

# Constraints via Projection and Decomposition

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# A Nasty Example

We used Lagrangian approaches to tackle constrained training problems:

$$\operatorname{argmin}_{\omega} \{ L(y) \mid g(y) \leq 0 \} \text{ with: } y = f(\hat{x}, \omega)$$

They work well, but:

- They require differentiability of  $g$  to use gradient descent
- ...And taking advantage of mini-batches is tricky

**Let's consider a particularly bad case**

Say we want to have perfectly balanced output in a binary classifier:

$$\sum_{i=1}^m \operatorname{round}(y_i) = \frac{m}{2}$$

- Where  $y_i$  is the positive-class output for example  $i$

# A Nasty Example

## First, the constraint is not differentiable

We can obtain a differentiable approximation by removing rounding:

$$\sum_{i=1}^m y_i = \frac{m}{2}$$

- But now we can satisfy the constraint by having  $y_i = 0.5$  for all examples!

## Second, the constraint is defined on the whole training set

We can restrict our focus to the example  $I_k$  in mini-batch  $k$ :

$$\sum_{i \in I_k} \text{round}(y_i) = \frac{|I_k|}{2}$$

- But now we'll have at best **stochastic** constraint satisfaction!

# A Nasty Example

## We could think of using the Projected Gradient Method

Let's consider our example from this point of view:

$$\sum_{i=1}^m \text{round}(y_i) = \frac{m}{2}, \text{ with: } y = f(\hat{x}, \omega)$$

- The constraint on  $\mathbf{y}$  is simple
  - ...But not so it's translation on  $\omega$
- The constraint is relational
  - Hence, using mini-batches leads to stochastic noise
  - ...And not using them may cause scalability issues
- The constraint is non-differentiable, non-convex, and non-separable
  - Hence, projecting can be an expensive operation

# Moving Targets

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

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

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

- Where  $\hat{y}$  is the target (or label) vector and  $L(y, \hat{y})$  is the loss function

**MT makes projection scalable by working in output space**

The method alternates between learner and master steps

- At every step  $k$ , we maintain a prediction  $y^k$  and an adjusted target  $z^k$
- In master steps, we move  $z^k$  so as to make it feasible and closer to  $\hat{y}$
- In learner steps, we train an ML model to make  $y^k$  close to  $z^k$

**Here we will present a revised version of the original algorithm**

# Moving Targets

The **master step** can be derived from a Taylor expansion

By assuming that  $L(y, \hat{y})$  is differentiable (as in the PGM) we can write:

$$L(y, \hat{y}) \simeq L(y^k, \hat{y}) + \nabla_y L(y^k, \hat{y})(z - y^k) + o(\|z - y^k\|_2^2)$$

Then we look for an adjusted target vector  $z$  that is:

- Feasible w.r.t. to  $C$ , improving in terms of loss w.r.t.  $\hat{y}$
- ...And close enough to  $y^k$  (for the linear approximation to be reliable)

**In practice, this is done by solving:**

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

- Which is obtained from the Taylor expansion by adding an  $\alpha$  parameter

# Moving Targets

Let's look closer at the master step problem

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

- By changing  $\alpha$ , we can control how close we are to  $y^k$ 
  - For  $\alpha = 0$ , we actually obtain a projection operator
- We can use **any solution technique** (including MILP, CP, SMT...)
  - Meaning that we can **apply** the method for basically any kind of constraint
  - ...Though convergence may be trickier in some cases
- The ML model  $f(x, \omega)$  is missing in the formulation
  - We are working **with the target vector alone** (i.e. in output space)
  - ...Which makes it much easier to deal with large-scale relational constraints

# Moving Targets

## The master step

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

- ...Can be thought of as merging gradient descent & projection from the PGM
- I.e. it's almost equivalent to performing:

$$z^{(k)} = \mathbf{proj}_C \left( y^{(k)} - \eta^{(k)} \nabla_z L(y^{(k)}, \hat{y}) \right)$$

**As a main difference, everything is done in output space**

- I.e. we change  $z^k$ , rather than changing  $\omega$

**But how do we actually update the ML model?**



# Moving Targets

Changing the ML model is purpose of the **learner step**

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

$$\operatorname{argmin}_{\omega} L(y, z^k) \text{ with: } y = f(\hat{x}, \omega)$$

...Which is a **traditional supervised learning** problem

The step can **also** be viewed as a for of projection:

$$\operatorname{argmin}_y \{ L(y, z^k) \mid y \in B \} \text{ with: } B = \{ y \mid \exists \omega, y = f(\hat{x}, \omega) \}$$

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

The overall method is as follows:

- $y^0 = \operatorname{argmin}_y \{ L(y, \hat{y}) \mid y \in B \}$
- For  $k = 1..n$ :
  - $z^k = \operatorname{argmin}_z \{ \alpha \frac{1}{k} \nabla_y L(y^k, \hat{y})(z - y^k) + \|z - y^k\|_2^2, \text{ s.t. } z \in C \}$
  - $y^{k+1} = \operatorname{argmin}_y \{ L(y, z^k) \mid y \in B \}$

## 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)
- $\alpha$  is divided by  $k$  at each iteration to ensure convergence

# Moving Targets

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- For  $k = 1..n$ :
  - $z^k = \operatorname{argmin}_z \{ \alpha \frac{1}{k} \nabla_y L(y^k, \hat{y})(z - y^k) + \|z - y^k\|_2^2, \text{ s.t. } z \in C \}$
  - $y^{k+1} = \operatorname{argmin}_y \{ L(y, z^k) \mid y \in B \}$

## Speaking of convergence

- At the momento of writing, a formal proof is still missing
- ...But the method is **still applicable** as a heuristic

# A Running Example

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# 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.:**

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

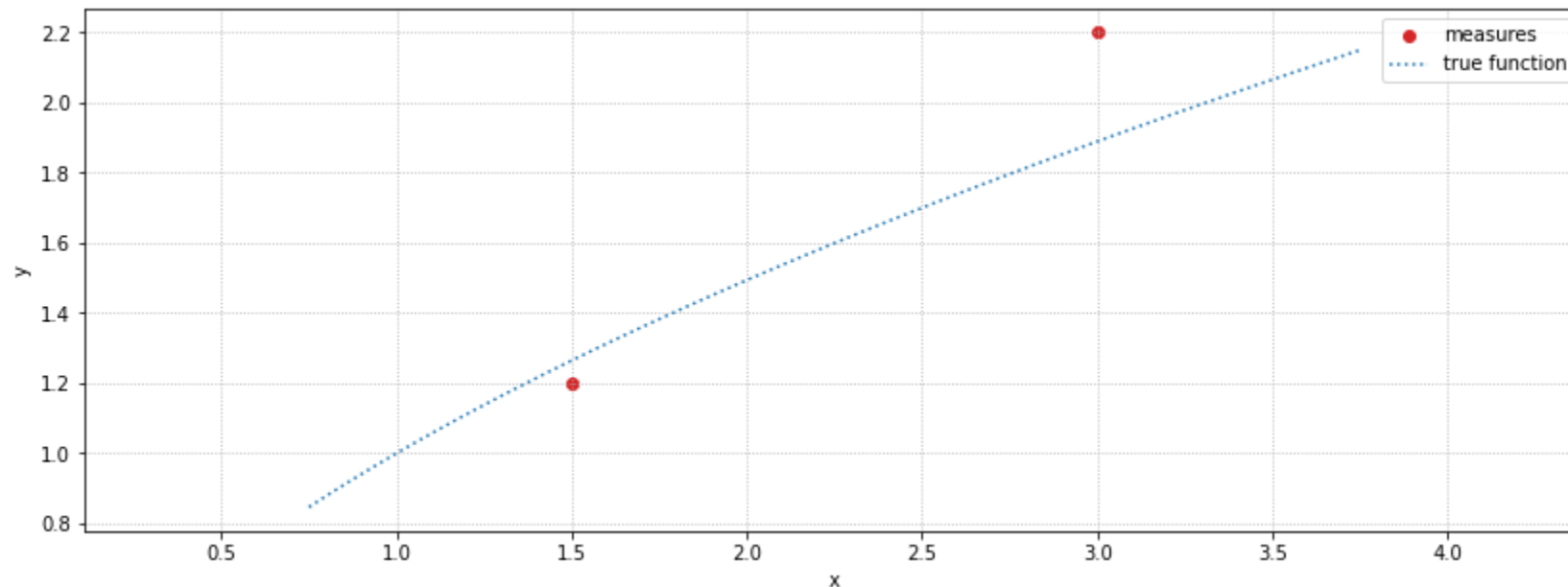
And hence we can obtain the true **y** values:

```
In [3]: 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 [4]: util.mtx_function_plot(xm, ym, f_true, figsize=figsize)
```



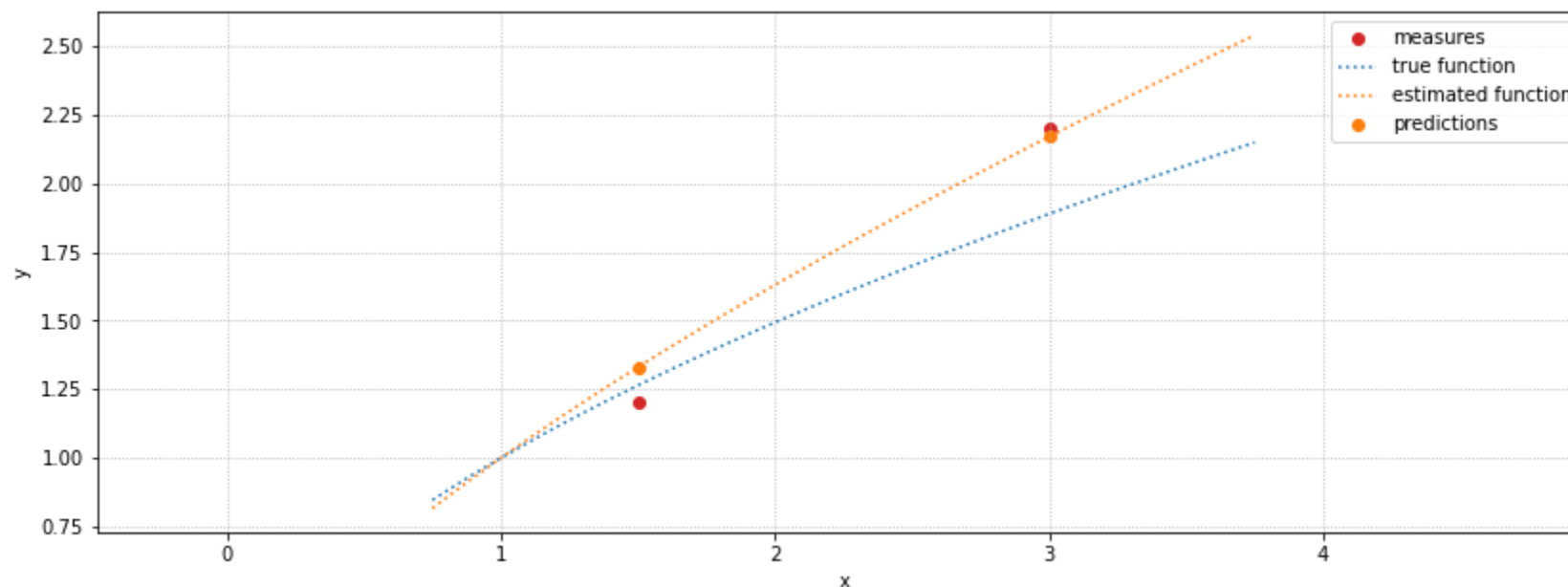
- We are underestimating the first point and overestimating the second
- ...Which may easily trick our simple model

# Learner Step

## We can now perform the first learner step

For this example, we can use any curve fitting method

```
In [5]: f_pred = util.mtx_learner_step(xm, ym)
util.mtx_function_plot(xm, ym, f_true, f_pred, figsize=figsize)
```



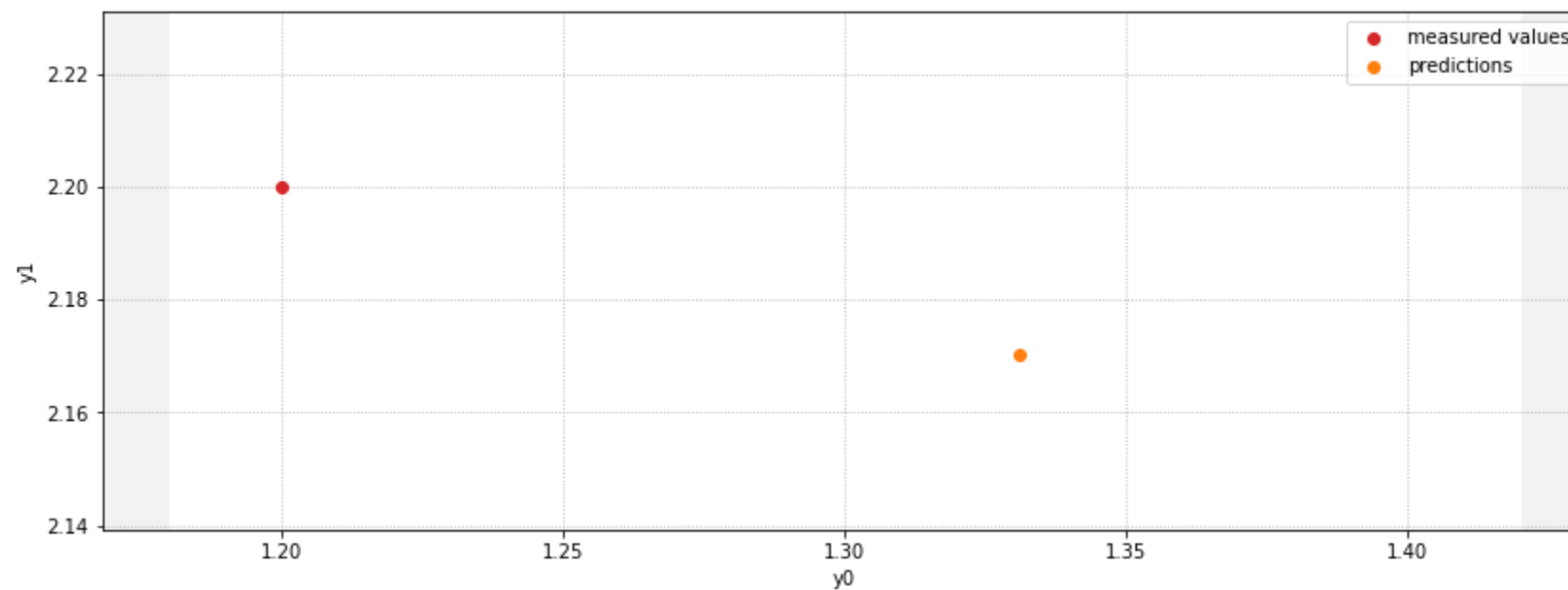
- The learner model indeed overestimates the curve slope
- More data could fix the issue, but we will rely instead on constraints

# Taking Advantage of Constraints

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

...Where they both look like **points**

```
In [6]: yp = f_pred(xm)
util.mtx_output_plot(xm, ym, yp, figsize=figsize)
```



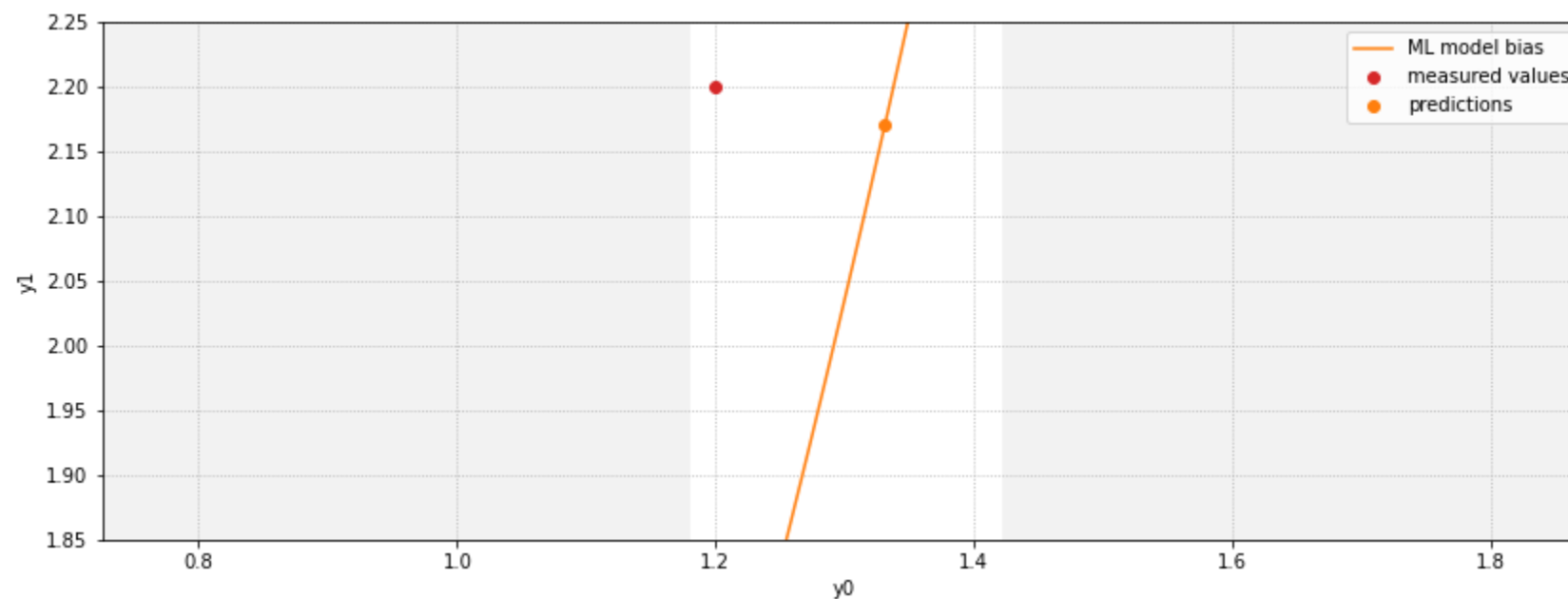


# Visualizing Model Bias

By changing the  $\beta$  in our model we can change the prediction vector

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

```
In [7]: yp = f_pred(xm)
util.mtx_output_plot(xm, ym, yp, plot_bias=True, figsize=figsize, ylim=(1.85, 2.25))
```



- This represents the bias  $\mathbf{B}$  of our ML model

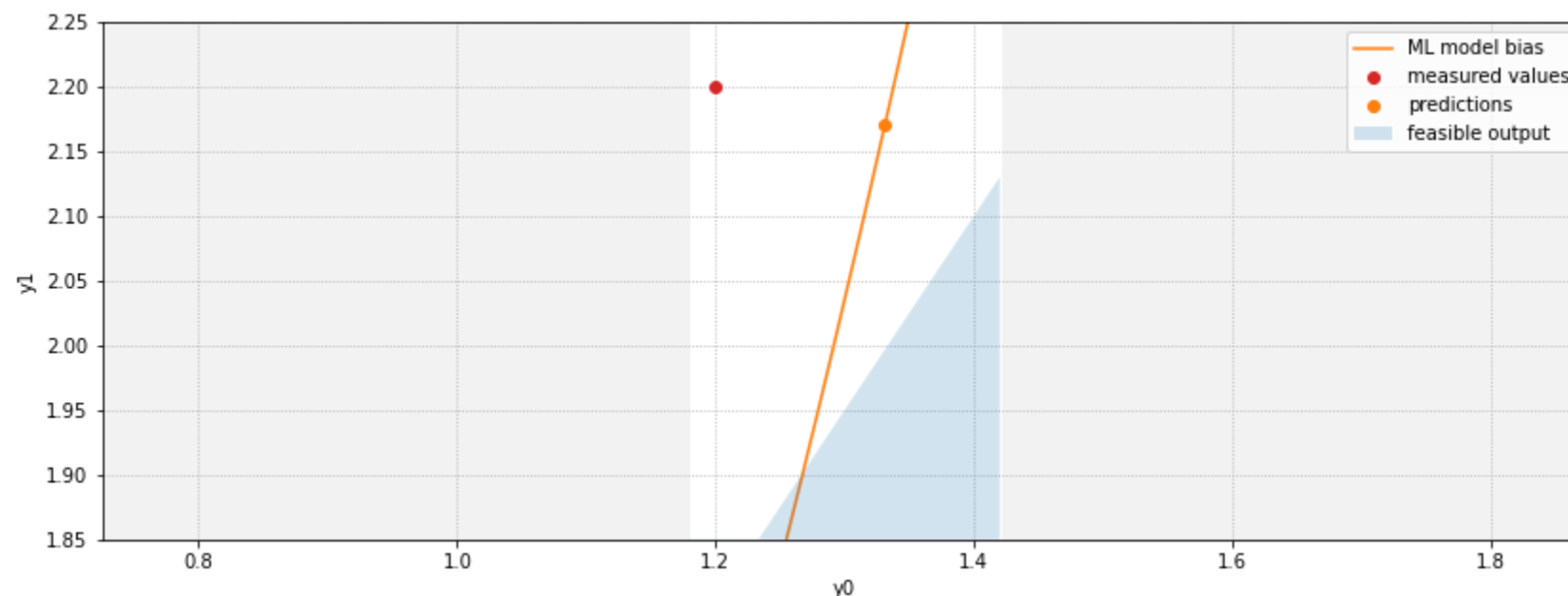
# Taking Advantage of Constraints

Say we know that our two measurements must obey

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

We can draw the feasible set  $\mathcal{C}$  in output space, too!

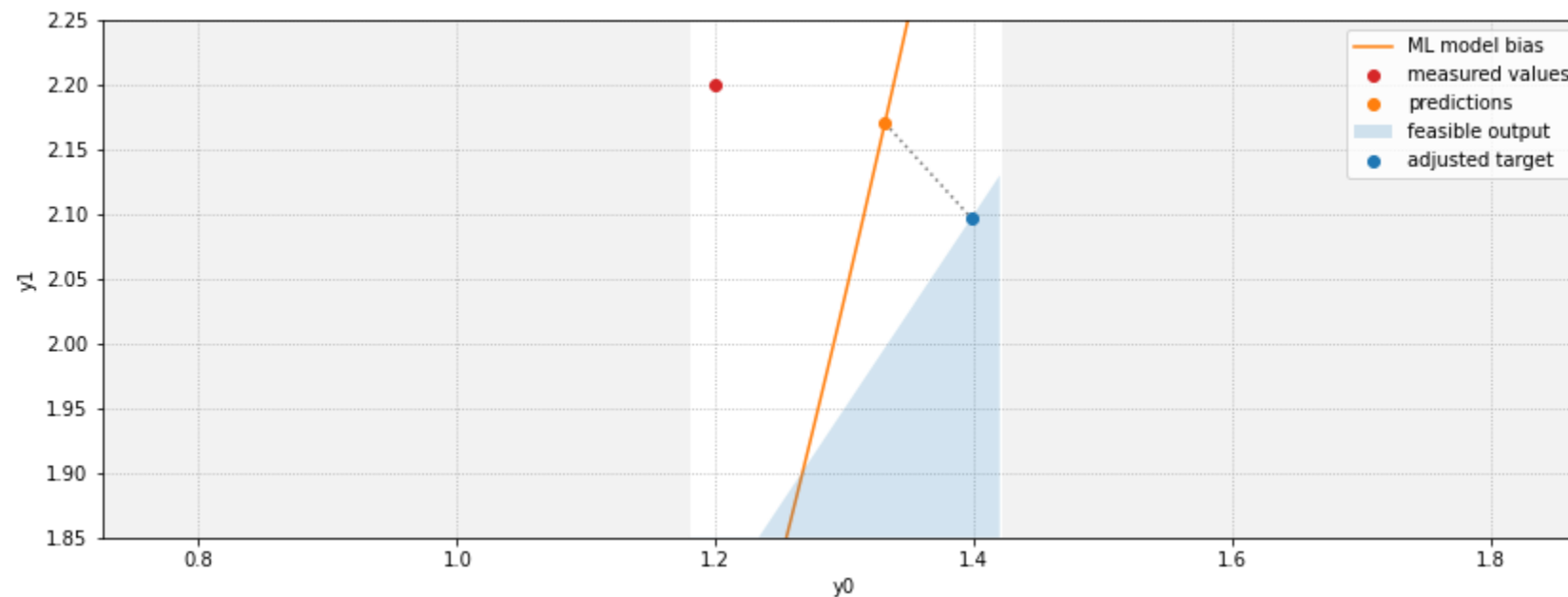
```
In [8]: f_bound = lambda y0: 1.5*y0  
util.mtx_output_plot(xm, ym, yp, plot_bias=True, f_bound=f_bound, figsize=figsize, ylim=(1.85, 2.25))
```



# Master Step

We can now perform the first master step

```
In [9]: yf = util.mtx_master_step_alpha(ym, yp, alpha=0.5)
util.mtx_output_plot(xm, ym, yp, plot_bias=True, f_bound=f_bound, yf=yf, figsize=figsize, ylim=
```

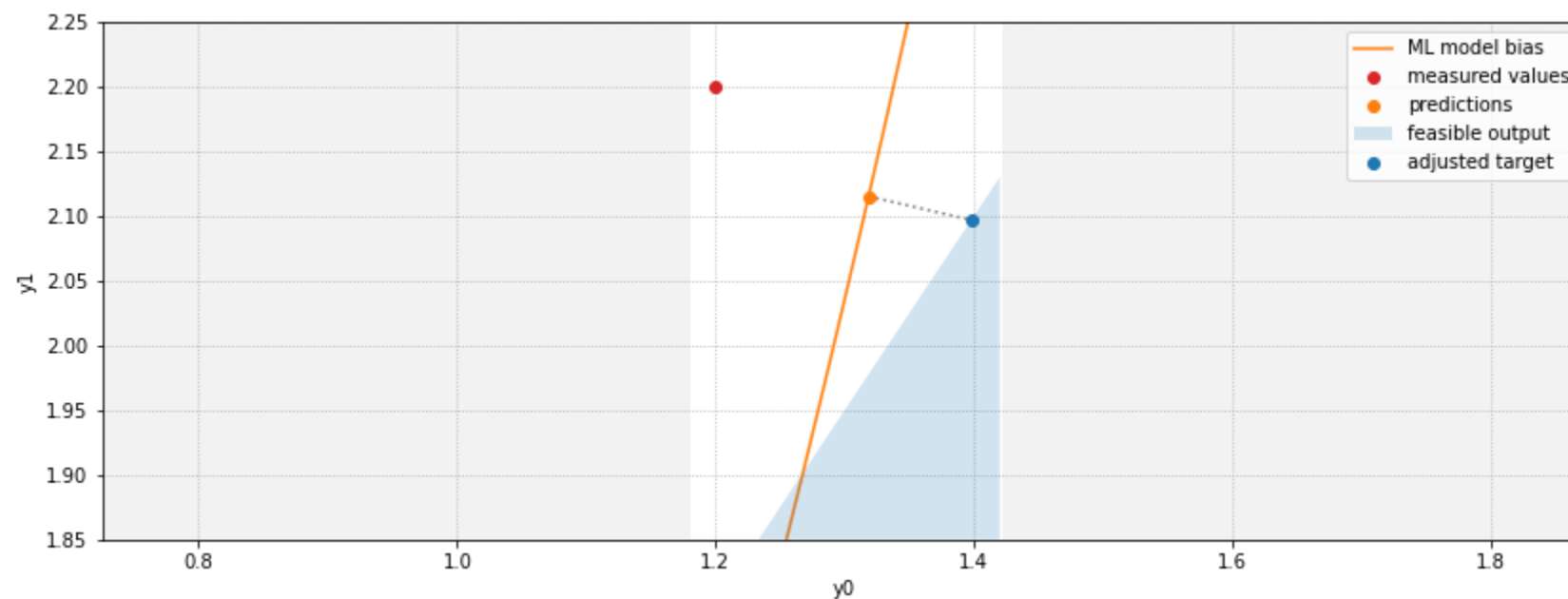


- The result is similar to a projection
- ...Except that it is a bit closer to the true target

## Second Learner Step

We can now perform and visualize a second learner step

```
In [10]: 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, ylim=
```

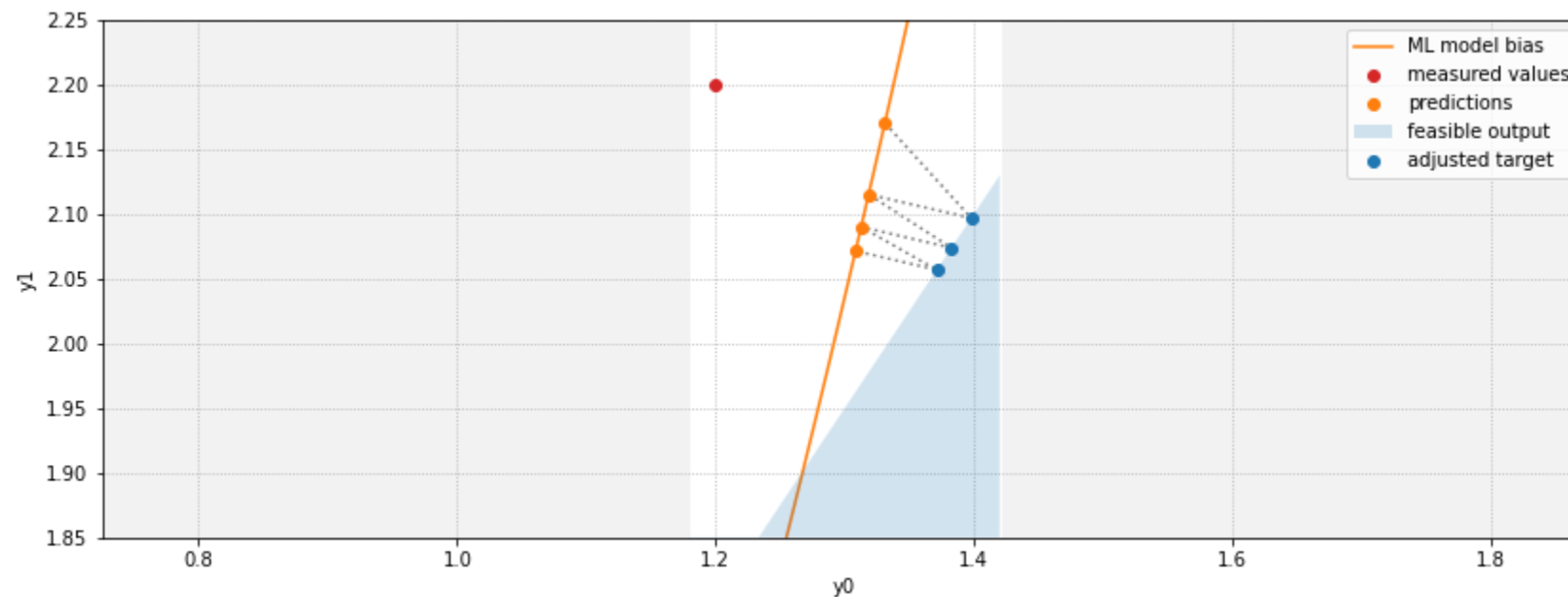


- This one is an actual projection on the model bias  $B$

# The Full Method

We can visualize a few iterations to see how MT works

```
In [11]: ypl, yfl, _ = util.mtx_moving_target_alpha(xm, ym, n=3, alpha=0.5)
util.mtx_output_plot(xm, ym, ypl, plot_bias=True, f_bound=f_bound, yf=yfl, figsize=figsize, ylin
```

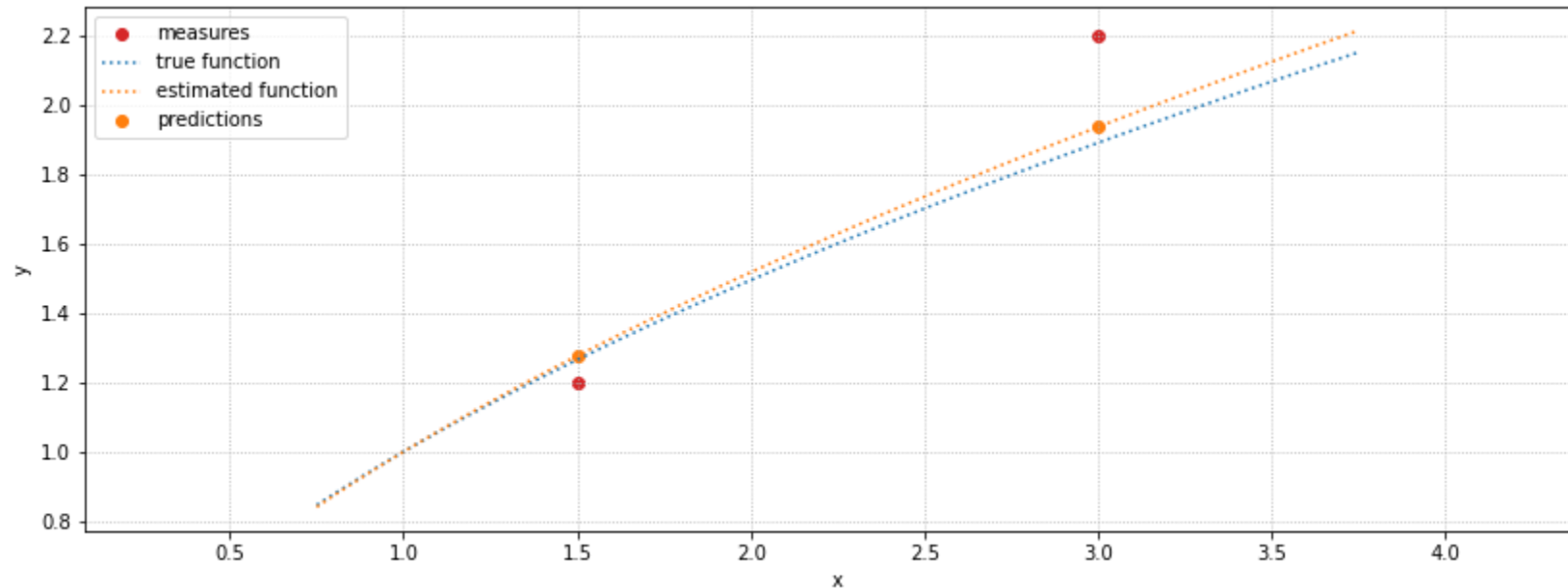


- Basically, MT zig-zags between the  $\mathbf{B}$  and the  $\mathbf{C}$  set
- This is not ideal, but it's the price we pay to enjoy a full decomposition

# The Final Outcome

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

```
In [12]: _, _, f_pred_final = util.mtx_moving_target_alpha(xm, ym, n=30, alpha=0.5)
util.mtx_function_plot(xm, ym, f_true, f_pred_final, figsize=figsize)
```



■ This is very close to the true function!