Constrained ML via Lagrangians

Fairness as a Constraint

Let's recap our goals:

We want to train an accurate regressor ($L = \text{MSE}$):

$$\text{argmin}_\theta \, \mathbb{E}_{x,y \sim P(X,Y)} \left[L(y, f(x, \theta)) \right]$$

We want to measure fairness via the DIDI:

$$\text{DIDI}(y) = \sum_{j \in J_p} \sum_{v \in D_j} \left| \frac{1}{m} \sum_{i=1}^{m} y_i - \frac{1}{|I_{j,v}|} \sum_{i \in I_{j,v}} y_i \right|$$

...And we want the DIDI to be low, e.g.:

$$\text{DIDI}(y) \leq \varepsilon$$

Fairness as a Constraint

We can use this information to re-state the training problem

$$\text{argmin}_\theta \{\mathbb{E}\left[L(y, f(x, \theta))\right] \mid \text{DIDI}(f(x, \theta)) \leq \varepsilon\}$$

- Training is now a constrained optimization problem
- We require the DIDI for ML output to be within acceptable levels

After training, the constraint will be distilled in the model parameters

We are requiring constraint satisfaction on the training set

...Meaning that we'll have no satisfaction guarantee on unseen examples

- This is suboptimal, but doing better is very difficult
- ...Since our constraint is defined (conceptually) on the whole distribution

We'll trust the model to generalize well enough

How to account for the constraint at training time?

How to account for the constraint at training time?

There's more then one method: we'll see the most famous one in ML

Constrained Machine Learning

Let's consider a ML problem with constrained output

In particular, let's focus on problems in the form:

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

Where:

- L is the loss (the notation omits ground truth label for sake of simplicity)
- x is the training input
- $\hat{y}$ is the ML model output, i.e. $f(x, \theta)$
- θ is the parameter vector (we assume a parameterized model)
- g is a constraint function

Constrained Machine Learning

Example 1: logical rules

E.g. hiearchies in multi-class classification ("A dog is also an animal"):

$$\hat{y}_{i,dog} \leq \hat{y}_{i,animal}$$

- This constraint is defined over individual examples

Example 2: shape constraints

E.g. input x_j cannot cause the output to decrease (monotonicity)

$$\hat{y}_i \leq \hat{y}_k \quad \forall i, k : x_{i,j} \leq x_{k,j} \wedge x_{i,h} = x_{k,h} \forall h \neq j$$

- This is a relational constraint, i.e. defined over multiple examples

Lagrangian Methods for Constrained ML

One way to deal with this problem is to rely on a Lagrangian Relaxation

Main idea: we turn the constraints into penalty terms:

- From the original constrained problem:

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

- We obtain the following unconstrained problem:

$$\text{argmin}_\theta L(\hat{y}) + \lambda^T \max(0, g(\hat{y})) \qquad \text{with: } \hat{y} = f(x, \theta)$$

- The new loss function is known as a Lagrangian (in penalty form)
- $\max(0, g(\hat{y}))$ is sometimes known as penalizer (or Lagrangian term)
- ...And the λ is a vector of multipliers

Lagrangian Methods for Constrained ML

Let's consider again the modified problem:

$$\text{argmin}_\theta L(\hat{y}) + \lambda^T \max(0, g(\hat{y})) \qquad \text{with: } \hat{y} = f(x, \omega)$$

- When the constraint is satisfied ($g(\hat{y}) \leq 0$), the penalizer is 0
- When the constraint is violated ($g(\hat{y}) \leq 0$), the penalizer is > 0
- Hence, in the feasible area, we still have the original loss
- ...In the infeasible area, we incur a penalty that can be controlled using λ

Therefore:

- If we choose λ large enough, under quite general conditions
- ...We can guarantee that a feasible or asymptotically feasible solution is found

This is the basis of the classical penalty method

Lagrangian Methods for Constrained ML

Some comments

Lagrangian approches are a classic in numeric optimization

- But their use in ML is much more recent
- One of the first instances is in the Semantic Based Regularization (SBR) paper

The constraints can depend on the sample input

- E.g. we use the protected attribute to define the fairness constraint
- They still count as out constraint, since the input is a-priori known

Constraint satisfaction can be framed in probabilistic terms

- This is one of the key ideas in most neuro-symbolic approaches
- The SBR paper is a good reference; also check Neural Markov Logic Networks

Lagrangian Methods for Constrained ML

Other comments:

For some specific cases, the $\max(\cdot)$ operator is not necessary

- The Lagrangian term is instead just $\lambda^T g(\hat{y})$
- When this is true, we say that strong duality holds
- When use use non-linear model, strong duality typically does not hold

Equality constraints (i.e. $g(\hat{y}) = 0$) can be modeled using two inequalities

- The two resulting penalizers can be simplified as $\lambda^T |g(\hat{y})|$
- Using a quadratic term, i.e. $g(\hat{y})^2$ is also possible
- The latter approach is common in augmented Lagrangian methods

Lagrangian Methods for Constrained ML

Yet more comments:

The feasibility guarantees have some caveats:

- In particular they assume that a feasible solution exists
- ...And that the problem is solved to optimality
- ...Which we will not do! So, some violation is possible

Beware of differentiability!

- The approach we discuss does not require it
- ...But our implementation will, since we'll be using SGD

A Practical Example

Back to Our Fairness Constraint

Ideally, we wish to train an ML model by solving

$$\text{argmin}_\theta \{\mathbb{E}\left[L(y, f(x, \theta))\right] \mid \text{DIDI}(f(x, \theta)) \leq \varepsilon\}$$

First, we obtain a Lagrangian term for our constraint:

$$\lambda \max\left(0, \text{DIDI}(f(x, \theta)) - \varepsilon\right)$$

- We just have one constraint, so λ is a scalar
- The threshold (i.e. ε) has been incorporated in the term
- The DIDI formula is differentiable, so we can use a NN for f
- ...Otherwise, we would have needed to use a differentiable approximation

Back to Our Fairness Constraint

With the Lagrangian term, we can modify the loss function:

$$\text{argmin}_\theta \, \mathbb{E}\left[L(y, f(x, \theta)) + \lambda \max\left(0, \text{DIDI}(f(x, \theta)) - \varepsilon\right)\right]$$

- So, in principle we can implement the approach with a custom loss function
- In practice, things are trickier due to how the DIDI works:

$$\text{DIDI}(y) = \sum_{j \in J_p} \sum_{v \in D_j} \left| \frac{1}{m} \sum_{i=1}^{m} y_i - \frac{1}{|I_{j,v}|} \sum_{i \in I_{j,v}} y_i \right|$$

- The computation requires information about the protected attribute
- ...Which is not part of the ground truth (at least not by default)

This makes things more complicated...

Fairness as a Semantic Regularizer

...To the point that is easier to use a custom Keras model

```
class CstDIDIRegressor(keras.Model):
    def __init__(self, base_pred, attributes, protected, alpha, thr): ...

    def call(self, data): ...

    def train_step(self, data): ...

    @property
    def metrics(self): ...
```

- In the `__init__` method we pass all the additional information we need
- The `call` method is called when evaluating the model
- The `train_step` method is called by Keras while training

The full code can be found in the support module

Fairness as a Semantic Regularizer

Let's have a deeper look at a few methods

```python
def __init__(self, base_pred, attributes, protected, alpha, thr):
    super(CstDIDIModel, self).__init__()
    self.base_pred = base_pred # Wrapped predictor
    self.alpha = alpha # This is the penalizer weight (i.e. lambda)
    self.thr = thr # This is the DIDI threshold (i.e. epsilon)
    self.protected = {list(attributes).index(k): dom for k, dom in protected.items()}
    ...

def call(self, data):
    return self.base_pred(data)
```

Our custom model is a wrapper (in software engineering terms)

- There's a second predictor stored as object field
- ...Which we call whenever we need to perform estimates
- Therefore, we can add our DIDI constraint on top of any NN model

Fairness as a Semantic Regularizer

The main logic is in the `train_step` method:

```
def train_step(self, data):
    x, y_true = data # unpack the input
    with tf.GradientTape() as tape: # loss computation
        ...
        loss = mse + self.alpha * cst

    grads = tape.gradient(loss, self.trainable_variables) # gradient computation
    self.optimizer.apply_gradients(zip(grads, tr_vars)) # update NN weights
    ...
```

- We compute the loss inside a `GradientTape` object
- This is used by TensorFlow to track tensor operations
- ...So that they can be differentiated using the `gradient` method
- We handle weight update using the usual optimizer

Fairness as a Semantic Regularizer

The main logic is in the `train_step` method:

```
def train_step(self, data):
    ...
    with tf.GradientTape() as tape:
        y_pred = self.base_pred(x, training=True) # obtain predictions
        mse = self.compiled_loss(y_true, y_pred) # compute base loss
        ymean = tf.math.reduce_mean(y_pred) # here we start computing the DIDI
        didi = 0
        for aidx, dom in self.protected.items():
            for val in dom:
                mask = (x[:, aidx] == val)
                didi += tf.math.abs(ymean - tf.math.reduce_mean(y_pred[mask]))
        cst = tf.math.maximum(0.0, didi - self.thr)
        loss = mse + self.alpha * cst
    ...
```

We use tensor operations for the DIDI (so its gradient can be computed by TF)

Building the Constrained Model

We start by building (and wrapping) our predictor

In [3]:
```
protected = {'race': (0, 1)}
didi_thr = 1.0
base_pred = util.build_nn_model(input_shape=len(attributes), output_shape=1, hidden=[])
nn = util.CstDIDIModel(base_pred, attributes, protected, alpha=5, thr=didi_thr)
```

Without a clear clue for choosing the Lagrangian multipliers

...We picked 5 as a guess

- Choosing a good weight is obviously an important issue
- We'll how to deal with that later

We will try to roughly halve the "natural" DIDI of the model

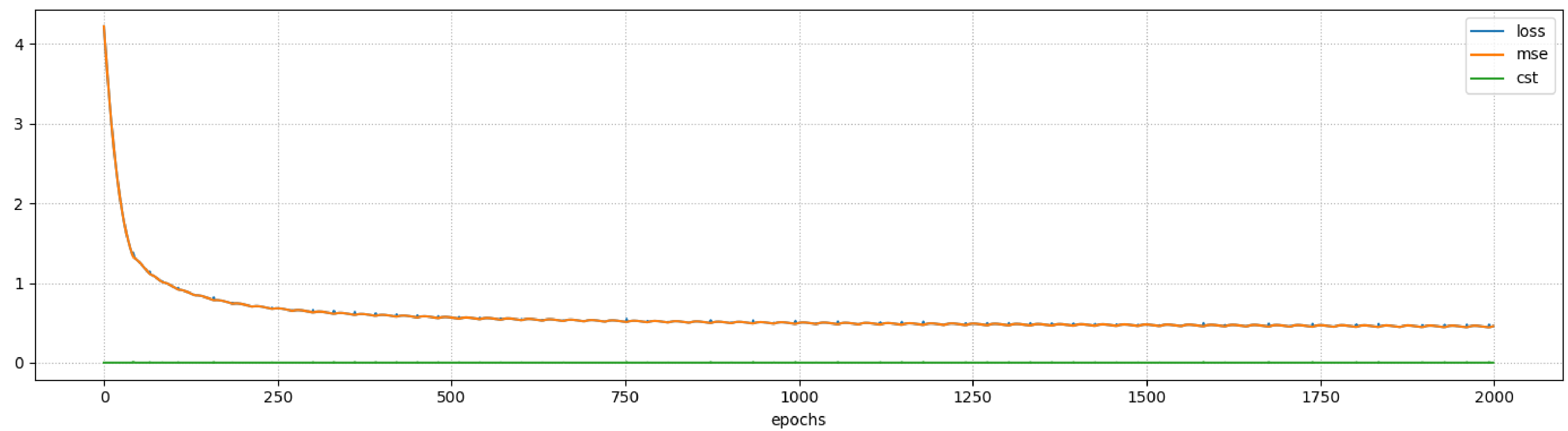
- Since for our baseline we have $\mathrm{DIDI}(y) \simeq 2$
- ...Then we picked $\varepsilon = 1$

Training the Constrained Model

We can train the constrained model as usual

- Since the constraint is for all the population, we have `batch_size=len(tr)`
- We could use mini-batches, but that would result in some noise

In [4]:
```
base_pred = util.build_nn_model(input_shape=len(attributes), output_shape=1, hidden=[])
nn = util.CstDIDIModel(base_pred, attributes, protected, alpha=5, thr=didi_thr)
history = util.train_nn_model(nn, tr[attributes], tr[target], loss='mse', validation_split=0
util.plot_training_history(history, figsize=figsize)
```




```
Final loss: 0.4592 (training)
```

Constrained Model Evaluation

Let's check both the prediction quality and the DIDI

In [5]:
```python
tr_pred = nn.predict(tr[attributes], verbose=0)
r2_tr = r2_score(tr[target], tr_pred)
ts_pred = nn.predict(ts[attributes], verbose=0)
r2_ts = r2_score(ts[target], ts_pred)
tr_DIDI = util.DIDI_r(tr, tr_pred, protected)
ts_DIDI = util.DIDI_r(ts, ts_pred, protected)

print(f'R2 score: {r2_tr:.2f} (training), {r2_ts:.2f} (test)')
print(f'DIDI: {tr_DIDI:.2f} (training), {ts_DIDI:.2f} (test)')
```

```
R2 score: 0.54 (training), 0.45 (test)
DIDI: 0.89 (training), 0.94 (test)
```

Constrained Model Evaluation

Let's check both the prediction quality and the DIDI

```
In [5]: tr_pred = nn.predict(tr[attributes], verbose=0)
        r2_tr = r2_score(tr[target], tr_pred)
        ts_pred = nn.predict(ts[attributes], verbose=0)
        r2_ts = r2_score(ts[target], ts_pred)
        tr_DIDI = util.DIDI_r(tr, tr_pred, protected)
        ts_DIDI = util.DIDI_r(ts, ts_pred, protected)

        print(f'R2 score: {r2_tr:.2f} (training), {r2_ts:.2f} (test)')
        print(f'DIDI: {tr_DIDI:.2f} (training), {ts_DIDI:.2f} (test)')
```

```
R2 score: 0.54 (training), 0.45 (test)
DIDI: 0.89 (training), 0.94 (test)
```

The constraint is satisfied (and the accuracy reduced, as expected)

...But why is there some slack in terms of constraint satisfaction?

- If λ were too small, we should have an infeasibility
- Otherwise, we should have optimal accuracy. Is this what is happening?

Lagrangian Dual Framework

Choosing Multiplier Values

We are currently solving this problem

$$\text{argmin}_\theta\, \mathbb{E}\left[L(y, \hat{y}) + \lambda \max\left(0, g(\hat{y})\right)\right] \qquad \text{with: } \hat{y} = f(x, \theta)$$

...By using (Stochastic) Gradient Descent

This is an important detail

- A large λ may be fine theoretically
- ...But it may cause the gradient to be unstable

Therefore:

- With a convex model, we should still reach convergence, but slowly
- With a non-convex model, we may end up in a poor local optimum

How can we deal with this?

Penalty Method

We can think of increasing λ gradually

...Which leads to the classical penalty method

- $\lambda^{(0)} = 1$
- $\theta^{(0)} = \text{argmin}_\theta \left\{ L(y, \hat{y}) + \lambda^{(0)T} \max(0, g(\hat{y})) \right\}$ with: $\hat{y} = f(x, \theta)$
- For $k = 1..n$
  - If $g(y) \leq 0$, stop
  - Otherwise $\lambda^{(k)} = r\lambda^{(k)}$, with $r \in (1, \infty)$
  - $\theta^{(k)} = \text{argmin}_\theta \left\{ L(y, \hat{y}) + \lambda^{(k)T} \max(0, g(\hat{y})) \right\}$ with: $\hat{y} = f(x, \theta)$

This can work, but there are a few issues

- λ grows quickly and may still become problematically large
- Early and late stages in SGD may call for different values of λ

Gradient Ascent to Control the Multipliers

A gentler approach consists in using gradient ascent for the multipliers

Let's consider our modified loss:

$$\mathcal{L}(\theta, \lambda) = L(y, f(x, \theta)) + \lambda^T \max(0, g(f(x, \theta)))$$

- This is actually differentiable in λ

The gradient is also a very simple expression:

$$\nabla_\lambda \mathcal{L}(\theta, \lambda) = \max(0, g(f(x, \theta)))$$

- For satisfied constraints, the partial derivative is 0
- For violated constraints, it is equal to the violation

Lagrangian Dual Approach

Therefore, we can solve our constrained ML problem

...By alternating gradient descent and ascent:

- $\lambda^{(0)} = 0$
- For $k = 1..n$ (or until convergence):
  - Obtain $\lambda^{(k)}$ via an ascent step with $\nabla_\lambda \mathcal{L}(\lambda, \theta^{(k-1)})$
  - Obtain $\theta^{(k)}$ via a descent step with $\nabla_\theta \mathcal{L}(\lambda^{(k)}, \theta)$

Technically, we are working with sub-gradients here

- When we optimize λ (outer optimization loop), we keep θ fixed
- ...Meaning we are going to under-estimate the gradient

Still, this is often good enough!

Lagrangian Dual Approach

Therefore, we can solve our constrained ML problem

...By alternating gradient descent and ascent:

- $\lambda^{(0)} = 0$
- $\theta^{(0)} = \text{argmin}_\theta \mathcal{L}(\lambda^{(0)}, \theta)$
- For $k = 1..n$ (or until convergence):
  - Obtain $\lambda^{(k)}$ via an ascent step with $\nabla_\lambda \mathcal{L}(\lambda, \theta^{(k-1)})$
  - Obtain $\theta^{(k)}$ via a descent step with $\nabla_\theta \mathcal{L}(\lambda^{(k)}, \theta)$

We might still reach impractical values for λ

...But the gentle updates will keep the gradient more stable

- At the beginning, SGD will be free to prioritize accuracy
- After some iterations, both θ and λ will be nearly (locally) optimal

Implementing the Lagrangian Dual Approach

We will implement the Lagrangian dual approach via another custom model

```
class LagDualDIDIRegressor(MLPRegressor):
    def __init__(self, base_pred, attributes, protected, thr):
        super(LagDualDIDIRegressor, self).__init__()
        self.alpha = tf.Variable(0., name='alpha')
        ...

    def __custom_loss(self, x, y_true, sign=1): ...

    def train_step(self, data): ...

    def metrics(self): ...
```

- We no longer pass a fixed `alpha` weight/multiplier
- Instead we use a trainable variable

Implementing the Lagrangian Dual Approach

We move the loss function computation in a dedicated method (`__custom_loss`)

```
def __custom_loss(self, x, y_true, sign=1):
    y_pred = self.base_pred(x, training=True) # obtain the predictions
    mse = self.compiled_loss(y_true, y_pred) # main loss
    ymean = tf.math.reduce_mean(y_pred) # average prediction
    didi = 0 # DIDI computation
    for aidx, dom in self.protected.items():
        for val in dom:
            mask = (x[:, aidx] == val)
            didi += tf.math.abs(ymean - tf.math.reduce_mean(y_pred[mask]))
    cst = tf.math.maximum(0.0, didi - self.thr) # regularizer
    loss = mse + self.alpha * cst
    return sign*loss, mse, cst
```

- The code is the same as before
- ...Except that we can flip the loss sign via a function argument (i.e. `sign`)

Implementing the Lagrangian Dual Approach

In the training method, we make two distinct gradient steps:

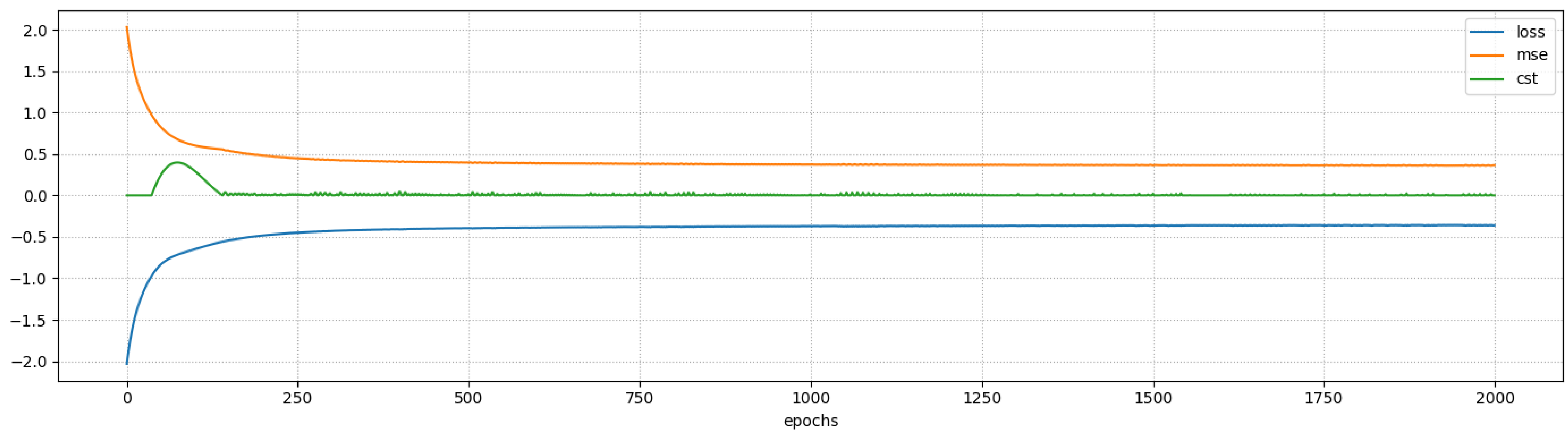
```
def train_step(self, data):
    x, y_true = data
    with tf.GradientTape() as tape: # first loss (minimization)
        loss, mse, cst = self.__custom_loss(x, y_true, sign=1)
    grads = tape.gradient(loss, self.trainable_variables)
    grads[-1] = 0 * grads[-1] # null multiplier gradient
    self.optimizer.apply_gradients(zip(grads, self.trainable_variables))
    with tf.GradientTape() as tape: # second loss (maximization)
        loss, mse, cst = self.__custom_loss(x, y_true, sign=-1)
    grads = tape.gradient(loss, self.trainable_variables)
    for i in range(len(grads)-1): # null weight gradient
        grads[i] = 0 * grads[i]
    self.optimizer.apply_gradients(zip(grads, self.trainable_variables))
    ...
```

- In principle, we could even have used two distinct optimizers

Training the Lagrangian Dual Approach

The new approach leads fewer oscillations at training time

In [34]:
```
base_pred = util.build_nn_model(input_shape=len(attributes), output_shape=1, hidden=[])
nn2 = util.LagDualDIDIModel(base_pred, attributes, protected, thr=didi_thr)
history = util.train_nn_model(nn2, tr[attributes], tr[target], loss='mse', validation_split=
util.plot_training_history(history, figsize=figsize)
```




```
Final loss: -0.3623 (training)
```

Lagrangian Dual Evaluation

Let's check the new results

```
In [33]: tr_pred2 = nn2.predict(tr[attributes], verbose=0)
r2_tr2 = r2_score(tr[target], tr_pred2)
ts_pred2 = nn2.predict(ts[attributes], verbose=0)
r2_ts2 = r2_score(ts[target], ts_pred2)
tr_DIDI2 = util.DIDI_r(tr, tr_pred2, protected)
ts_DIDI2 = util.DIDI_r(ts, ts_pred2, protected)

print(f'R2 score: {r2_tr2:.2f} (training), {r2_ts2:.2f} (test)')
print(f'DIDI: {tr_DIDI2:.2f} (training), {ts_DIDI2:.2f} (test)')
```

```
R2 score: 0.64 (training), 0.57 (test)
DIDI: 0.98 (training), 1.12 (test)
```

- The DIDI has the desired value (on the test set, this is only roughly true)
- ...And the prediction quality is much higher than before!

Some Comments

This is not the only approach for constrained ML

- There approaches based on projection, pre-processing, iterative projection...
- ...And in some cases you can enforce constraints through the architecture itself

...But it is simple and flexible

- You just need your constraint to be differentiable
- ...And some good will to tweak the implementation

The approach can be used also for symbolic knowledge injection

- Perhaps domain experts can provide you some intuitive rule of thumbs
- You model those as constraints and take them into account at training time
- Just be careful with the weights, as in this case feasibility is not the goal