Let's load the required dataset

The Projected Gradient Method

Constrained ML, Again

We used Lagrangian approaches to tackle constrained training problems:

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

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:

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

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

A Particularly Bad 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:

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

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

Projected Gradient Method

A potential alternative is the projected gradient method

...Which can target ML problems in the form:

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

Here C is a generic feasible set

- We no longer need to define constraints
- ...Using differentiable functions $g(y)$

In terms of 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:

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

$$\mathbf{proj}_C(\omega) = \text{argmin}_{\omega'} \left\{ \frac{1}{2} \|\omega' - \omega\|_2^2, \quad \text{s.t. } f(\hat{x}, \omega') \in C \right\}$$

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

The key point is that we use projection (not a penalty) for the constraints

$$\mathbf{proj}_C(\omega) = \text{argmin}_{\omega'} \left\{ \frac{1}{2}\|\omega' - \omega\|_2^2, \quad \text{s.t. } f(\hat{x}, \omega') \in C \right\}$$

In some cases, solving this projection problem is very easy

- E.g. constraint = non-negative weights ($\omega \geq 0$)
- Projection = clip each individual weight at 0

In more complex situation, we can project using gradient descent

- E.g., lattice models provide support for monotonicity constraints
- These correspond to inequalities over the model parameters
- ...And they are enforced via projection (using gradient descent)

Projected Gradient Method

...But in other cases we still have problems

Let's consider again our example:

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

- The constraint on y is simple
  - ...But not so it's translation on ω
- 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 (and non-convex)
  - Hence, projecting can be an expensive operation

Moving Targets

Moving Targets

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

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

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

- Where $\hat{y}$ is the target (or label) vector

MT makes projection scalable by working in output space

The method alternates between learner and master steps

- At evey 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:

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

- Which is obtained from the Taylor expansion by adding an α parameter

Moving Targets

Let's look closer at the master step problem

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

- By changing α, 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

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

- ...Can be thought 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 ω

But 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:

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

...Which is a traditional supervised learning problem

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

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

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:

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

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

Moving Targets

The overall method is as follows:

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

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

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:

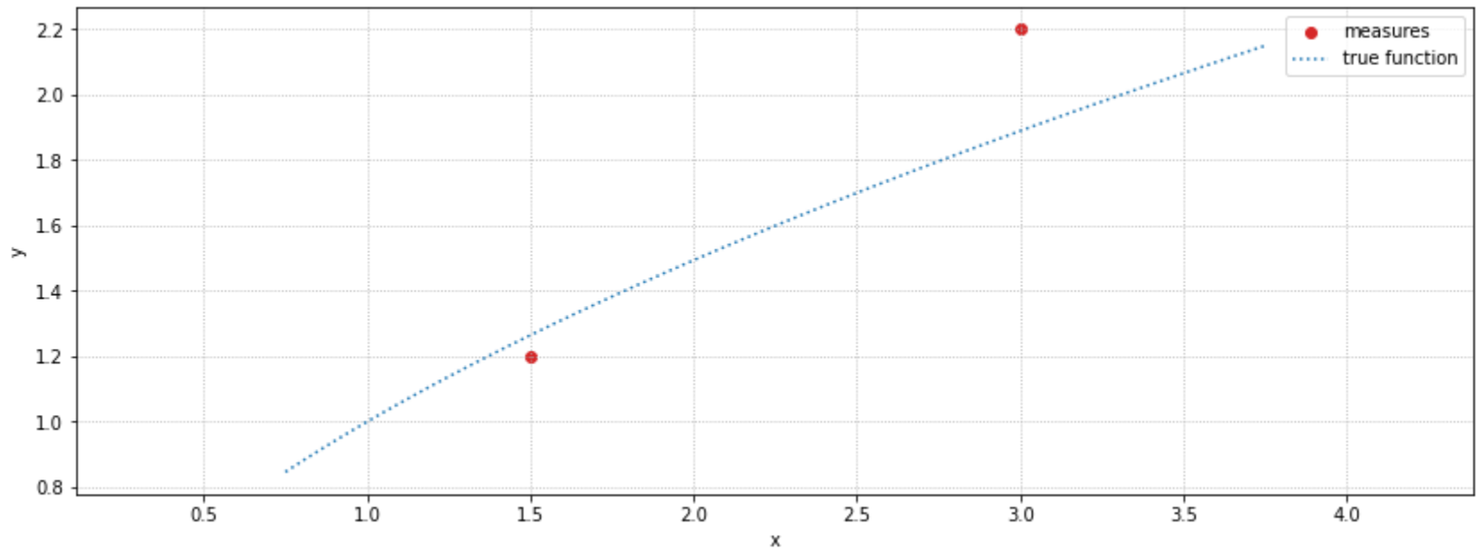
In [2]:
```
xm = np.array([1.5, 3])
ym = np.array([1.2, 2.2])

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



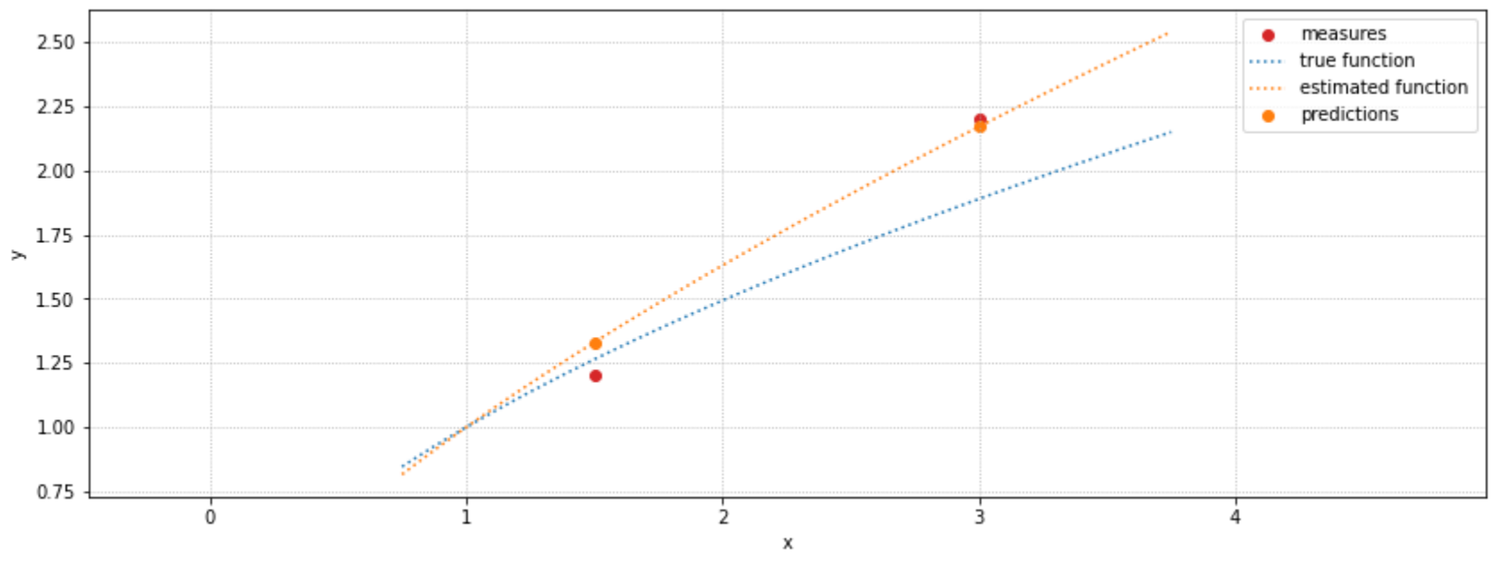
- We are underestimating the first point and overestimatng the second
- ...Which may easily trick our simple model

Learner Step

We can now perform the first learner step

For this example, we can use any curve fitting method

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



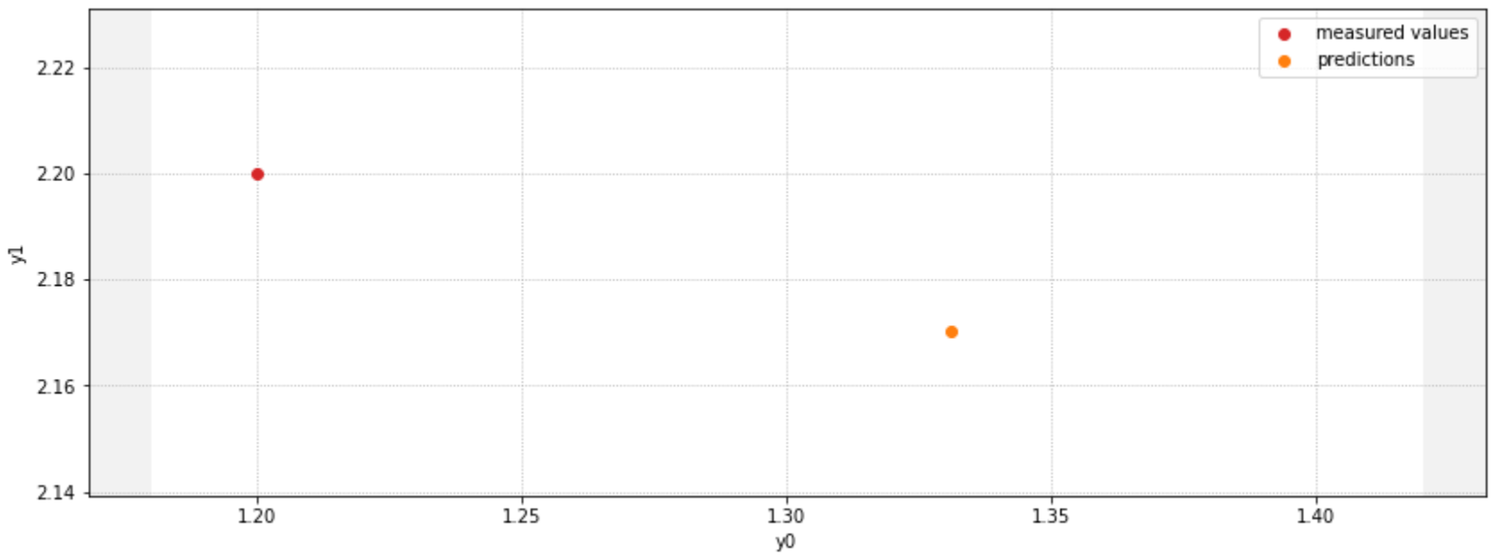
- The learner model indeed overestimates the curve slope
- More data could fix the issue, but we will rely instead on constraints

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)
```

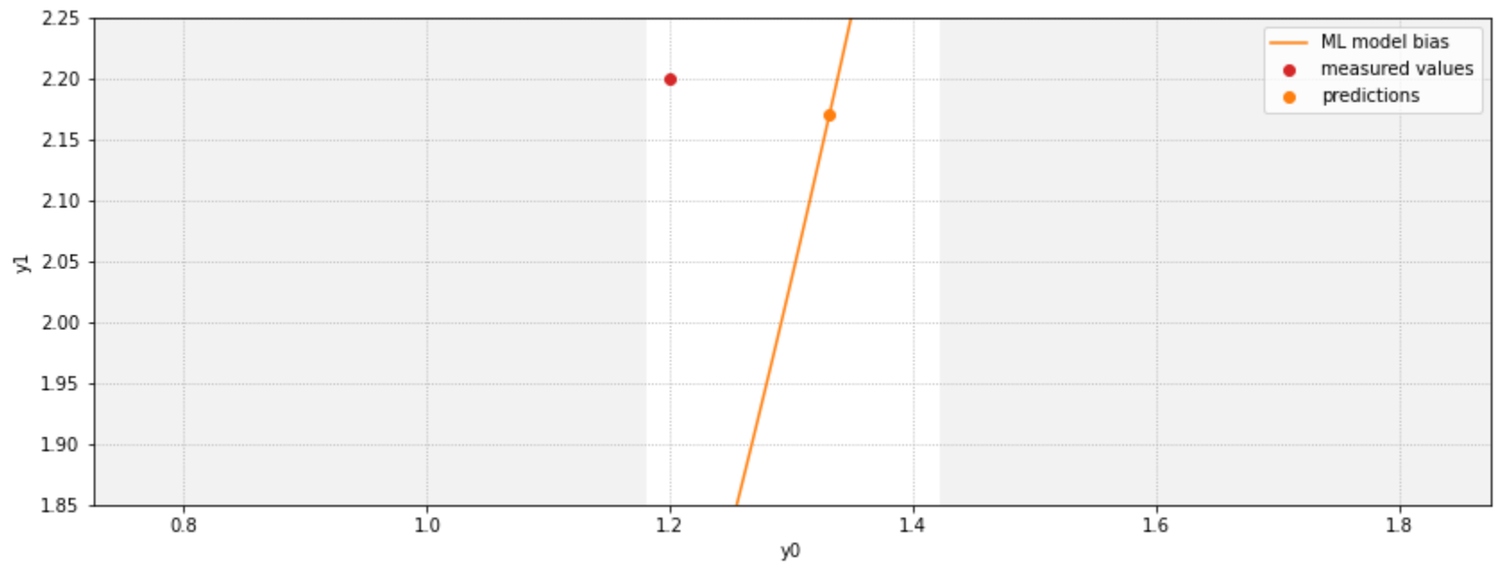


Visualizing Model Bias

By changing the 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 [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 $\boldsymbol{B}$ of our ML model

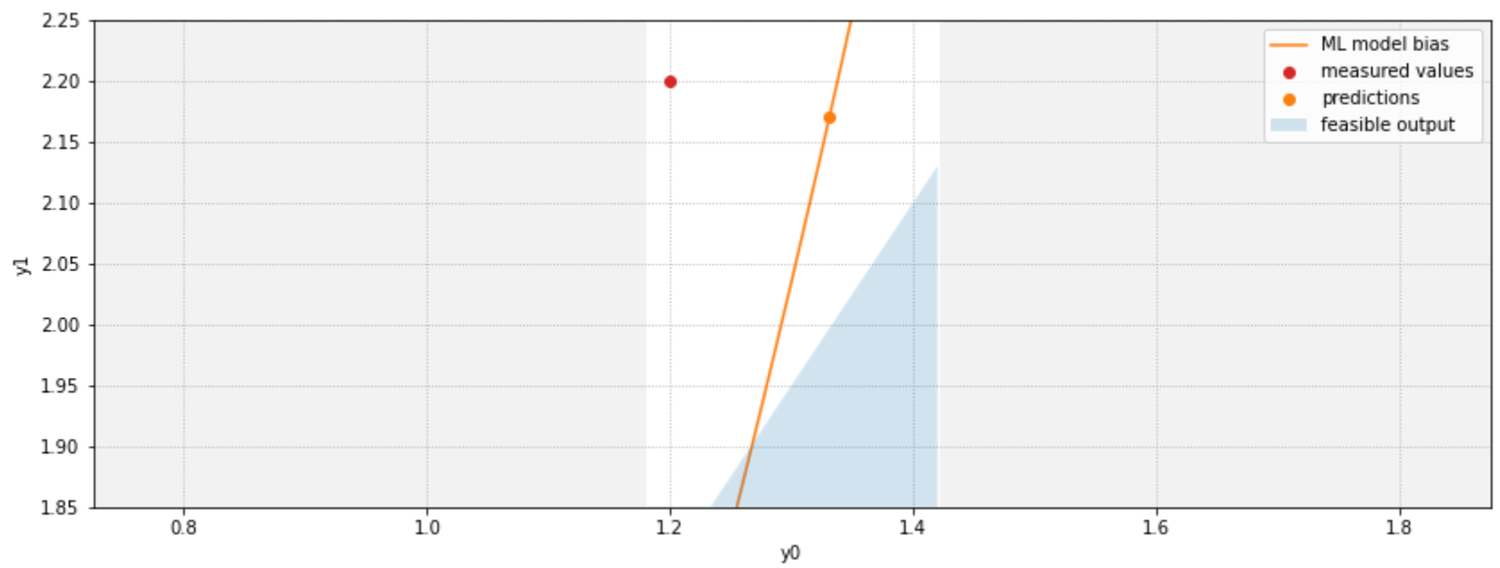
Taking Advantage of Constraints

Say we know that our two measurements must obey

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

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

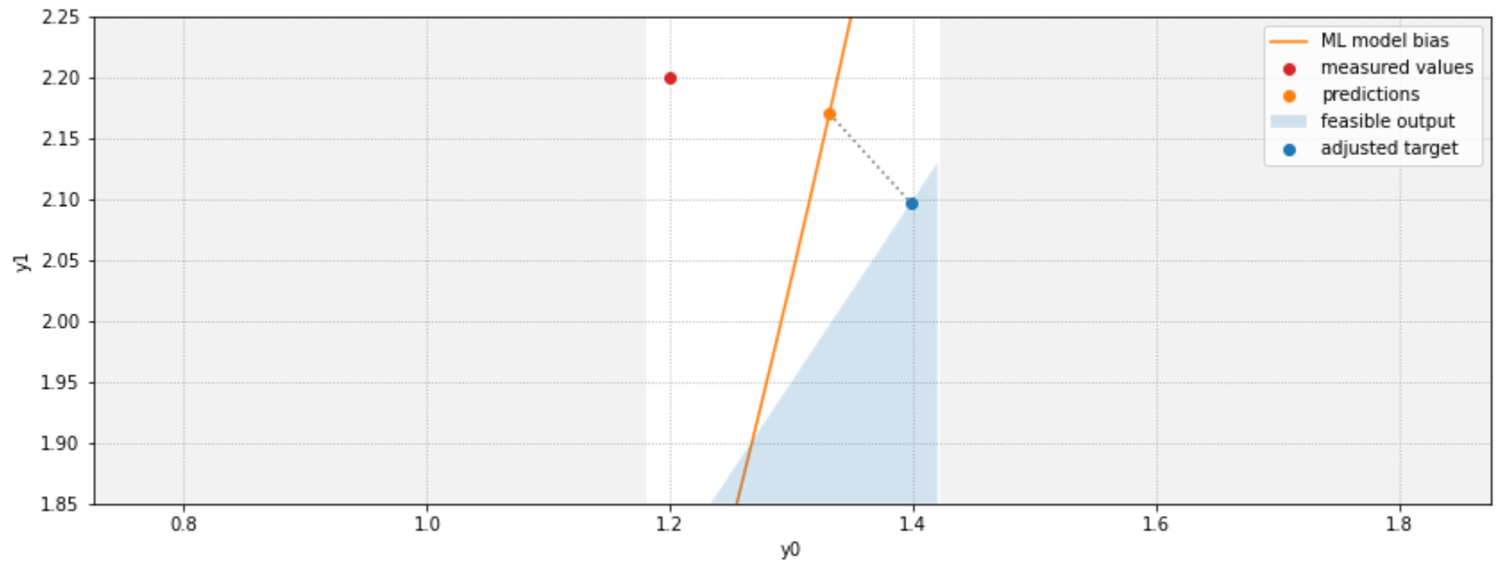
In [8]:
```
f_bound = lambda y0: 1.5*y0
util.mtx_output_plot(xm, ym, yp, plot_bias=True, f_bound=f_bound, figsize=figsize, ylim=(1.85, 2
```



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=
```

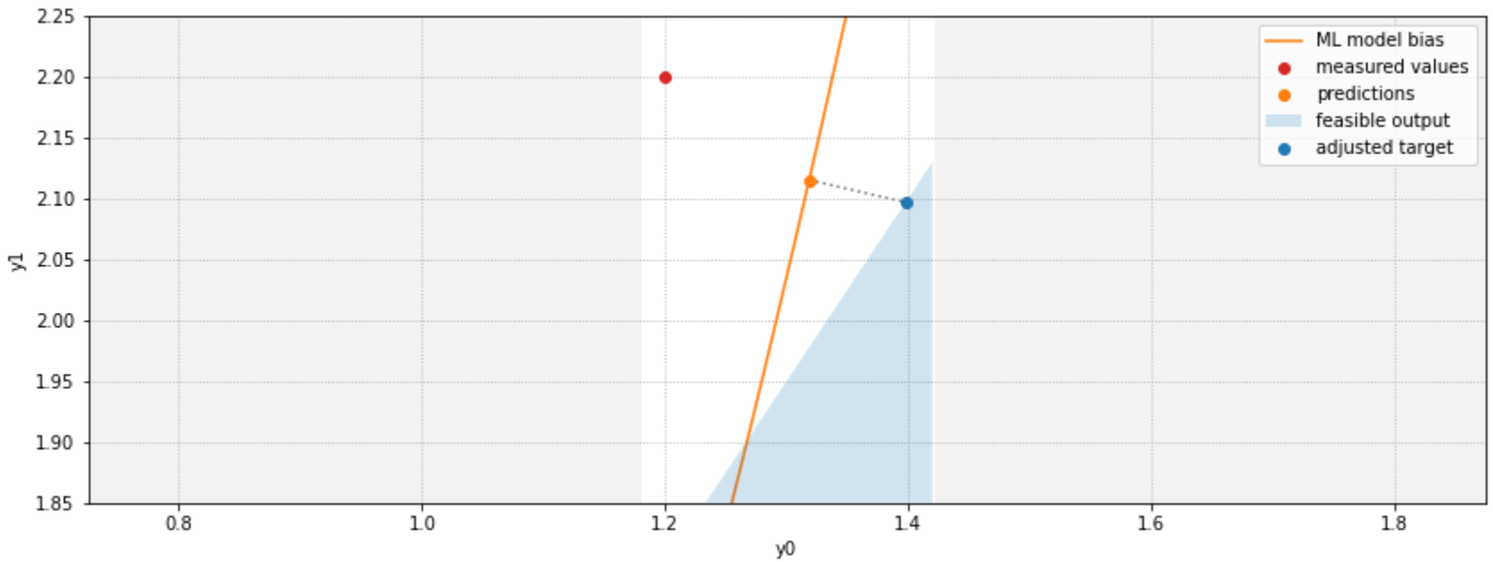


- The result is similar to a projection
- ...Except that it is a bit closer to the true target

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=
```

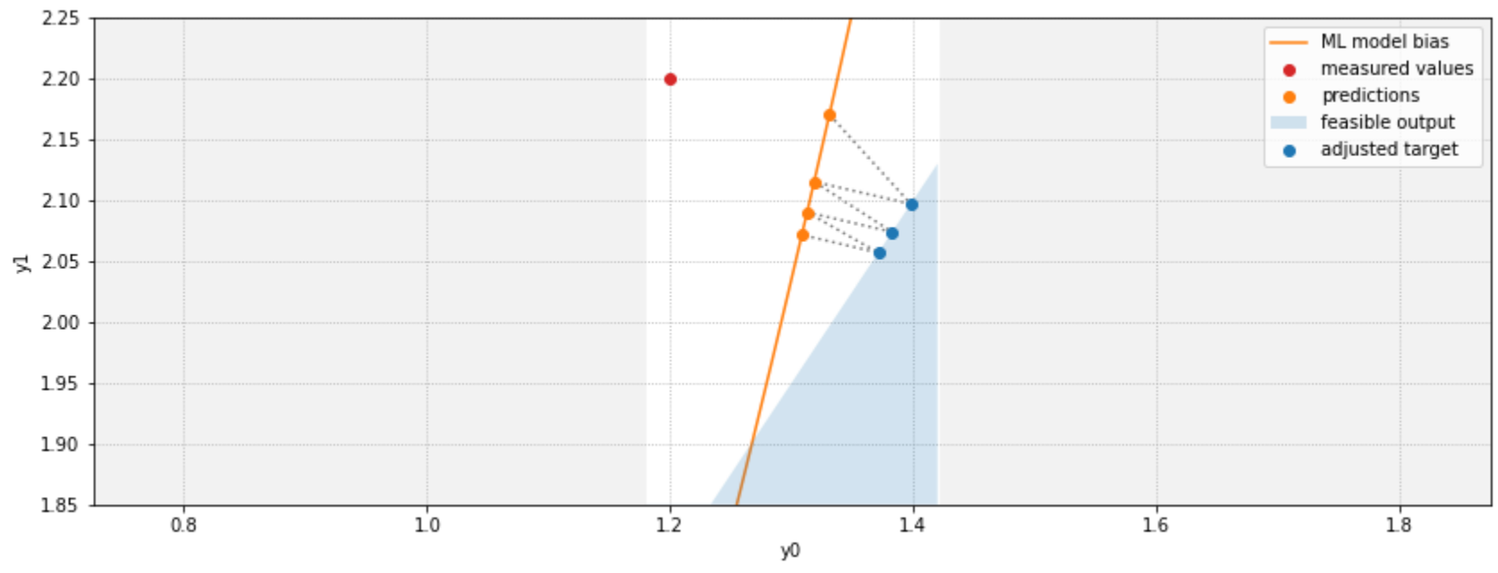


- This one is an actual projection on the model bias $\boldsymbol{B}$

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, ylir
```

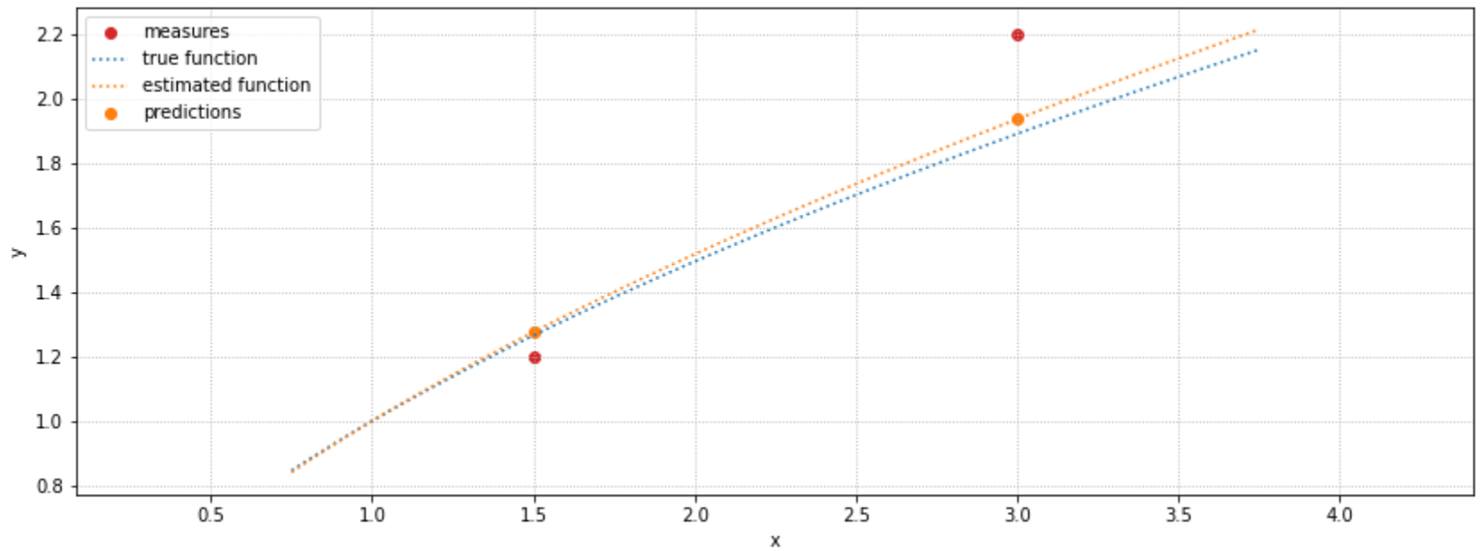


- Basically, MT zig-zags between the $\boldsymbol{B}$ and the $\boldsymbol{C}$ set
- This is not ideal, but it's the price we pay to enjoy a full decomposition

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!