Invariant mass evaluation for e^+e^- events

Optimization of a Neural Network regression model

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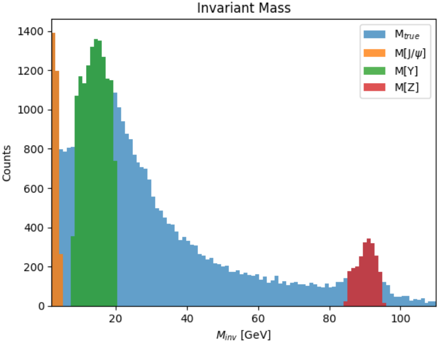
Index

Data and goal

Data used in this work are taken from a selection of *pp* collisions simulated for the LHC experiments resulting in e^+e^- measured in the detector.
The goal of the project is to build a model able to make a prediction of the invariant mass of the couple e^+e^- generated in the range $2 - 110$GeV. This is particularly important to identify hadronic resonances produced in the collisions. Since the final state has no electrical charge and produces 2 leptons ($+$ neutrinos eventually since it is not back-to-back emission) the resonance produced must be a neutral meson or boson.

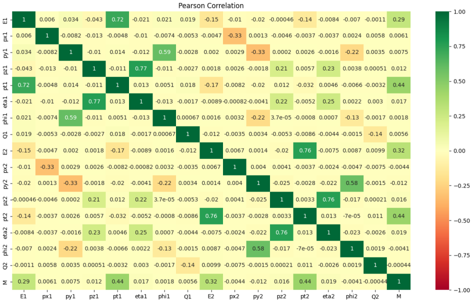


Meson	Theoretical Mass
J/ψ	~ 3 GeV
$\Upsilon(1,2,3S)$	~ 10 GeV
Z	~ 91 GeV

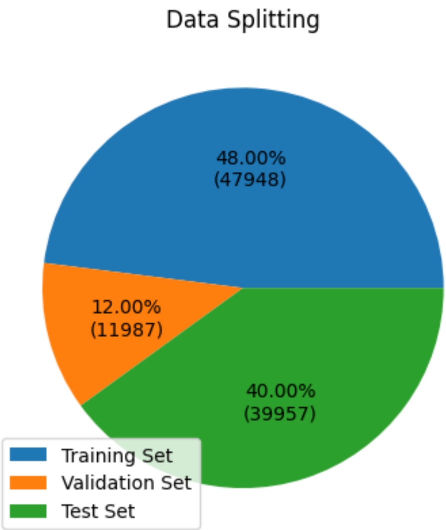
Name	Physical quantity
Run, Event	Event identifiers (not used for model evaluation)
E1, E2	Total energies [GeV]
px1, py1, pz1, px2, py2, pz2	Components of the 4-momenta [GeV]
pt1, pt2	Transverse momenta [GeV]
eta1, eta2	Pseudorapidities
phi1, phi2	Azimuthal angles
Q1, Q2	Charge of the particles (e^+/e^-)
M	Invariant mass [GeV]

No linear correlation between features and target

- $\Rightarrow$ Difficult to solve with analytical techniques
- $\Rightarrow$ Need to develop non-linear models



Dataset - PreProcessing



- *Data cleaning*: delete rows with NaN mass and duplicated events
- *Splitting data*: divide training, validation and test sets
- *Features normalization*: apply MinMaxScaler (range 0-100)

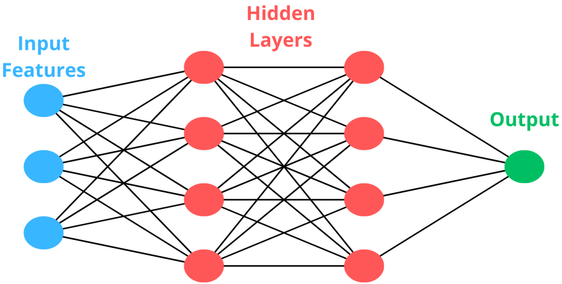
Model Architecture - Shallow Neural Network

Advantages

- General purpose model
- Faster training compared to deep learning models
- Reduce overfitting for simple taget functions

Disadvantages

- Possibly not the most CPU efficient model (e.g. Decision Trees)
- Need to find the correct architecture (layers/nodes)



Model Architecture - Basic Design

Parameter	Choice
Activation	ReLU
Initializer	Glorot-Bengio
Optimizer	AdamW
Loss/Metric	MeanSquaredError
Batch size	32

Glorot-Bengio Initializer

Initial weights are drawn from a uniform normalized distribution to avoid extreme results during parameters training

$$W \sim U\left[-\frac{\sqrt{6}}{\sqrt{n_j + n_{j+1}}}, \frac{\sqrt{6}}{\sqrt{n_j + n_{j+1}}}\right]$$

AdamW implements weight decay for Adam optimizer

$\Rightarrow$ Avoid large weights

$\Rightarrow$ Significant improvements in generalization performance

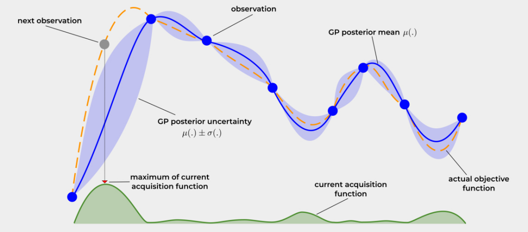
Algorithm 2 Adam with L_2 regularization and Adam with weight decay (AdamW)

given $\alpha = 0.001, \beta_1 = 0.9, \beta_2 = 0.999, \epsilon = 10^{-8}, w \in \mathbb{R}$
initialize time step $t \leftarrow 0$, parameter vector $\boldsymbol{x}_{t=0} \in \mathbb{R}^n$, first moment vector $\boldsymbol{m}_{t=0} \leftarrow \boldsymbol{0}$, second moment vector $\boldsymbol{v}_{t=0} \leftarrow \boldsymbol{0}$, schedule multiplier $\eta_{t=0} \in \mathbb{R}$
repeat
  $t \leftarrow t + 1$
  $\nabla f_t(\boldsymbol{x}_{t-1}) \leftarrow \text{SelectBatch}(\boldsymbol{x}_{t-1})$ ▷ select batch and return the corresponding gradient
  $\boldsymbol{g}_t \leftarrow \nabla f_t(\boldsymbol{x}_{t-1})$ $+w\boldsymbol{x}_{t-1}$
  $\boldsymbol{m}_t \leftarrow \beta_1 \boldsymbol{m}_{t-1} + (1-\beta_1)\boldsymbol{g}_t$ ▷ here and below all operations are element-wise
  $\boldsymbol{v}_t \leftarrow \beta_2 \boldsymbol{v}_{t-1} + (1-\beta_2)\boldsymbol{g}_t^2$
  $\hat{\boldsymbol{m}}_t \leftarrow \boldsymbol{m}_t/(1-\beta_1^t)$ ▷ β_1 is taken to the power of t
  $\hat{\boldsymbol{v}}_t \leftarrow \boldsymbol{v}_t/(1-\beta_2^t)$ ▷ β_2 is taken to the power of t
  $\eta_t \leftarrow \text{SetScheduleMultiplier}(t)$ ▷ can be fixed, decay, or also be used for warm restarts
  $\boldsymbol{x}_t \leftarrow \boldsymbol{x}_{t-1} - \eta_t \left(\alpha \hat{\boldsymbol{m}}_t/(\sqrt{\hat{\boldsymbol{v}}_t} + \epsilon) +w\boldsymbol{x}_{t-1}\right)$
until *stopping criterion is met*
return optimized parameters $\boldsymbol{x}_t$

Model Architecture - Hyperparameters Tuning

Bayesian Optimization

Sequential design strategy for global optimization of black-box functions that does not assume any functional forms



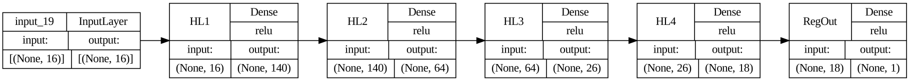
Research algorithm:

1. Define range of parameters $\Rightarrow$ Parameters space is limited
2. Define a surrogate gaussian model for the objective function
3. Pick some random sets of hyperparameters to evaluate the model
4. Update hyperparameters by evaluating the covariance matrix of the model $\Rightarrow$ Balance exploitation and exploration

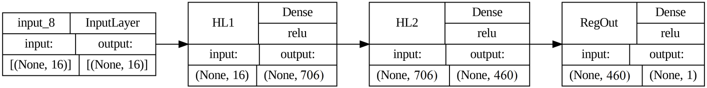
Model Architecture - Hyperparameters Results

HyperPar	Unconstrained Model		Constrained Model	
	Range	Best values	Range	Best values
N Layer	1 - 4	2	2 - 4	4
Node 0	1 - 1000	706	90 - 140	140
Node 1	1 - 1000	460	50 - 80	64
Node 2	1 - 1000	/	20 - 40	26
Node 3	1 - 1000	/	10 - 20	18
LearningRate	10^{-4} - 10^{-3}	$5 \cdot 10^{-4}$	10^{-4} - 10^{-3}	$5 \cdot 10^{-4}$
RMSE [GeV]	0.74 ± 0.09		0.80 ± 0.08	
Exec Time [s]	2700 ± 400		980 ± 300	

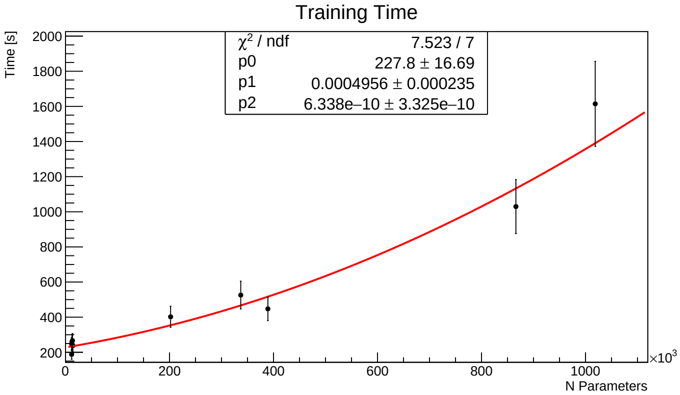
Small Layers Model



Large Layers Model

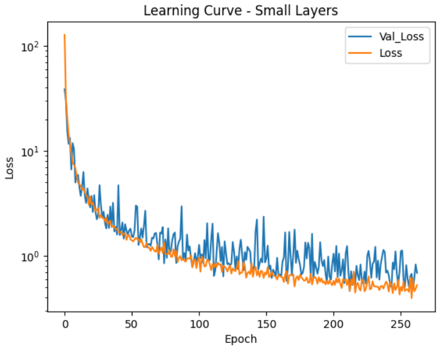


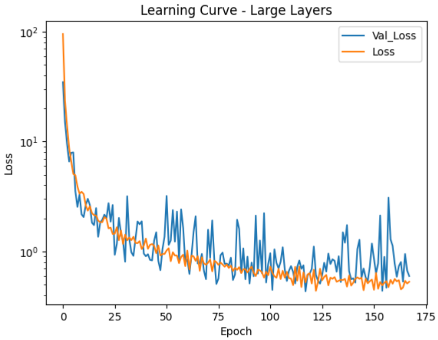
Model Architecture - Training Time scaling



Training time scales as $\mathcal{O}\left(N_{par}^2\right)$ while the performance improvement is small
$\Rightarrow$ Large models are inefficient for linear regression tasks

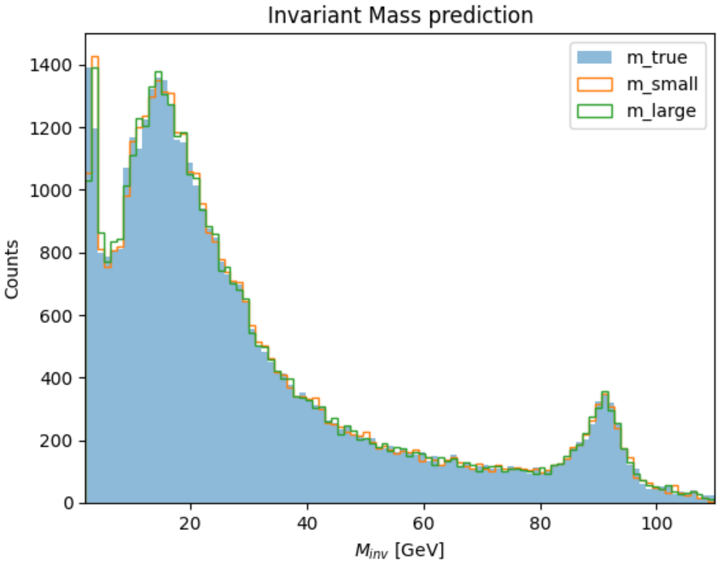
Results - Training





Oscillation in the loss function evaluation is caused by the presence of local minima during the optimisation of the parameters.
EarlyStopping criteria (patience = 50 epochs) were implemented on both `loss` and `val_loss` functions to avoid getting stuck in local minima.

Results - Invariant mass prediction



Conclusions

Achieved goals:

- Testing different models proved that shallow models are more efficient for linear regression tasks thanks to the limited number of free parameters to train
- Hyperparameters tuning resulted in significant improvements for the training of the model (especially for learning rate)
- The achieved error (RMSE $\leq 0.8 GeV$) is coherent with the experimental error usually found for $M_{inv} \gtrsim 10 GeV$ ($\Delta E/E < 10\%$)

Possible improvements:

- Compare other algorithms to improve performance and/or efficiency (e.g. DecisionTrees)
- Try different features (e.g. invariants)
- Dataset with experimental error on the features may result in better performance

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