification have the same structure!

...And Yet an Annoying One

We cannnot easily use Lagrangians

...At least not in a differentiable ML setting

- The original constraint is non-differentiable when $\hat{y}_i = 0$
- ...And has 0-gradient everywhere else

This is all caused by the rounding operator

We can obtain a differentiable approximation by removing rounding

$$\sum_{i=1}^{m} \hat{y}_i = \frac{m}{2}$$

- But now we can satisfy the constraint by having $y_i = 0.5$ for all examples
- So, the constraint might conflict with the main loss function

...And Yet an Annoying One

Projection has a better time dealing with non-differentiable constraints

...But we cannnot easily use inference-time projection!

- This is a distribution constraint
- ...And cannot be enforced easily by working on individual examples

Data projection might also be in trouble

...Because it may fail to account for the input-output correlation

$$\sum_{i=1}^{m} \text{round}(\hat{y}_i) \leq (1 + \varepsilon)\frac{m}{2}$$

- There are many rounded vectors that satisfy the constraint
- ...And data projection might pick one that is uncorrelated with the input

What can we do about this?

First: at least give the know methods a chance! If that fails, however...

Moving Targets

One way around these issues is provided by the Moving Targets method

...Which is designed for constrained supervised learning, i.e.:

$$\text{argmin}_\theta \left\{ L(\hat{y}, y) \mid y \in C \right\} \text{ with: } \hat{y} = f(x, \theta)$$

- Where $\hat{y}$ is the prediction vector
- ...And $(x, y) = \{x_i, y_i\}_{i=1}^m$ is the training data

The method alternates between learner and master steps

- At evey step k, we keep a prediction $\hat{y}^{(k)}$ and a feasible adjusted target $z^{(k)}$
- In master steps, we move $z^{(k)}$ closer to te ground truth y
- In learner steps, we train an ML model to make $y^{(k)}$ close to z

Moving Targets

The master step consists in solving:

$$z^{(k+1)} = \text{argmin}_z \left\{ L(z, y) + \frac{1}{\rho} L(\hat{y}^{(k)}, z) \mid z \in C \right\}$$

We search for a z vector such that:

- z is close to y, as measured by the loss function L
- z is feasible w.r.t. the constraints C

Additionally, we keep z close to the current prediction $\hat{y}^{(k)}$

- We use the loss function to measure the proximity
- ...And we can control how close we want to stay by changing ρ

Moving Targets

The problem can be viewed as an approximate proximal operator

$$\mathbf{prox}_{\rho(I_C(z)+L(z,y))}(\hat{y}^{(k)})$$

- $I_C(z)$ is the constraint indicator function for C
- ...And the operator is computed w.r.t. the current prediction $\hat{y}$

Applying the proximal operator would lead to:

$$z^{(k+1)} = \operatorname{argmin}_z \left\{ L(z, y) + \frac{1}{\rho}\|z - \hat{y}^{(k)}\|_2^2 \mid z \in C \right\}$$

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This is similar to what we did in data projection

- In the master step, the L2 norm is replaced by the loss function
- ...Exactly like in the data projection approach

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...With one key difference

- We consider proximity w.r.t. the prediction $\hat{y}^{(k)}$
- ...And we account for the loss w.r.t. the ground truth y

Moving Targets

In the learner step we make the prediction closer to $z^{(k+1)}$

Given a target vector z^k, this consists in solving:

$$\hat{y}^{(k+1)} = \operatorname*{argmin}_{\theta} L(\hat{y}, z^{(k+1)}) \qquad \text{with: } \hat{y} = f(x; \theta)$$

...Which is just a traditional supervised learning problem

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The step can also be viewed as a form of projection:

$$\hat{y}^{(k+1)} = \operatorname{argmin}_{\hat{y}} \left\{ L(\hat{y}, z^{(k+1)}) \mid \hat{y} \in B \right\} \ \text{with: } B = \{\hat{y} \mid \exists \theta, \hat{y} = f(x; \theta)\}$$

Where B (model bias) is the set of output that can be reached by the model

- This perspective is useful to understand the algorithm behavior
- ...But of course it does not alter the way we train

Moving Targets

Overall, the method is as follows:

- $y^{(0)} = \text{argmin}_{\hat{y}}\left\{L(\hat{y}, y) \mid \hat{y} \in B\right\}$
- For $k = 0..n-1$:
  - $z^{(k+1)} = \text{argmin}_z\left\{L(z, y) + \frac{1}{\rho}L(\hat{y}^{(k)}, z) \mid z \in C\right\}$
  - $\hat{y}^{(k+1)} = \text{argmin}_{\hat{y}}\left\{L(\hat{y}, z^{(k+1)}) \mid \hat{y} \in B\right\}$

Some highlights

- You can use any technique for either step (it's a full decomposition)
- Non differentiable constraints can be handled via CP, SMT, MP, meta-heuristics
- Batching is not needed in the master step (when constraints are handled)
- α is divided by k at each iteration to ensure convergence

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Speaking of convergence

- If L, B, C are convex and target are continuous...
  - ...Then the method can be proved to converge to a global optimum
- When these conditions are not met
  - ...The method is still applicable as a heuristic

Let's see a running example

A Toy Learning Problem

Say we want to fit a model in the form:

$$\tilde{f}(x, \beta) = x^{\beta}$$

...Based on just two observations

For evaluation purpose, we assume we know the true curve, i.e.:

$$f(x) = x^{0.579}$$

And hence we can obtain the true y values:

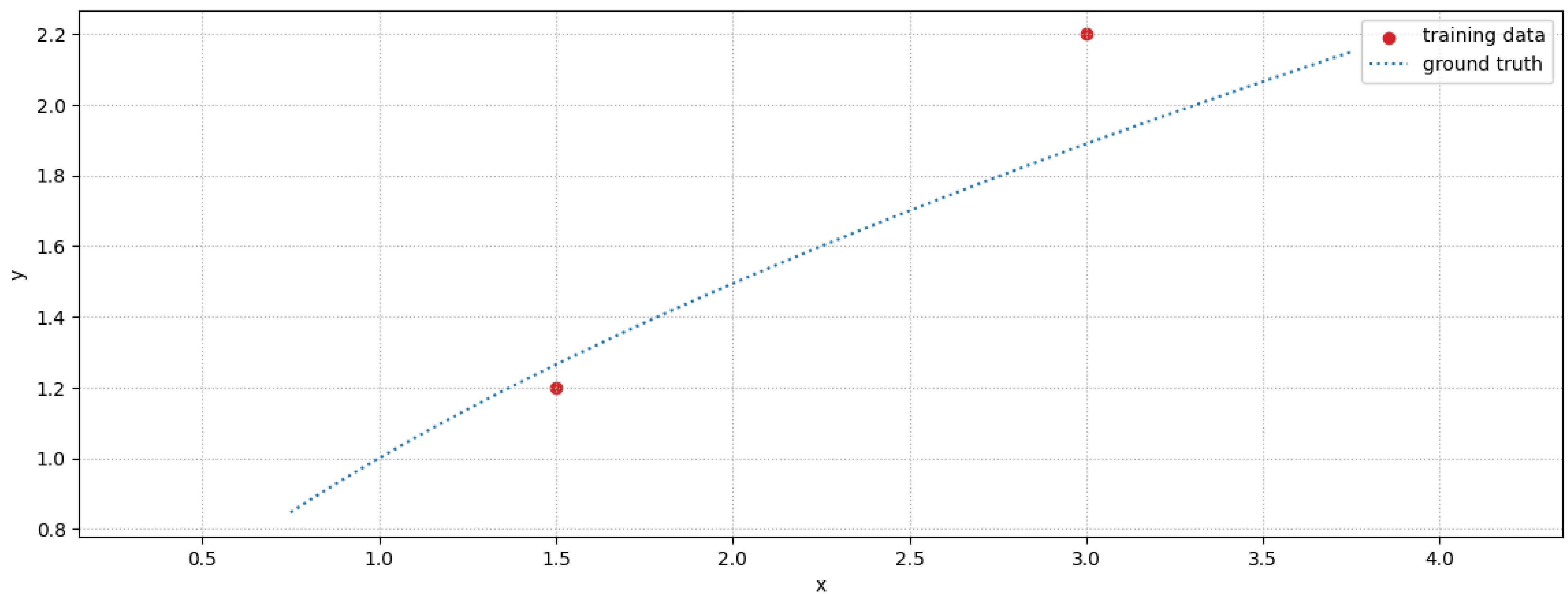
In [2]:
```
xm = np.array([1.5, 3])
ym = np.array([1.2, 2.2])

f_true = lambda x: x**0.579
yt = f_true(xm)
```

A Toy Learning Problem

We can now plot both the true curve and the measured x, y points:

```
In [6]: util.mtx_function_plot(xm, ym, f_true, figsize=figsize)
```



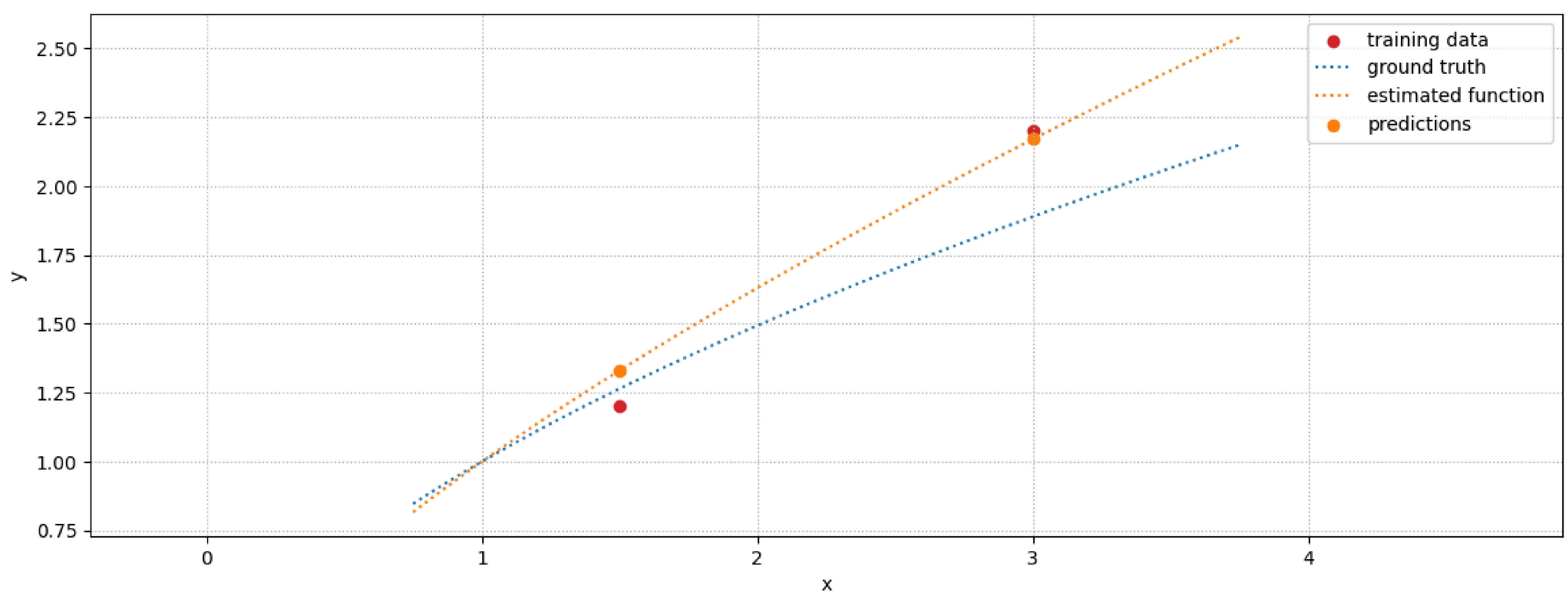
- We are underestimating the first point and overestimatng the second
- ...Which may easily trick our simple model

Learner Step

We can now perform the first learner step

For this example, we can use any curve fitting method

In [8]:
```
f_pred = util.mtx_learner_step(xm, ym)
util.mtx_function_plot(xm, ym, f_true, f_pred, figsize=figsize)
```

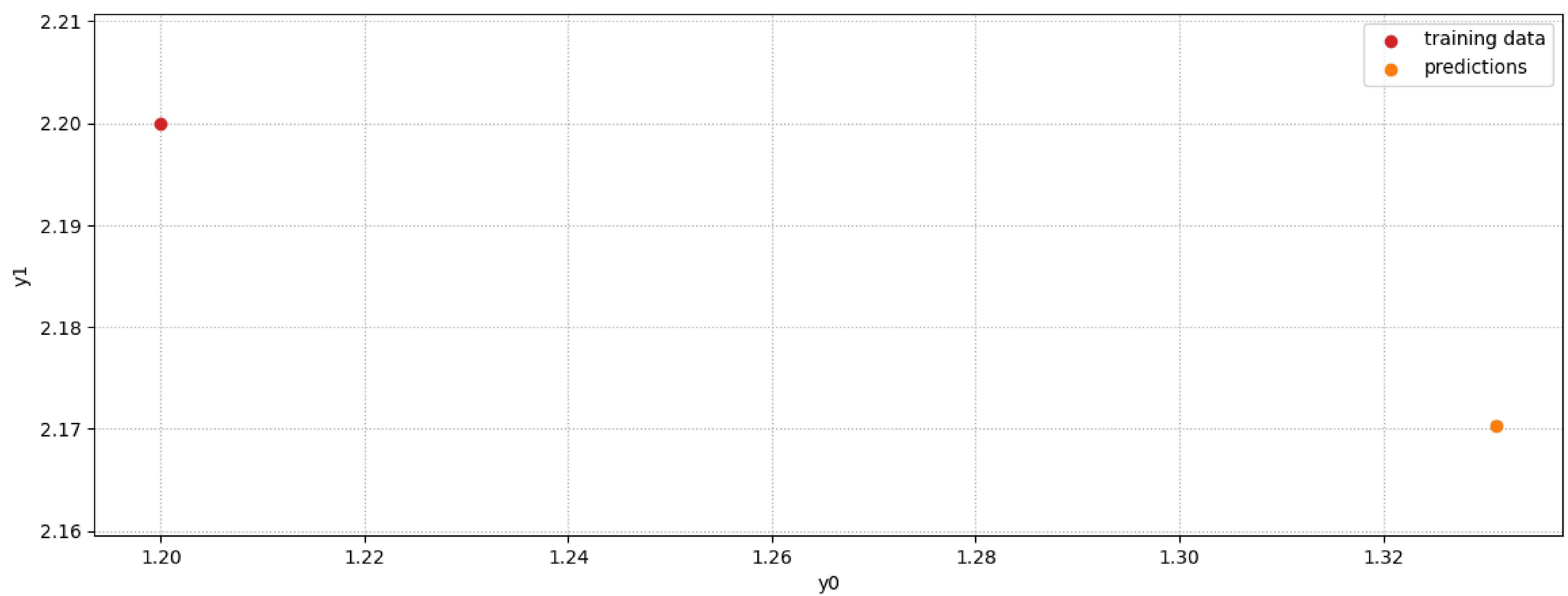


Taking Advantage of Constraints

Before that, let's view measurements and predictions in output space

...Where they both look like points

In [11]:
```
yp = f_pred(xm)
util.mtx_output_plot(xm, ym, yp, figsize=figsize)
```

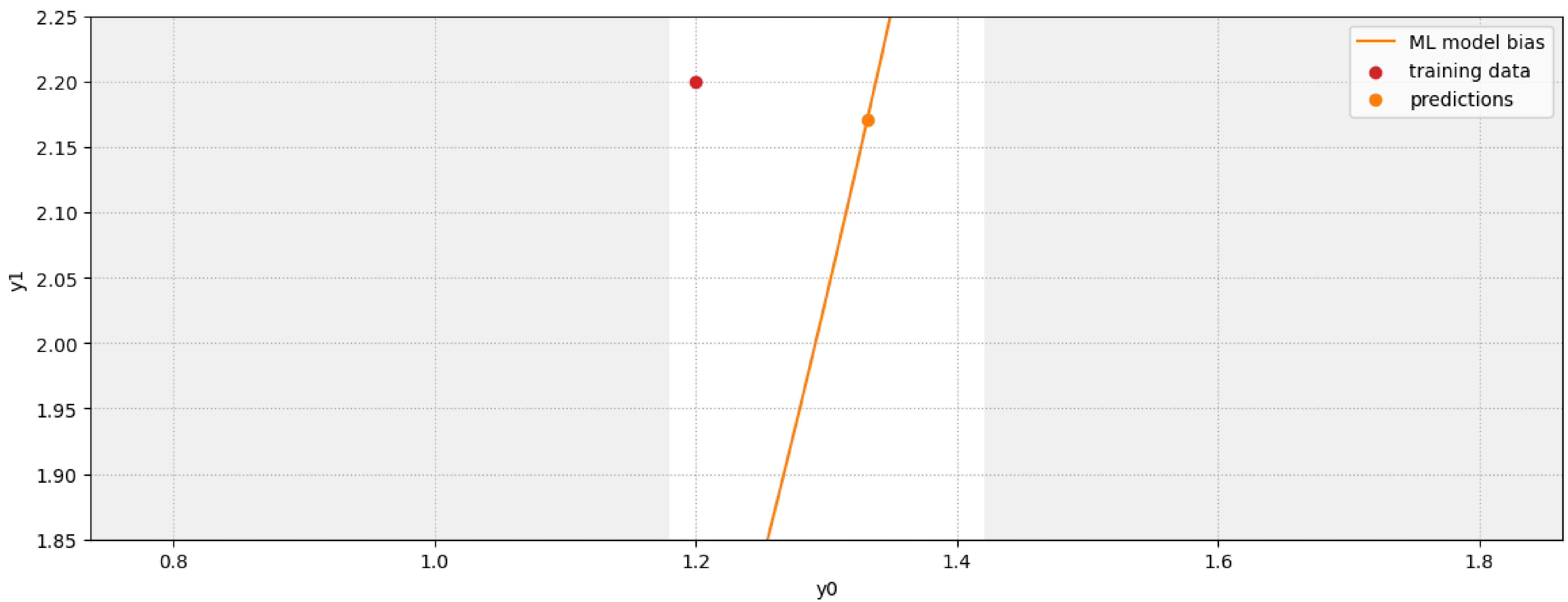


Visualizing Model Bias

By changing the β in our model we can change the prediction vector

We can draw a range of potential predictions in output space (part of $\boldsymbol{B}$)

```
In [13]: yp = f_pred(xm)
         util.mtx_output_plot(xm, ym, yp, plot_bias=True, figsize=figsize, ylim=(1.85, 2.25))
```



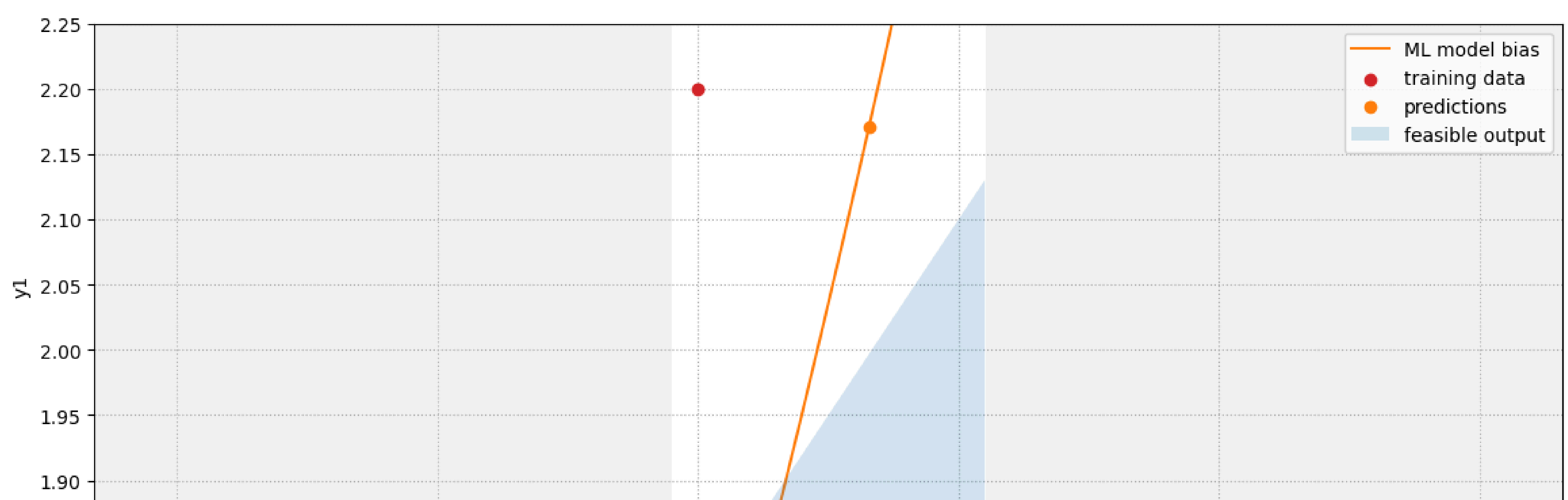
Taking Advantage of Constraints

Say we know that our two measurements must obey

$$y_1 \leq \frac{3}{2} y_0$$

We can draw the feasible set C in output space, too!

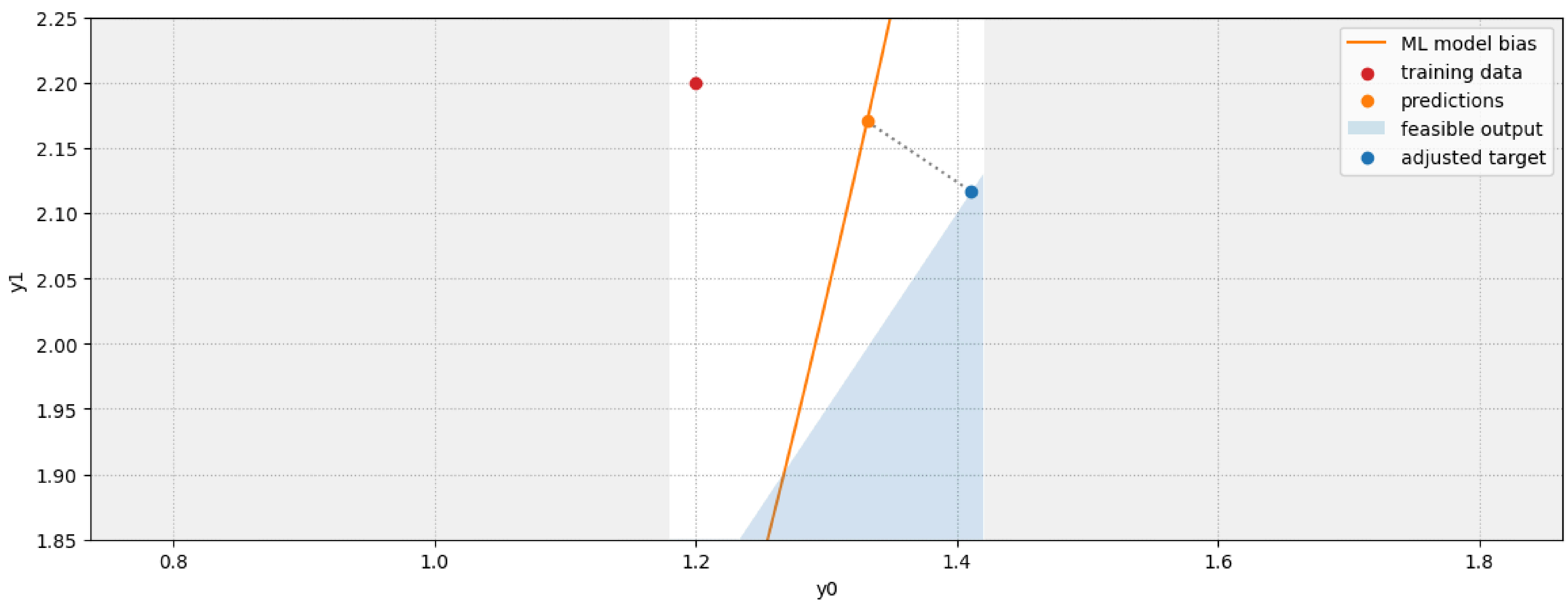
```
In [47]: f_bound = lambda y0: 1.5*y0
         util.mtx_output_plot(xm, ym, yp, plot_bias=True, f_bound=f_bound, figsize=figsize, ylim=(1.8
```



Master Step

We can now perform the first master step

```
In [46]: yf = util.mtx_master_step_alpha(ym, yp, rho=0.01)
         util.mtx_output_plot(xm, ym, yp, plot_bias=True, f_bound=f_bound, yf=yf, figsize=figsize, y
```

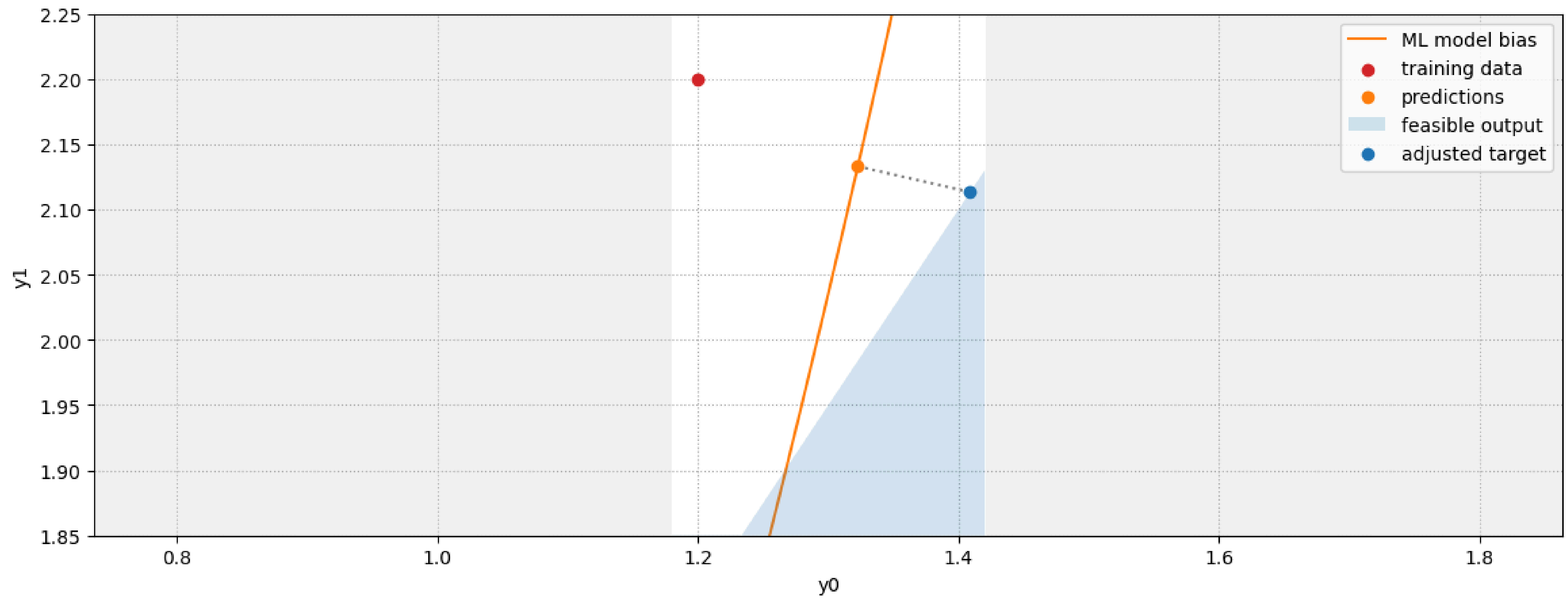


- The result is similar to a projection, but it is a bit closer to the true target

Second Learner Step

We can now perform and visualize a second learner step

```
In [39]: f_pred2 = util.mtx_learner_step(xm, yf)
         yp2 = f_pred2(xm)
         util.mtx_output_plot(xm, ym, yp2, plot_bias=True, f_bound=f_bound, yf=yf, figsize=figsize, y
```

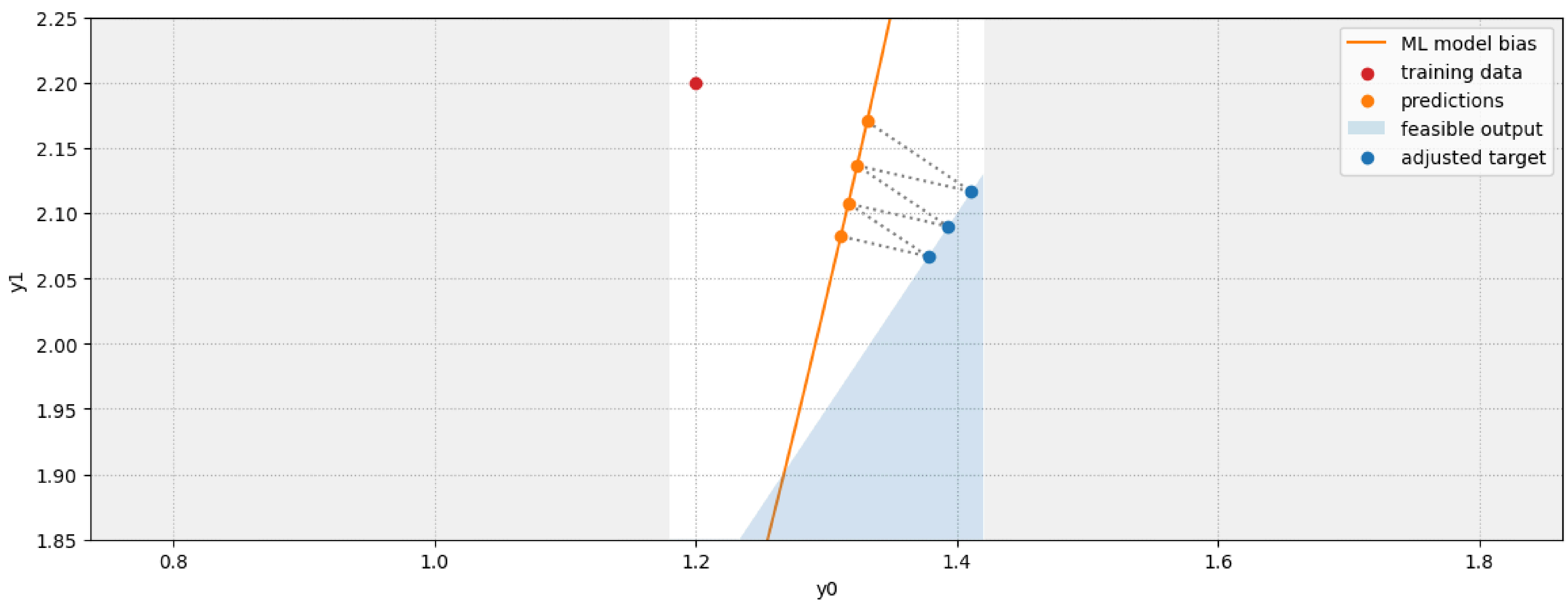


- This one is an actual projection on the model bias B

The Full Method

We can visualize a few iterations to see how MT works

In [45]:
```
ypl, yfl, _ = util.mtx_moving_target_rho(xm, ym, n=3, rho=0.01)
util.mtx_output_plot(xm, ym, ypl, plot_bias=True, f_bound=f_bound, yf=yfl, figsize=figsize,
```

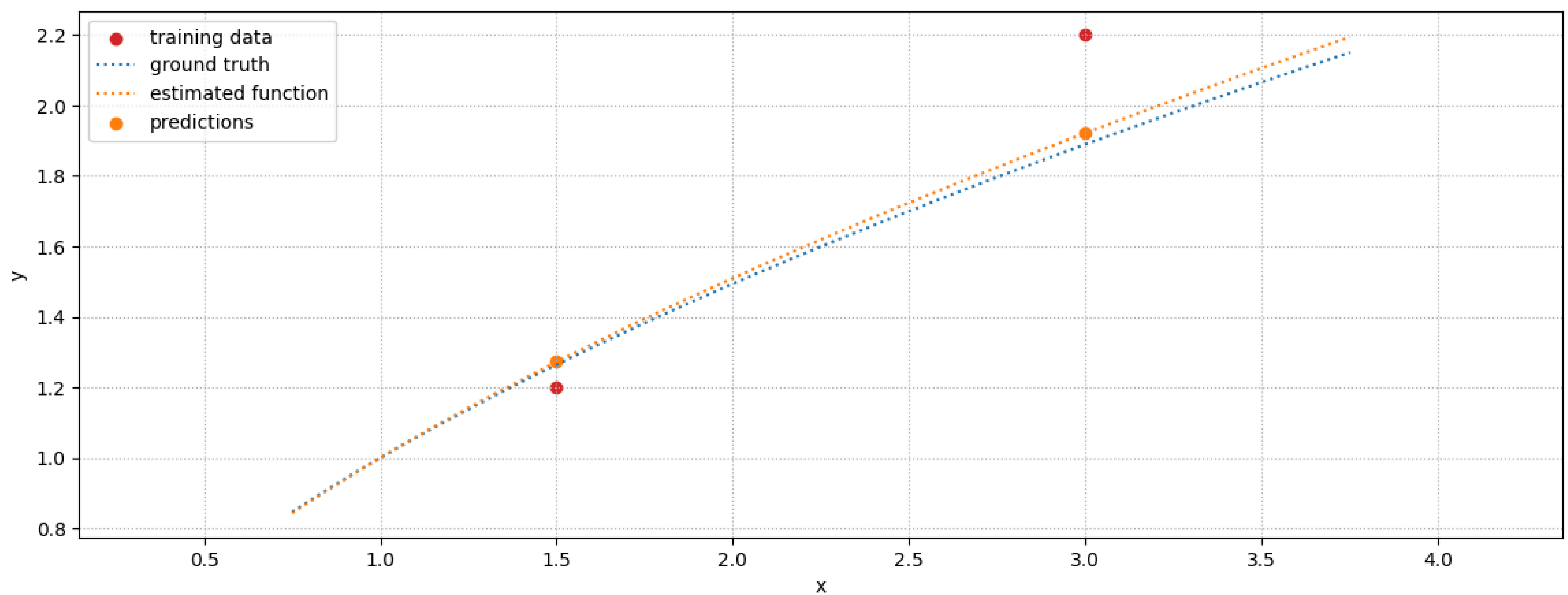


- Basically, MT zig-zags between the $\boldsymbol{B}$ and the $\boldsymbol{C}$ set

The Final Outcome

We can now inspect which kind of model we can obtain after some iterations

```
In [44]: _, _, f_pred_final = util.mtx_moving_target_rho(xm, ym, n=30, rho=0.01)
         util.mtx_function_plot(xm, ym, f_true, f_pred_final, figsize=figsize)
```



- This is very close to the true function!