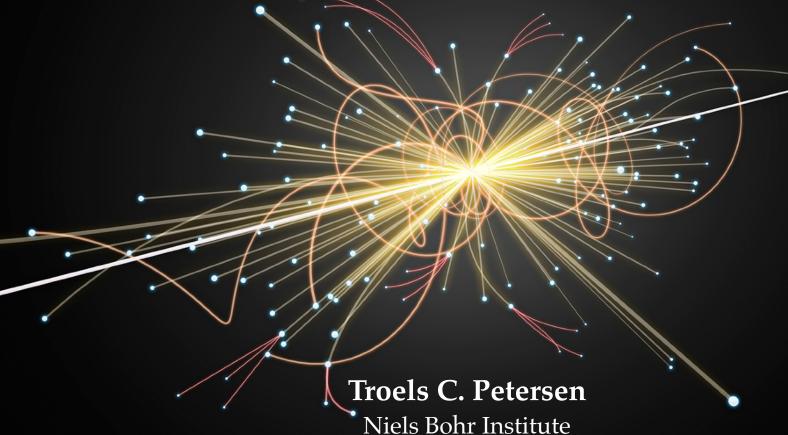


# 

# Past experiences





# On experience

#### Sentence:

"Experience is simply the name we give our mistakes", [Oscar Wilde]

#### Lemma:

"I didn't fail. It was a learning experience",

[Anonymous]

#### First encounters

On a dark and stormy night in 2001, PostDoc Andreas Hoecker called me into his office: "Troels, come and see this..."

It was a piece of Fortran code, that he had gotten in an Email:

It was a Neural Network!

For context, I was working on the BaBar experiment at SLAC, focusing on B to DKpi decays:

```
\begin{array}{c}
V_{us} \\
\overline{d} \\
\overline{d} \\
\overline{d} \\
\pi^{+} \\
u \\
D^{-}
\end{array}
```

```
PROGRAM TPK
! The TPK Algorithm
! Fortran 90 style
 IMPLICIT NONE
 INTEGER
 REAL
                           :: Y
 REAL, DIMENSION (0:10)
 READ (*,*) A
 DO I = 10, 0, -1
                           ! Backwards
   Y = FUN(A(I))
   IF ( Y < 400.0 ) THEN
     WRITE(*,*) I, ' Too large'
   END IF
 END DO
                            ! Local function
 CONTAINS
   FUNCTION FUN(T)
     REAL, INTENT(IN) :: T
      FUN = SQRT(ABS(T)) + 5.0*T**3
 END PROGRAM TPK
```

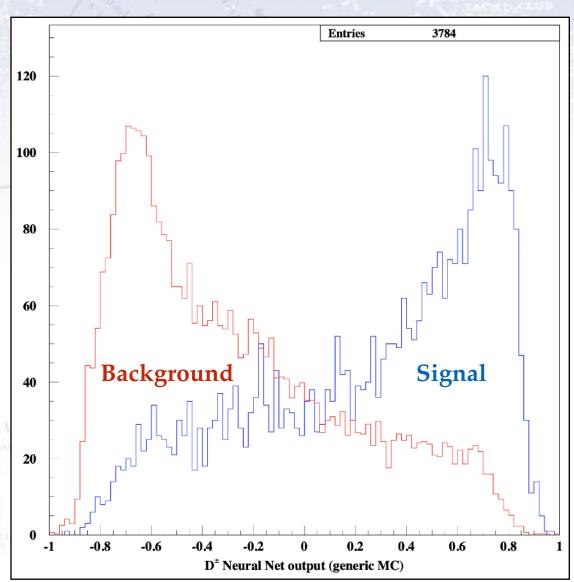
#### First encounters

Not having any experience with ML, I did a lot of mistakes:

- No description of architecture!
- No HP optimisation.
- No check of data-MC correspondence.
- No loss / epoch plot.

I had not thought of any way to cross check and calibrate the output.

But... simply throwing myself at it was a great experience to build on.



# Higgs Search/Discovery

#### Motivation

#### Problem:

Given a number of clean ZZ events, determine if they are Higgs or SM diboson events!

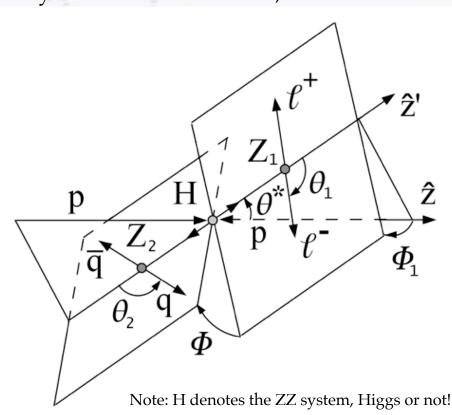
#### Possible solution:

Since Higgses are produced quite differently then SM diboson ZZ, their angular distributions differ!

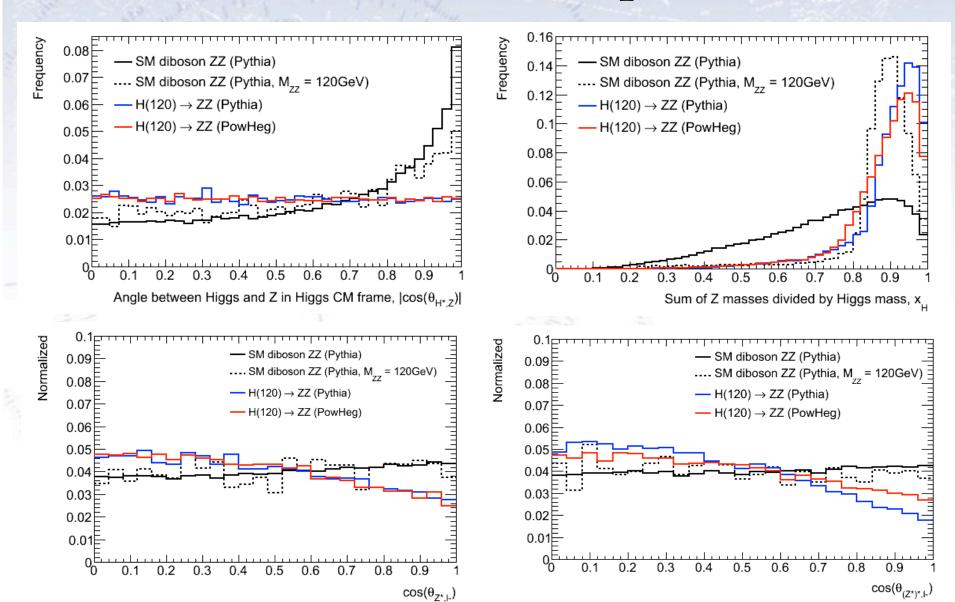


#### Variables available/used:

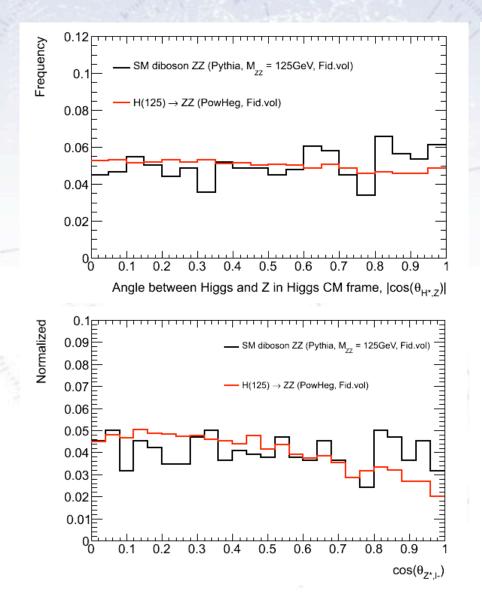
- Higgs rapidity
- Angle Z to Higgs in Higgs CM
- Angle lep- to Z in Z CM
- Angle lep- to Z\* in Z\* CM
- Fraction of mZ+mZ\* to mHiggs

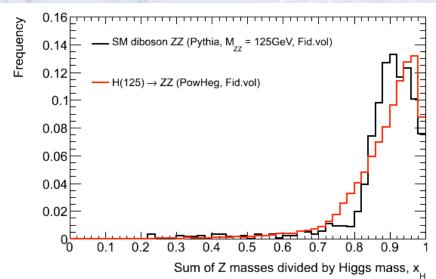


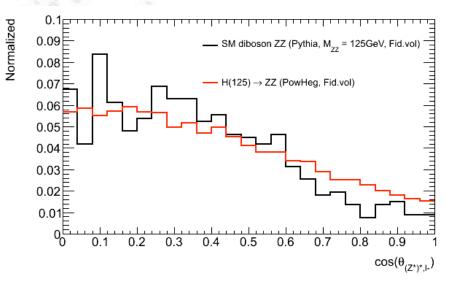
#### Generator level comparison



# After fiducial requirements

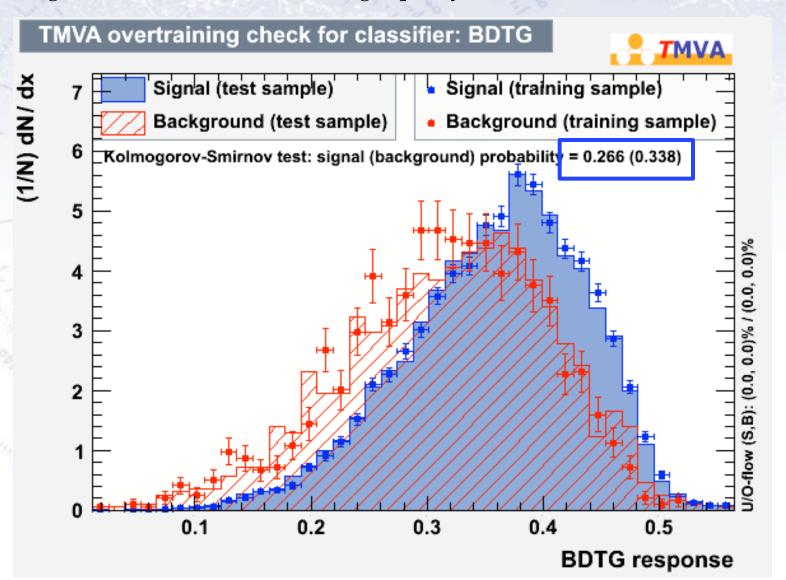




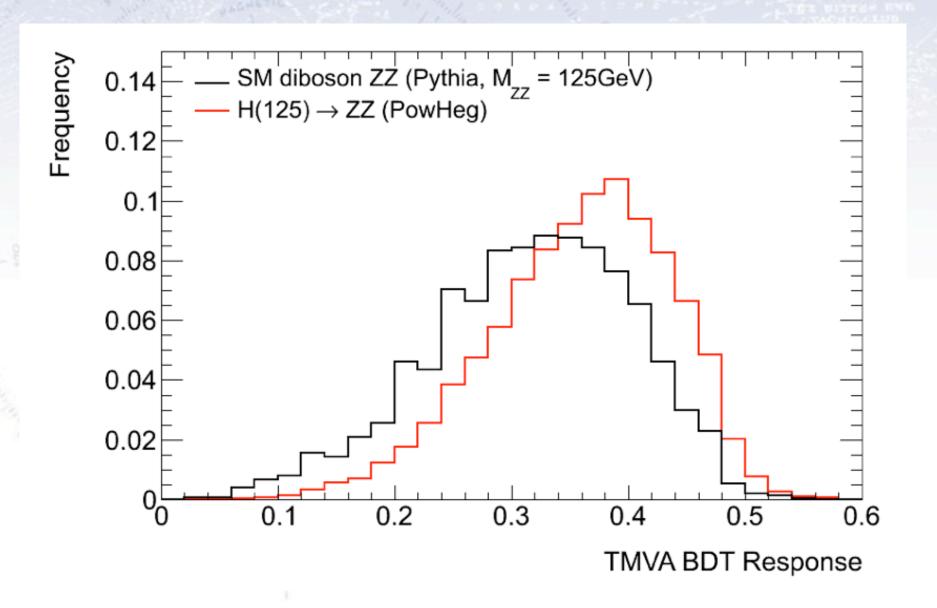


# Combining variables

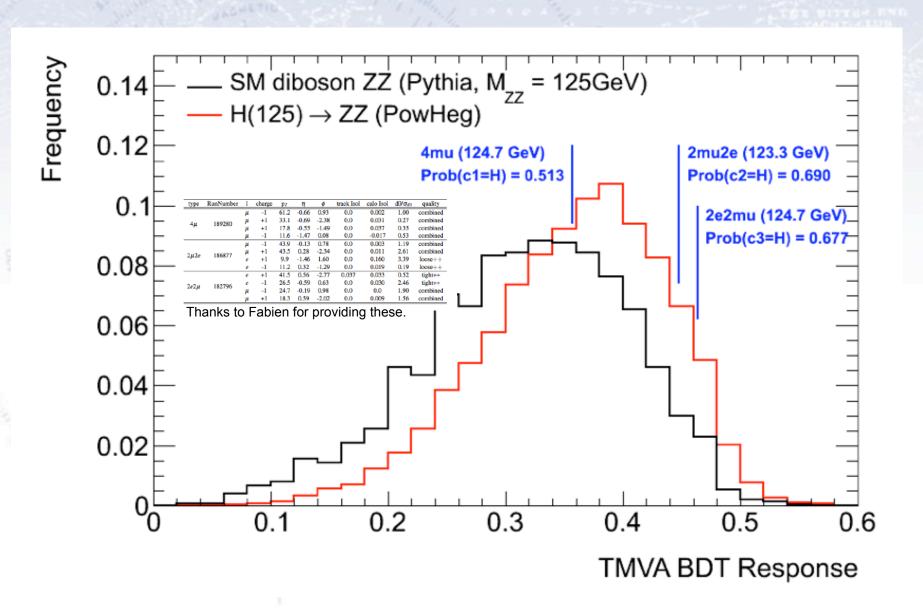
Using the 5 variables (i.e. including rapidity) in a BDT (100 trees, 4 nodes):



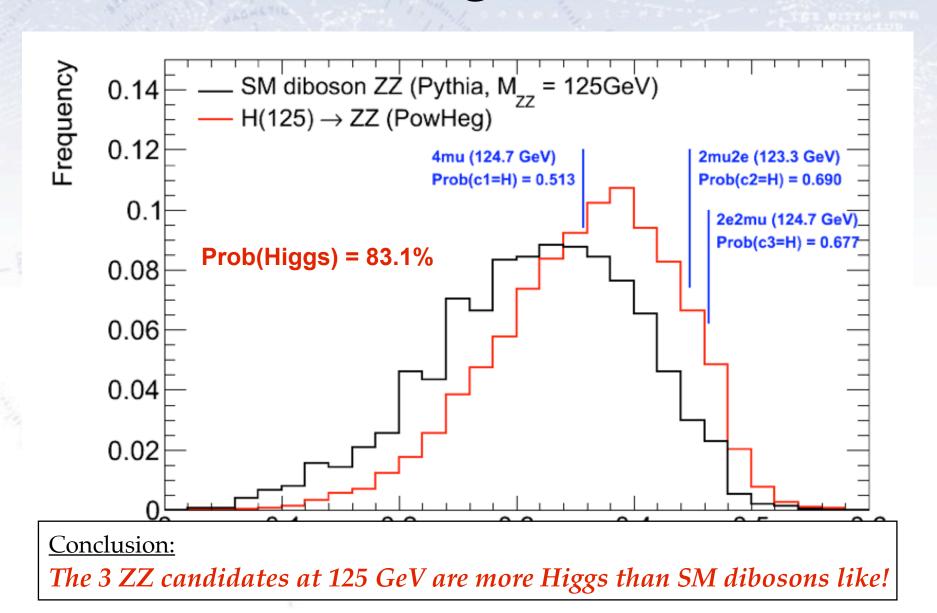
# Combined angular variable



# Combined angular variable

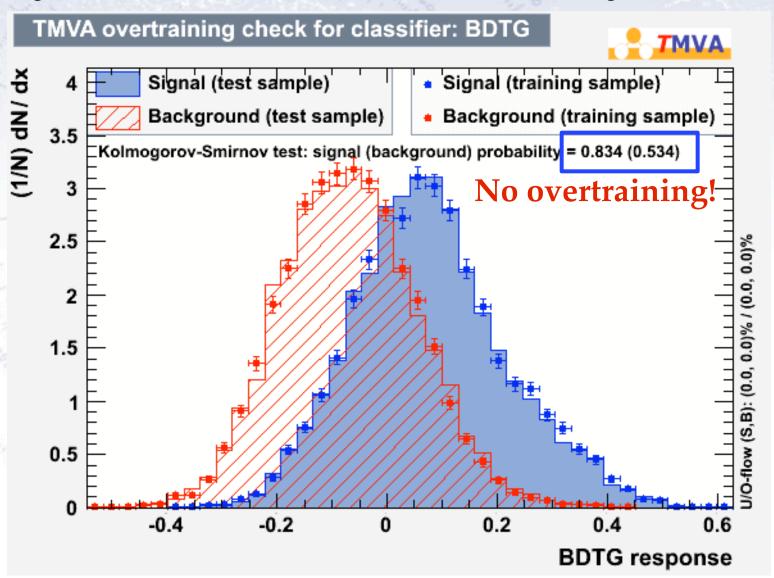


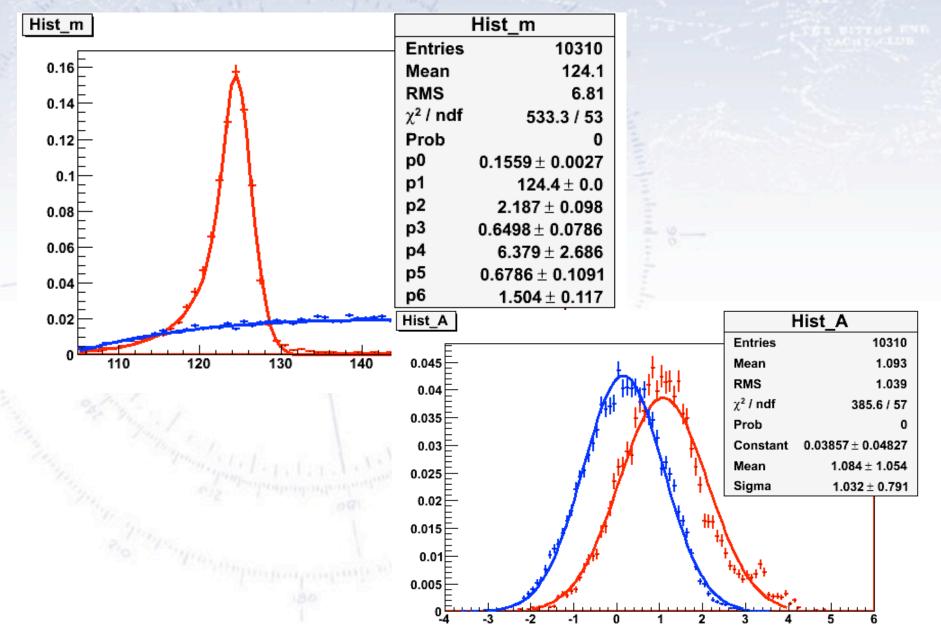
# Combined angular variable

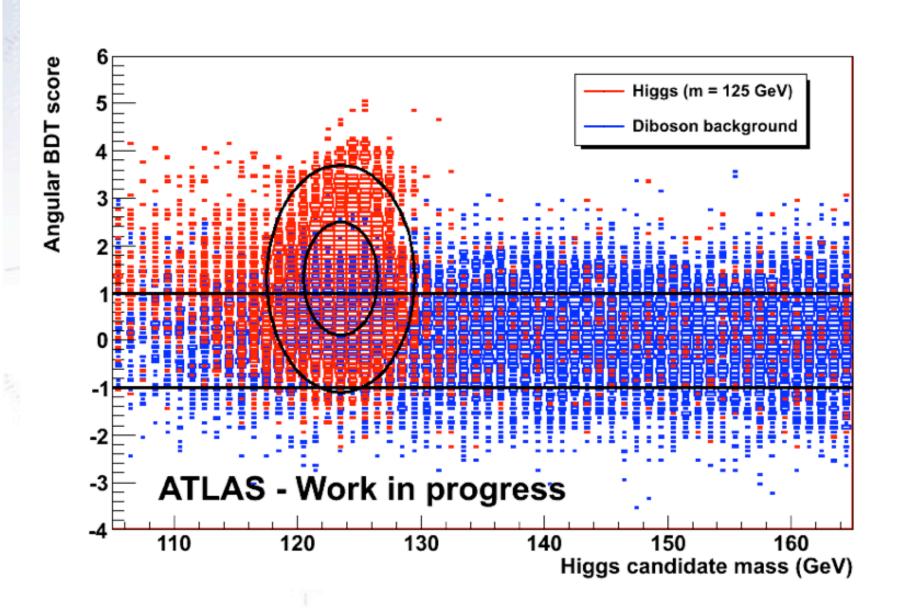


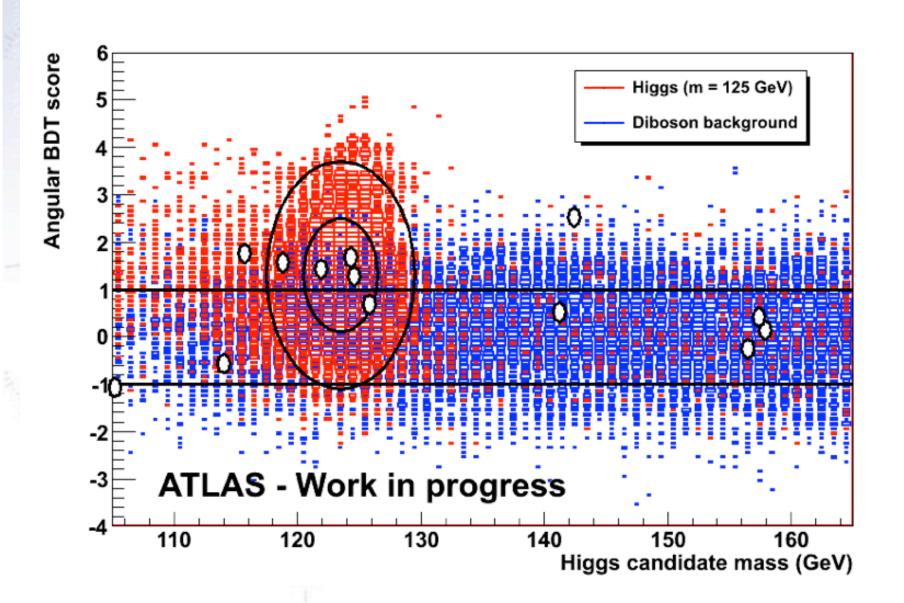
# Check for overtraining

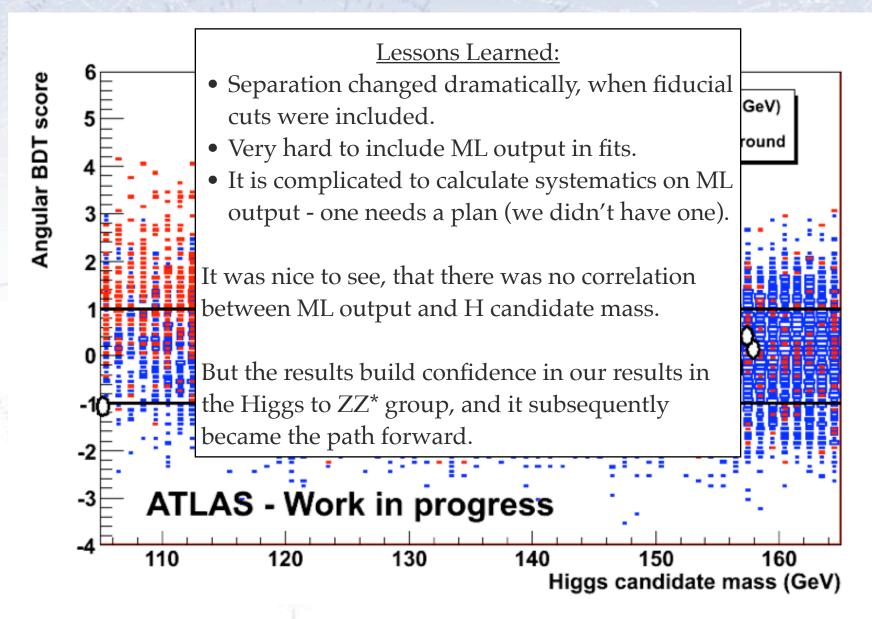
Using 9 variables in a BDT (200 trees, 4 nodes) and checking for overtraining:

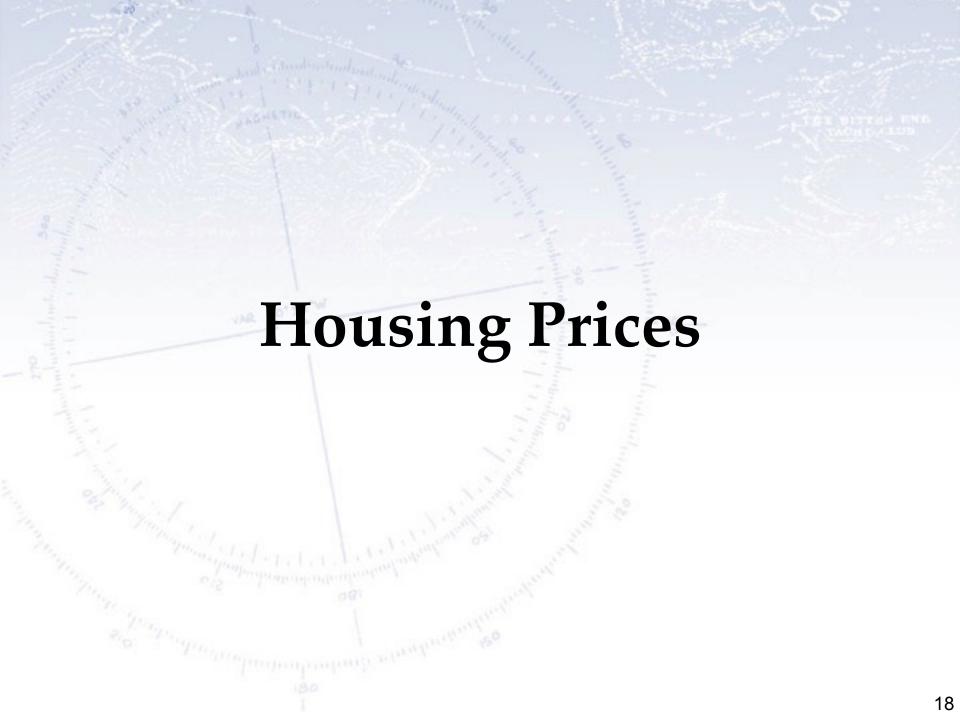






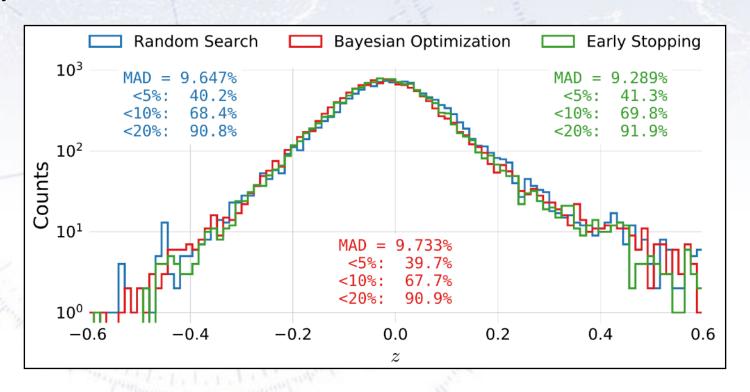






# **Estimating Housing Prices**

Slightly by coincidence, we got in contact with BoligSiden and collaborated. They had data on 0.5M house sales 2008-2019 (90+% of all).

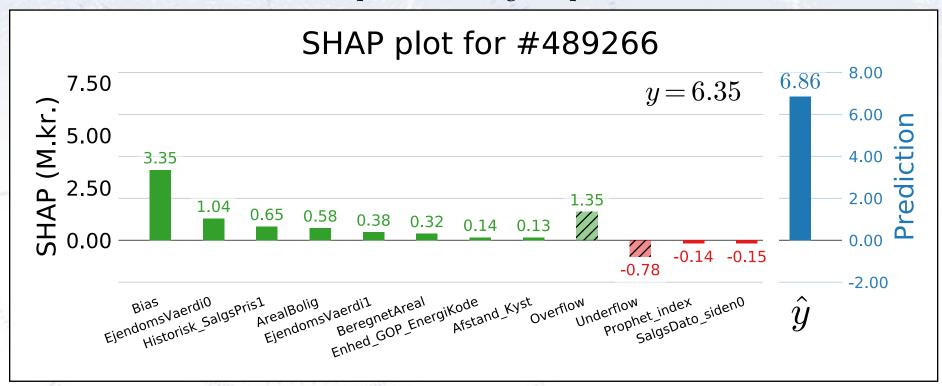


We used XGBoost to build a model: Dealt well with categories and NaNs.

For apartments, we managed to "break" the tough 10% uncertainty limit.

#### Individuel estimates

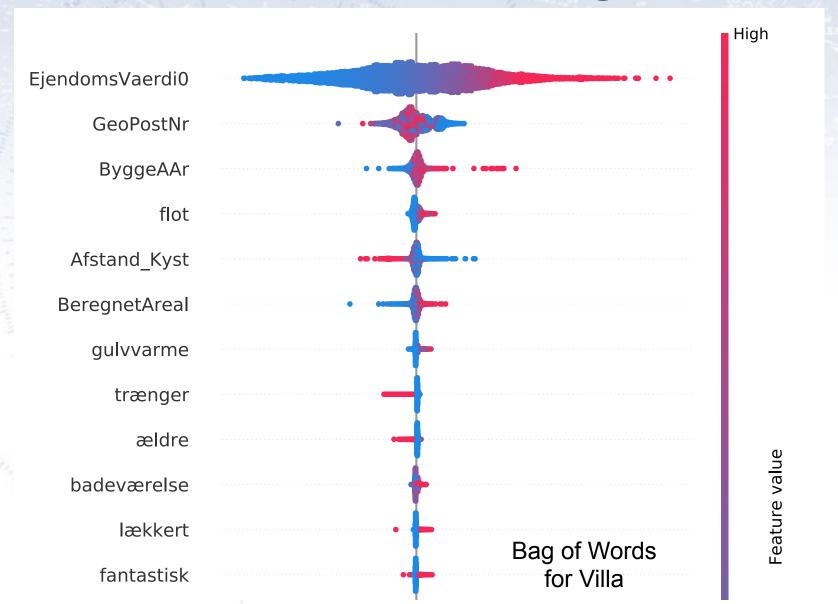
Shapley-values also gives the possibility to see the reason behind **individuel estimates**. Below is an example, illustrating this point.



Above is shown which factors that influences the final estimate of the sales price (and how much). The estimate is the sum of the contributions (here 6.86 MKr.).

This is a fantastic tool to get insight into the ML workings!!!

# Word ranking



# Result of including text

#### **Natural Language Processing**

Term Frequency - Inverse Document Frequency: *TF-IDF* 

Natural weighting of words

CountVectorizer, TfidfVectorizer

Assign a weight to each word, according to its frequency of use. weight\_IDF =  $log(N_{all} / N_{appearances})$ 

MAD(XGB, numerics only) = 0.165

MAD(XGB, text only, BOW) = 0.254

MAD(XGB, combined) = 0.147

(Numerics: GeoPostNr, BeregnetAreal, ByggeAAr, EjendomsVaerdi0, Afstand\_Kyst)

# Result of including text

Lessons Learned:

**Natural Lat** • The ML part of the project was fun and BDTs worked really well.

Term F • Including text was (at the time) harder, but we had a way to cross check, if it worked.

• We were not at all prepared for the reluctance to use this in the real world.

Cour

"Big ships turn very slowly!"

-IDF

each word, quency of use. Nall / Nappearances)

MAD(XGB, numerics only) = 0.165

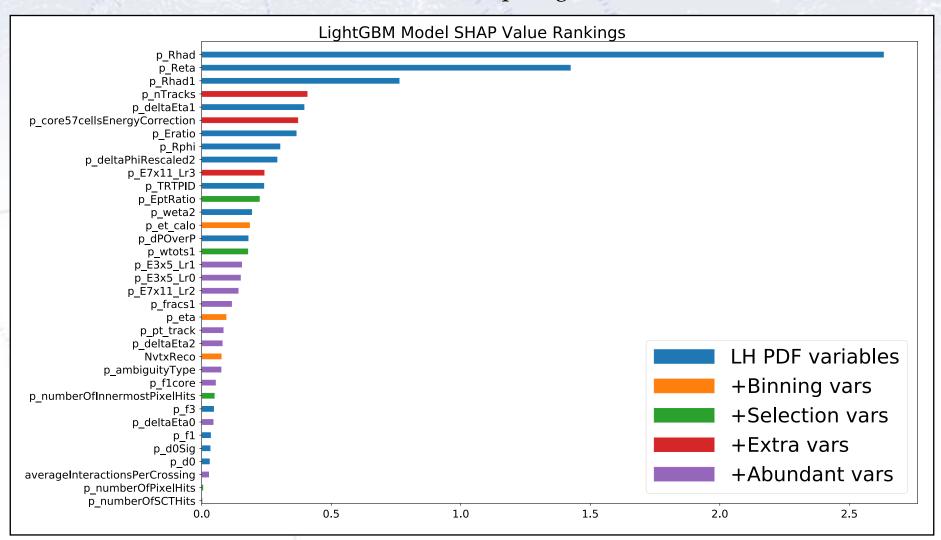
MAD(XGB, text only, BOW) = 0.254

MAD(XGB, combined) = 0.147

# **Electron Identification**

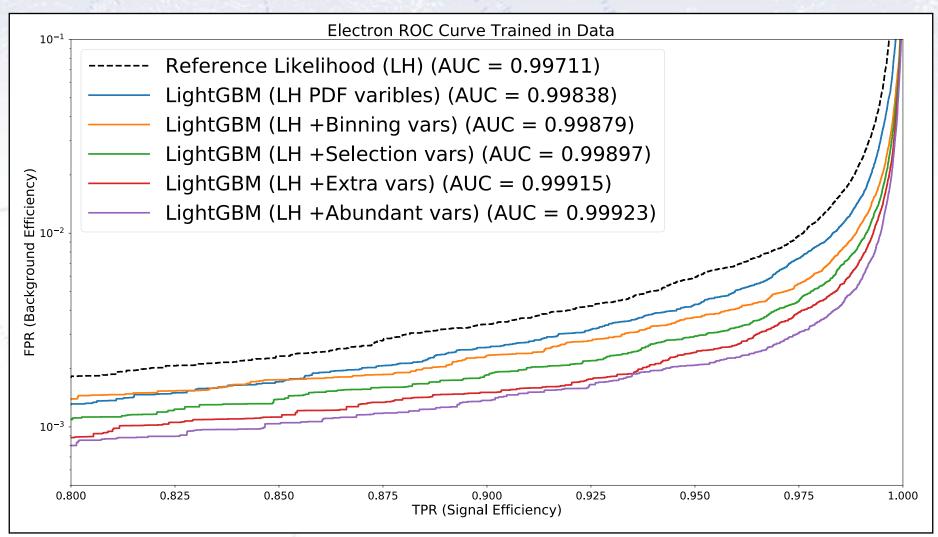
#### Input Feature Ranking

Here is an example from particle physics. The blue variables were "known", but with SHAP we discovered three new quite good variables in data.

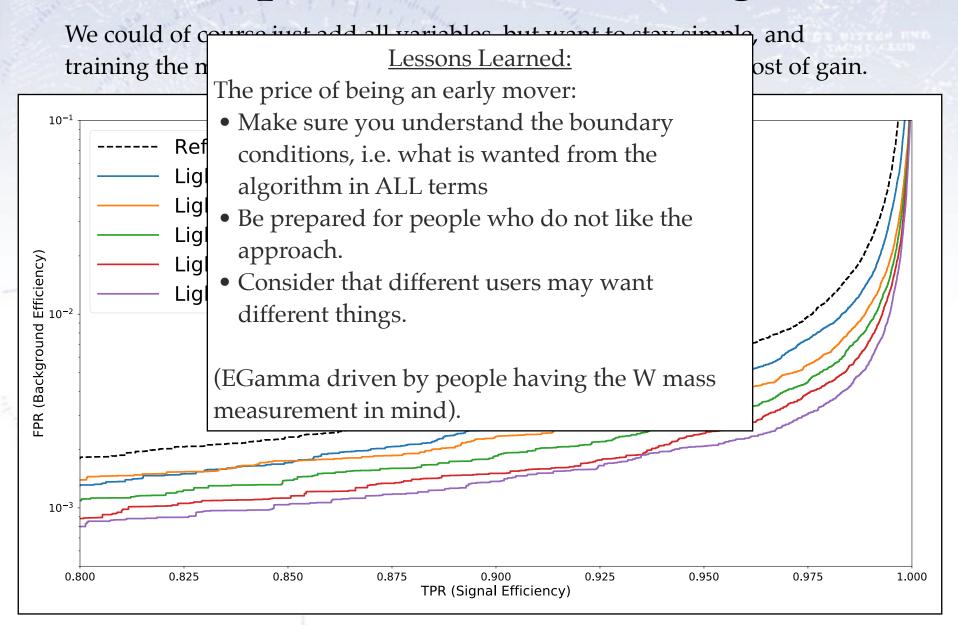


#### Input Feature Ranking

We could of course just add all variables, but want to stay simple, and training the models, we see that the three extra variables gives most of gain.



### Input Feature Ranking



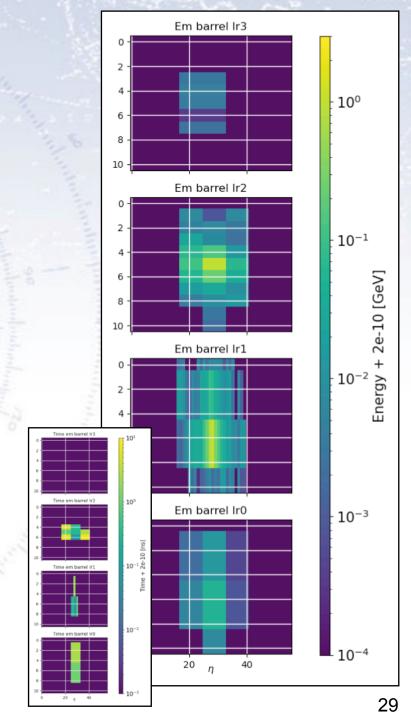
# **Electron Regression**

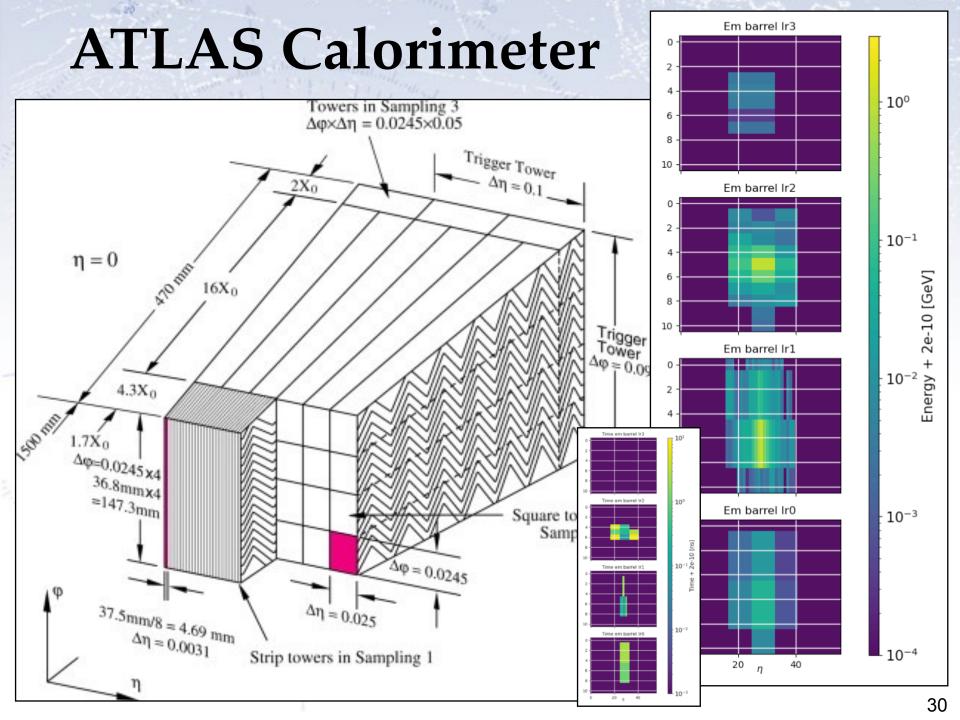
28

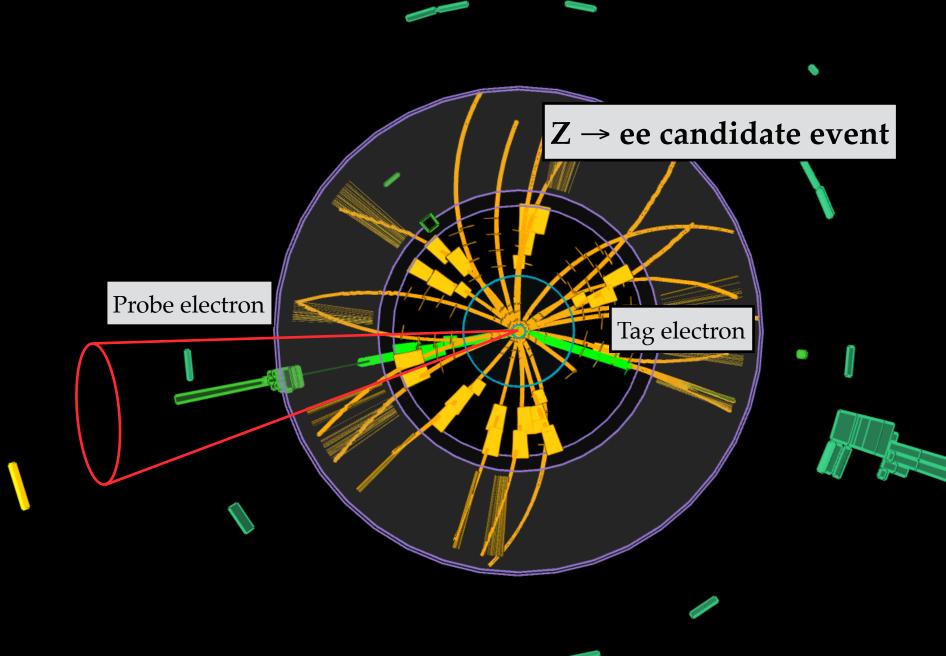
#### CNNs at work

The ATLAS calorimeter data looks like images.

Can we use CNNs to get a better energy measurement?







## The input variables

We consider the cell energies as pixels in four images. The cells contain two (used) types of information:

- Energy (primary variable)
- Time of cell energy

The variables are both scalar and cell based. The scalars

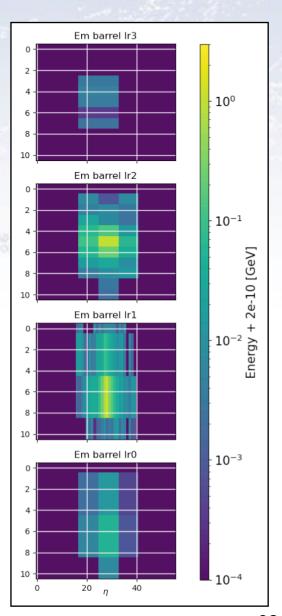
can be seen in table on the right.

Finally, we consider the (up to)
10 nearest tracks in a "TrackNet"

input:

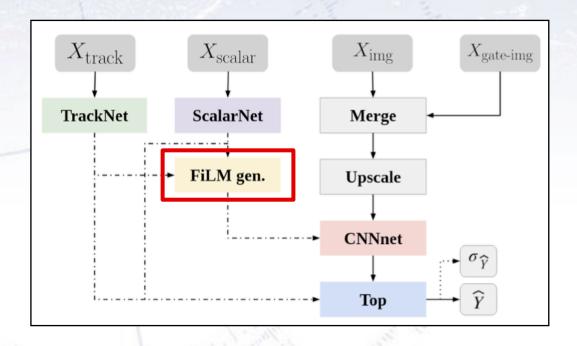
Туре	Name	Description
Energy	$p_{t,track}/q_{track}$	Transverse momentum of track divided by its charge $q$
Geometric	$d_0/\sigma_{d0}$	$d0$ is the signed transverse distance between the point of closest approach and the z-axis where $\sigma_{d0}$ is its uncertainty
	$\Delta R$	$\Delta R = \sqrt{(\phi_0 - \phi)^2 + (\eta_0 - \eta)^2}$
	$vertex_{track}$	Reconstructed vertex of the track
	20	Longitudinal distance between the point of closest approach and the z-axis.
	$\eta_{track}$	Reconstructed $ \eta $ of tracks.
	$\phi_{track}$	Reconstructed $\phi$ of tracks.
Misc.	$n_{pixel}$	Number of hits in the pixel detector
	$n_{SCT}$	Number of hits in the SCT
	$n_{TRT}$	Number of hits in the TRT

Type	Name	Description
Energy	$E_{acc}$	Energy deposit in layer 1-3 of ECAL.
	$\eta_{index}$	$\eta$ cell index of cluster of layer 2.
	$f0_{cluster}$	Ratio of energy between layer 0 and $E_{acc}$ in $ \eta $ 1.8 (end of layer 0).
	R12	Ratio of energy between layer 1 and 2 in ECAL.
	$p_1^{track}$	$p_T$ estimated from tracking for the particle (e).
	$E_{TG3}$	Ratio between the energy in the crack scintillal and $E_{acc}$ within $1.4 <  \eta  < 1.6$ .
	$E_{tile-gap}$	Sum of the energy deposited in the tile-gap.
	η	Pseudorapidity of the particle.
	$\Delta \phi_2^{rescaled}$	Difference between $\phi$ , as extrapolated by traing, use for ECAL momentum estimation an of the ECAL cluster.
	$\eta_{ ext{ModCalo}}$	Relative $\eta$ position w.r.t. the cell edge of layer the ECAL*.
Geometric	$\Delta\eta_2$	Difference between $\eta$ , as extrapolated by track use for ECAL momentum estimation and $\eta$ of ECAL cluster (only $e$ ).
	poscs <sub>2</sub>	Relative position of $\eta$ within cell in layer 2 ECAL. $2(\eta_{cluster} - \eta_{maxEcell})/0.025 - 1$ , $\eta_{cluster}$ $\eta$ of the barycenter of the cluster and $\eta_{maxEce}$ $\eta$ of the most energetic cell of the cluster.
	$\Delta \phi_{TH3}$	Relative position in $\phi$ in a cell. mod(2 $\pi$ $\phi$ , $\pi/32$ ) – $\pi/32$ .
Misc.	$\langle \mu \rangle$	Average proton-proton interaction per bu crossing.
	$n_{tracks}$	# of tracks assigned (only $e$ ).
	$n_{vertexReco}$	Number of reconstructed vertices.

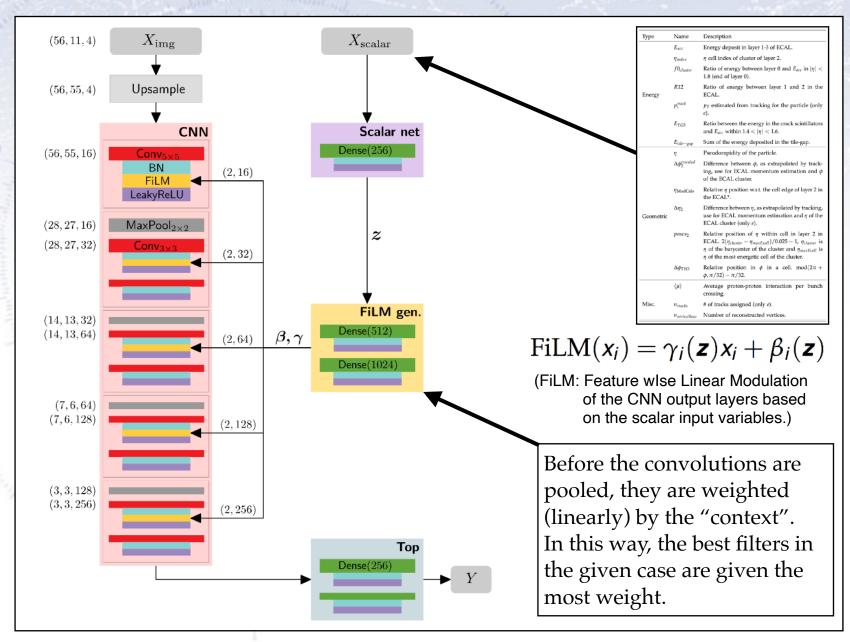


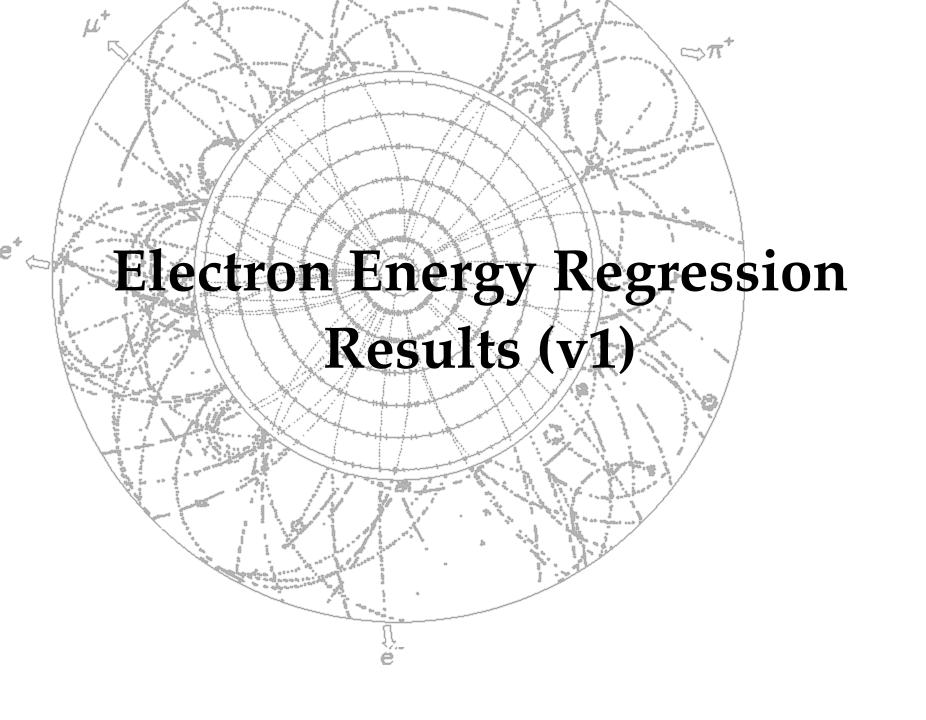
#### The network architecture

There are many ways to combine the input variables, and we have considered the following architectures, where the dashed lines are the considerations.



#### Feature wIse Linear Modulation





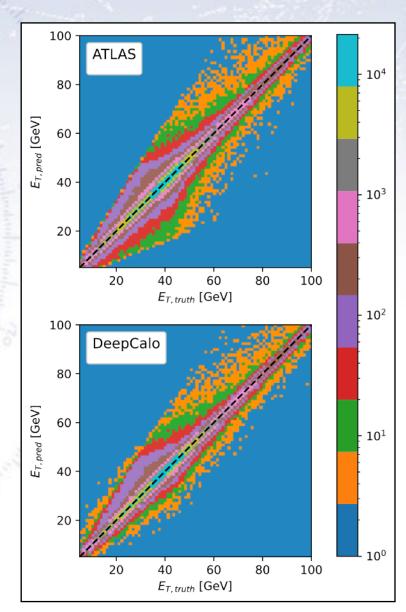
#### The results in 2D - MC

The  $E_T$  distribution for truth (x-axis) and reconstruction (y-axis) can be compared for the current ATLAS and the DeepCalo algorithms.

As the figure shows, both algorithms do well, and improve with energy.

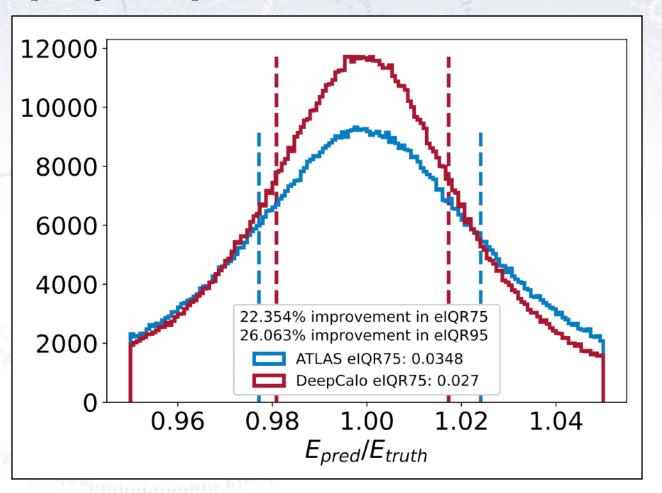
As the statistics is largest around 40 GeV, this is where the comparison is most detailed, and here DeepCalo visibly has a significantly reduced lower edge.

Thus, the DeepCalo more rarely undershoots the energy.



### The results in 1D - MC

Integrating the previous plot into 1D considering the RE distribution, we see a general sharpening. The improvement in relative eIQR (reIQR) is about 22%.

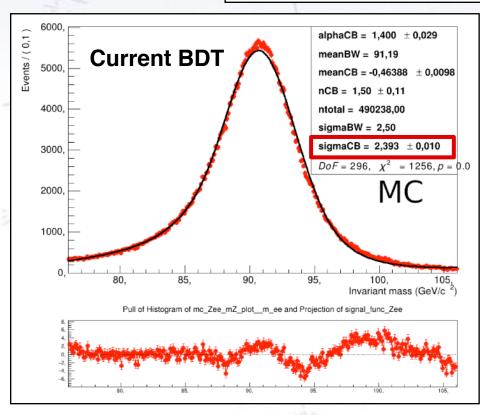


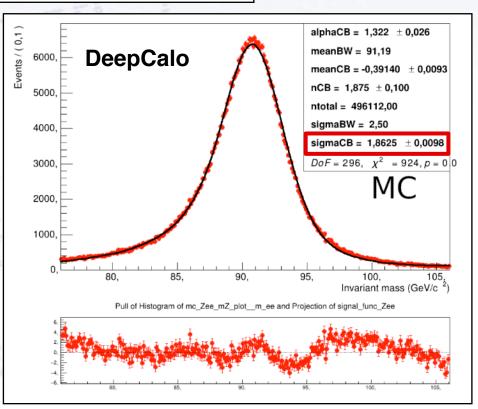
Naively, we would of course love to see a similar number in data!

### Result in Zee - MC

On the Zee peak, we evaluate the improvement by fitting with a BW⊗CB fit, considering the CB width (sigmaCB) as the performance parameter. We get:

$$\langle 1 - rac{\sigma_{CB}^{DeepCalo}}{\sigma_{CB}^{ATLAS}} 
angle = 1 - rac{1.8310 \pm 0.006}{2.393 \pm 0.01} = 23.5 \pm 0.4\%$$

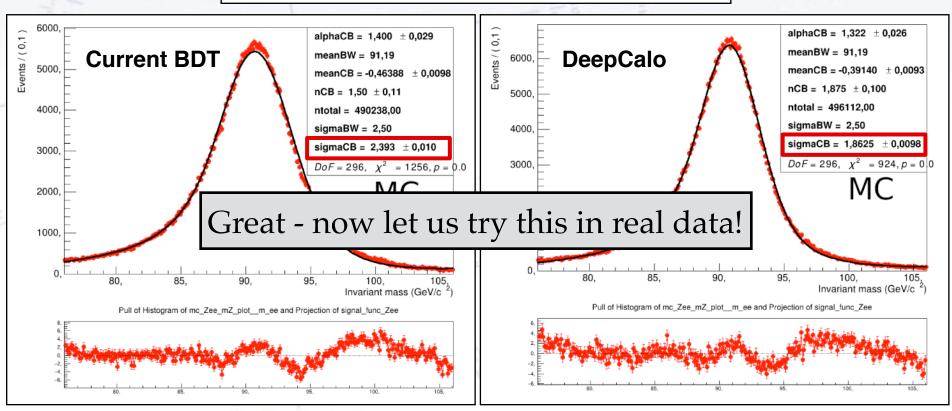




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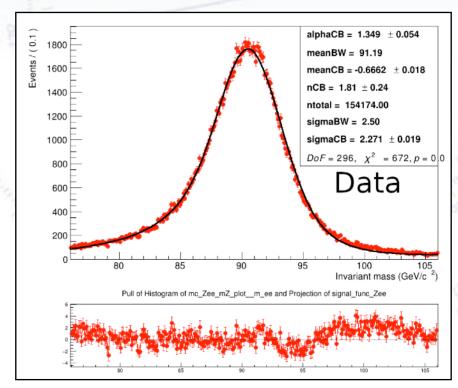


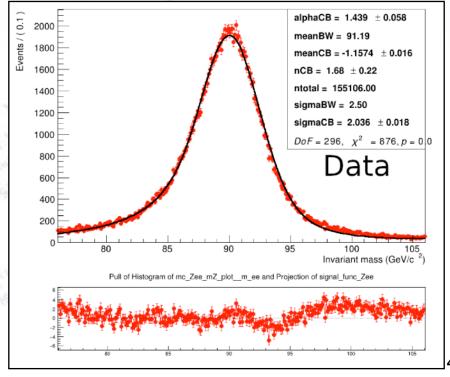
### Results on Zee - data (v1)

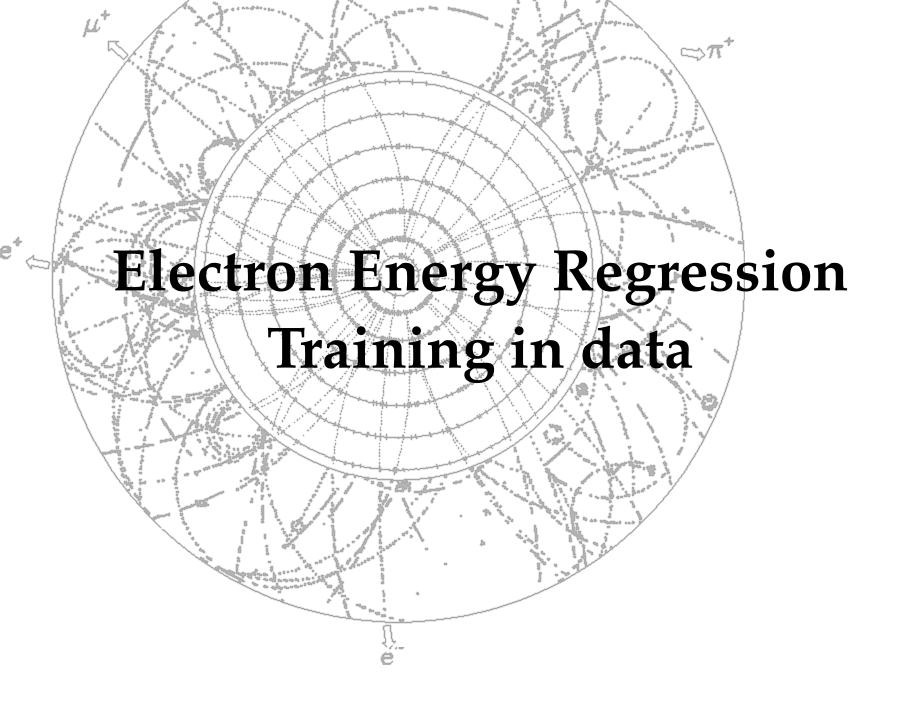
The result we get is a much more modest improvement:

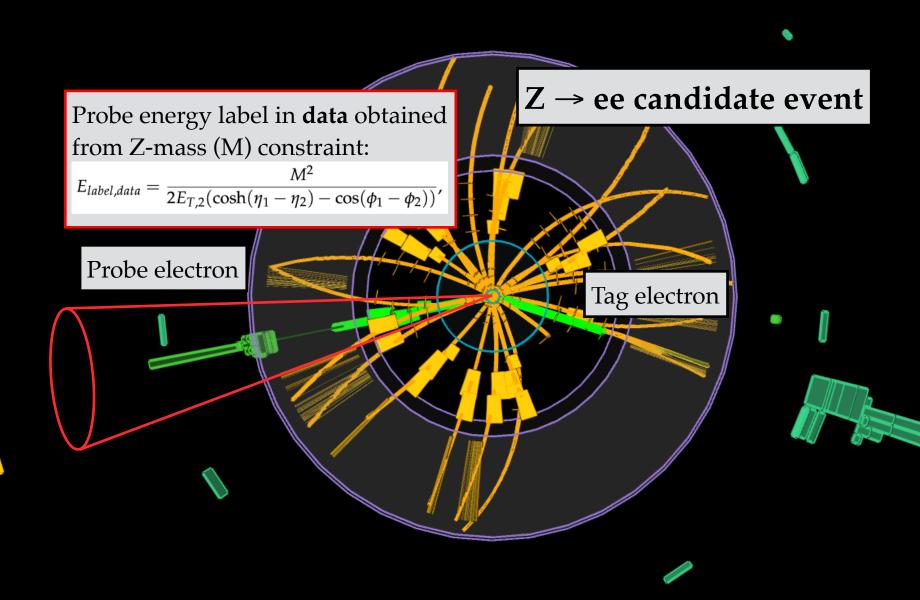
$$\langle 1 - rac{\sigma_{CB}^{DeepCalo}}{\sigma_{CB}^{ATLAS}} 
angle = 1 - rac{2.058 \pm 0.010}{2.271 \pm 0.019} = 9.4 \pm 0.9\%.$$

Though perhaps a little disappointing, this is not surprising, as we can not expect the MC to mimic data perfectly in the very large space considered.









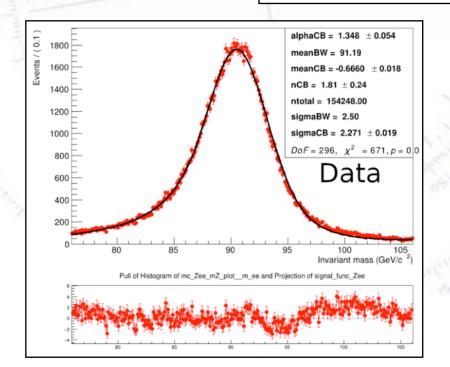
## Training in data

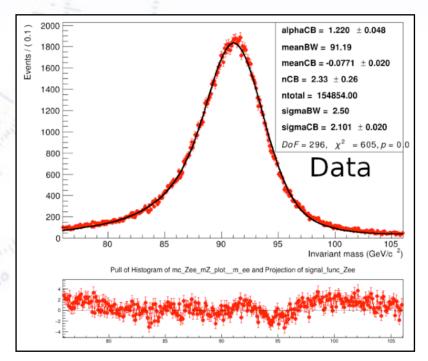
Using Zee events with invariant masses 86-97 GeV, one can get "approximate labels" in data, by assuming the true Z mass:  $M^2 = 2p_{T,1}p_{T,2}(\cosh(p_1-p_2)-\cos(p_1-p_2))$ 

Using such labels, we train in data and get...

$$\begin{split} M^2 &= 2p_{T,1}p_{T,2}(\cosh(\eta_1 - \eta_2) - \cos(\phi_1 - \phi_2)), \quad p_T = E_T \updownarrow \\ E_{label,data} &= \frac{M^2}{2E_{T,2}(\cosh(\eta_1 - \eta_2) - \cos(\phi_1 - \phi_2))'} \\ \text{with } E_{T,2} &= E\text{calib}^{(BDT)} \text{ and } M^2 = 91.19^2 \end{split}$$

$$\langle 1 - rac{\sigma_{CB}^{DeepCalo}}{\sigma_{CB}^{ATLAS}} 
angle = 5.9 \pm 0.9\%$$





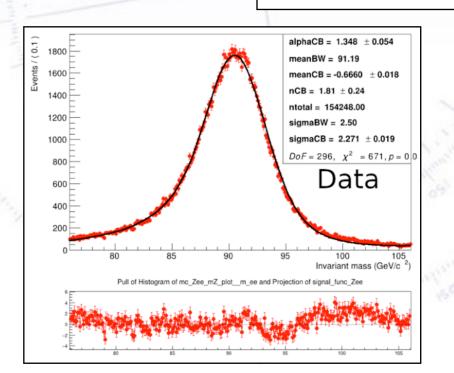
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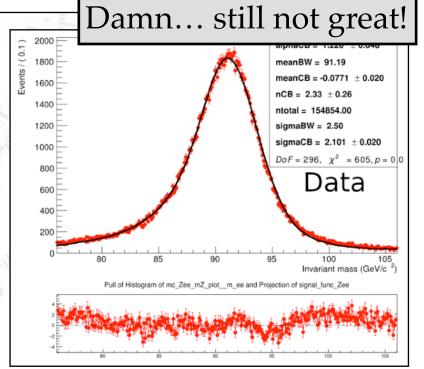
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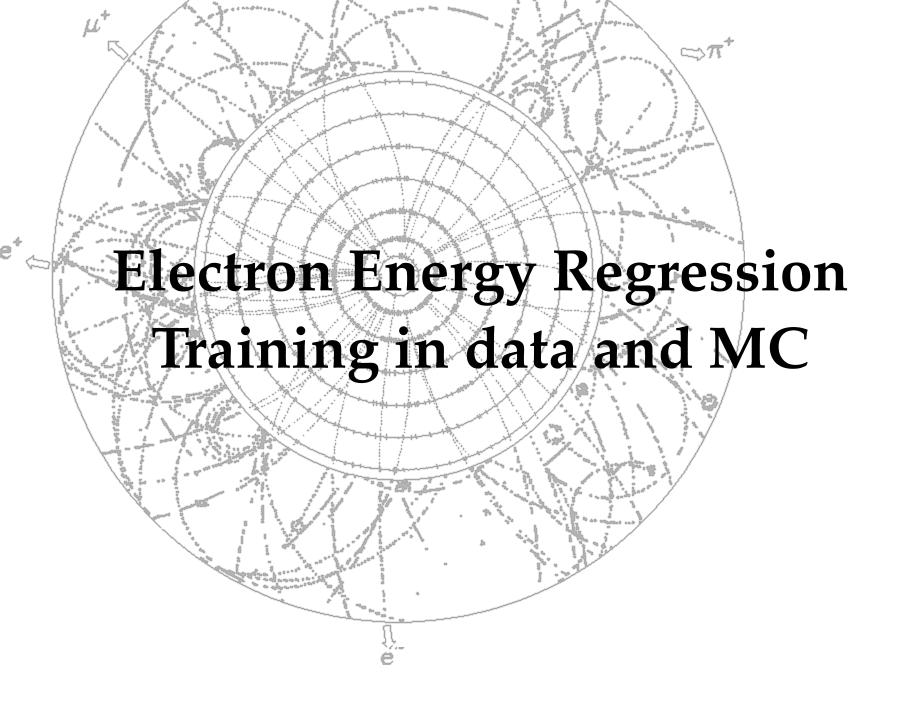
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$$\langle 1 - rac{\sigma_{CB}^{DeepCalo}}{\sigma_{CB}^{ATLAS}} 
angle = 5.9 \pm 0.9\%$$







## Training in data and MC

Once we have labels in data, there is nothing keeping us from combining the loss functions of MC and data (they even have the same form), and thus training **simultaneously** in data and MC:

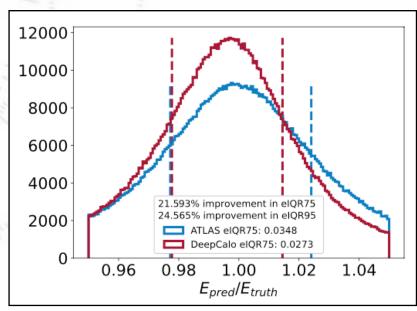
$$\mathcal{L}(y, \hat{y}) = \mathcal{L}(y_{(\text{Zee, MC})}, \hat{y}_{(\text{Zee, MC})}) + \mathcal{L}(y_{(\text{Zee, Data})}, \hat{y}_{(\text{Zee, Data})})$$

This allows the model to both use the "strength" of MC, but also learn the differences between MC and real data.

Doing this and trying out the result in MC first yields:

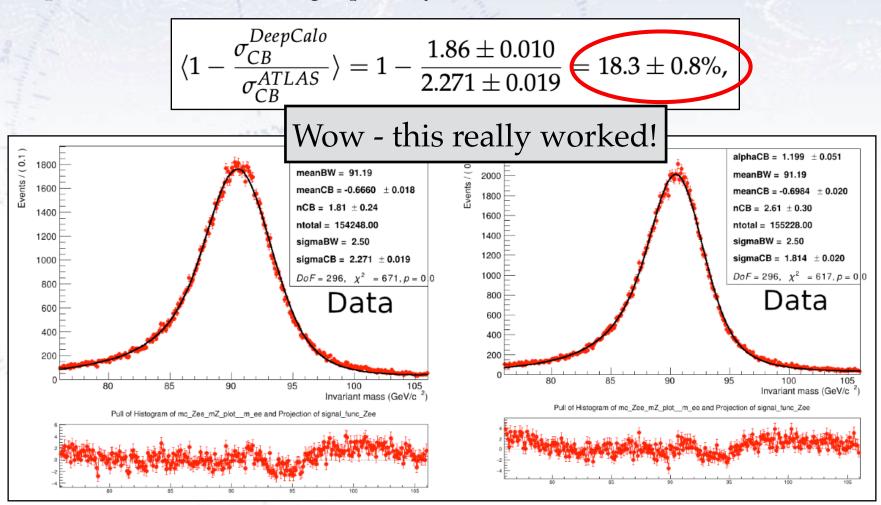
$$\langle reIQR_{75}^{DeepCalo} \rangle = 22.1 \pm 0.3\%$$

OK, so at least it doesn't ruin the model for MC. Now let us try data...



### Result in data (v2)

The result in data is rather encouraging, and greater than the sum of the improvements from training separately in MC (9.4%) and data (5.9%).



### Outlook

While this is still "only" an improvement in the electron energy regression, and only for lower energies (Zee range), the simultaneous training allows for extending the energy range, by including the Electron Gun MC.

Furthermore, this training might be extended to include photons, as these behave much the same as electrons, and suffer the same sources of uncertainties and smearing.

For improving the H  $\rightarrow \gamma \gamma$  resolution, one might use the following loss function and related training samples:

$$\begin{split} \mathcal{L}(y, \hat{y}) &= \mathcal{L}(y_{(\text{Zee, MC})}, \hat{y}_{(\text{Zee, MC})}) + \mathcal{L}(y_{(\text{Zee, Data})}, \hat{y}_{(\text{Zee, Data})}) + \\ \mathcal{L}(y_{(\text{Z}\mu\mu\gamma, \text{MC})}, \hat{y}_{(\text{Z}\mu\mu\gamma, \text{MC})}) + \mathcal{L}(y_{(\text{Z}\mu\mu\gamma, \text{Data})}, \hat{y}_{(\text{Z}\mu\mu\gamma, \text{Data})}) + \\ \mathcal{L}(y_{(H\gamma\gamma, \text{MC})}, \hat{y}_{(H\gamma\gamma, \text{MC})}) \end{split}$$

Meanwhile, we are trying to write this up somehow (but Malte is now a Ph.D. in Geneva).

#### Outlook

While this is st only for lower extending the

Furthermore, to behave much to and smearing.

**Lessons Learned:** 

• Remember to think about publishing. Even what may seem "a fun little example" at the time, may turn out to inspire a new line of thinking.

• Remember to think about the longevity of any approach. In this case, the storage of cell information was discontinued shortly after!

gression, and ws for

as these f uncertainties

For improving the first of the following loss function and related training samples:

$$\begin{split} \mathcal{L}(y, \hat{y}) &= \mathcal{L}(y_{(\text{Zee, MC})}, \hat{y}_{(\text{Zee, MC})}) + \mathcal{L}(y_{(\text{Zee, Data})}, \hat{y}_{(\text{Zee, Data})}) + \\ \mathcal{L}(y_{(\text{Z}\mu\mu\gamma, \text{MC})}, \hat{y}_{(\text{Z}\mu\mu\gamma, \text{MC})}) + \mathcal{L}(y_{(\text{Z}\mu\mu\gamma, \text{Data})}, \hat{y}_{(\text{Z}\mu\mu\gamma, \text{Data})}) + \\ \mathcal{L}(y_{(H\gamma\gamma, \text{MC})}, \hat{y}_{(H\gamma\gamma, \text{MC})}) \end{split}$$

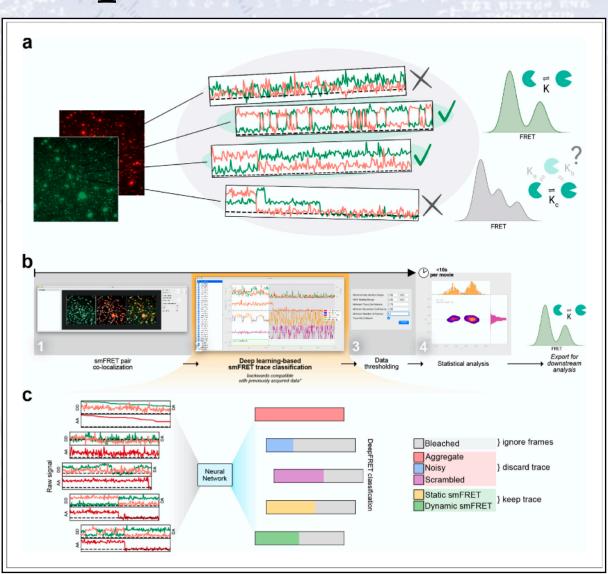
Meanwhile, we are trying to write this up somehow (but Malte is now a Ph.D. in Geneva).

# DeepFRET

FRET is a technique used to study and dynamics of biomolecules.
The data is a "trace", which is a time series with possible phase transitions.

The group would go through 10000 traces and select about 250 of these... by hand!!!
This took a few people about a week, and was neither reproducible nor optimal.

So we made DeepFRET.



# DeepFRET

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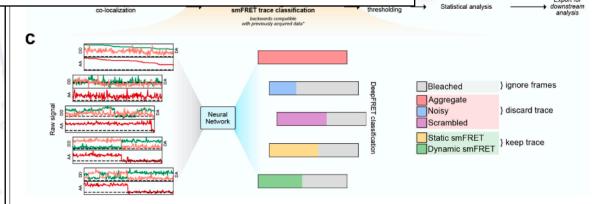
This took a few people about a week, and was neither reproducible nor optimal.

So we made DeepFRET.



а

- The experience was rather good, as the group really wanted to go this way, and was amazed at how well it worked.
- However, the field was dubious to say the least! No one published how they classified traces. No one published their raw data either.



# Knee- & Hip surgery

### The data

The analysis is based on V1.0 of the data:

Dtasæt\_NBI\_Predict\_PrimæreTXA\_16\_17\_MASTER\_ WORK.csv

																Dtasæt_Ni	BI_Predict_Prima	ereTXA_16_17_MA	STER_	WORK													
Ken Ci	vilstatus	Height	Weight	нь н	lb_g_dL	Anæmi	Rygni	ing Al	lkohol G	angredskab	Udhv	filet Sno	orken I	DM_type	Hypertension_ja_ell_recept	Hyperkolesterol	Cardiac_disease	Pulmonary_disease	Psych_	D Psi	recept_Ps	D Cer	rebral_attack Tidl_V	/TE Fa	m_VTE_AK_t	eh Pote	entAK	Cancer	Nyre I	ed A	der BMI	Årstal Hosp	ital Medical_outcome
0	1	165	56	6,9	11,109	1		0	0	1	1	0	2	0	0	0		0		1	1	1	1	0	1	0	0	0	0	0	81 20,5693296602388	2016	7 0
0	0	168	77	8,2	13,202	0		0	0	0	)	1	0	0	1	0		0		0	0	0	0	0	0	0	0	0	0	0	81 27,281746031746	2017	5 0
0	1	160	70	8,7	14,007	0		0	0	1	1	1	2	D	1	1	1	0		0	D	0	0	0	0	0	0	0	0	0	81 27,34375	2017	7 0
1	0	170	85	9,5	16,296	0		0	0	0	)	1	0	2	0	0		0		0	1	1	0	0	0	1	1	0	0	1	78 29,4117647058824	2016	4 0
1	0	168	73	8,8	14,168	0		0	0	0	)		0	0	0	0		0		0	D	0	0	0	0	0	0	0	0	0	76 25,8645124716553	2016	4 0
1	0	183	96	7,8	12,558	- 1		0	0	0	0	1	1	1	1	1	1			0	0	0	0	0	0	0	0	0	0	0	77 28,3675236644868	2017	3 0
1	0	173	96	9	14,49	0		0	0	1	1	1	1	0	1	1	1	0		0	0	0	1	0	0	1	0	0	1	1	75 32,075912994086	2016	1 0
0	0	164	75	8	12,88	- 1		0	0	0	0	0	0	0	0	0		0		0	0	0	0	0	0	0	0	0	0	1	74 27,8851873884593	2016	4 0
1	0	169	77	8,7	14,007	0		0	1	0	0	1	2	0	0	0		0		1	1	0	0	0	0	0	0	0	0	1	73 26,9598403417247	2016	1 0
0	1	170	53	7,8	12,558	- 1		0	0	0	)	1	0	0	0	0		0		0	0	0	0	0	0	0	0	0	0	0	73 18,3391003460208	2017	7 0
0	0	168	85	8,2	13,202	0		0	0	0	0	1	0	0	1	1		0		0	0	0	0	0	0	0	0	0	0	0	72 30,1162131519274	2017	7 0
0	1	163	63	7,8	12,558	- 1		0	0	0	0	1	2	2	1	1		0		0	0	0	0	0	0	0	0	0	0	0	71 23,7118446309609	2016	1 0
1	0	176	83	9,6	15,456	0		0	0	0	0	1	2	0	1	1		1		0	0	0	0	0	0	0	0	0	0	1	71 26,7949380165289	2016	4 0
0	0	158	80	7,9	12,719	1		0	0	0	)	0	0	0	1	1	1	0		1	1	1	0	0	1	0	0	0	0	0	71 32,0461464508893	2016	6 0
0	0	170	68	8,5	13,685	0		0	1			1	2	0	0	1		0		1	1	1	0	0		0	0	0	0	0	71 23,5294117647059	2016	7 0
0	0	157	69	7,3	11,753	1		0	0	1	1		0	0	1	1		0		0	0	0	0	0	0	0	0	0	0	0	72 27,9930220292912	2017	7 0
0	0	157	92	6,8	10,948	- 1		0	0	1	1	0	1	2	1	1	1	0		0	0	0	1	0	0	0	0	0	0	1	72 37,3240293723883	2017	9 0

There were 10573 entries with 32 variables in the data, and we tried to give a prediction for the medical outcome (stay more than 4 nights or returning within 30 days). The data is **quite imbalanced**, with only 5.7% in one class.

We have so far used a "simple" setup (algorithm: LightGBM with focal loss), and not done a lot of optimisation... yet!

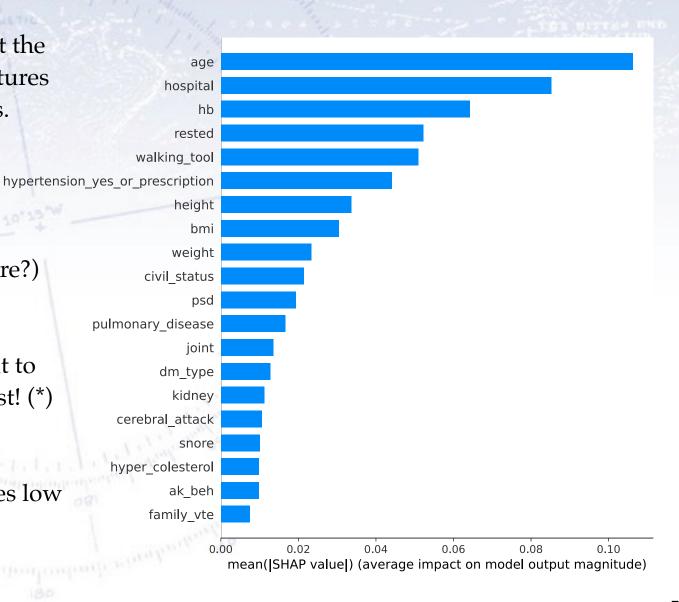
# Ranking of features

Here we show what the most important features were in the analysis.

Age is no surprise! HB (= blood pressure?) also ranks high.

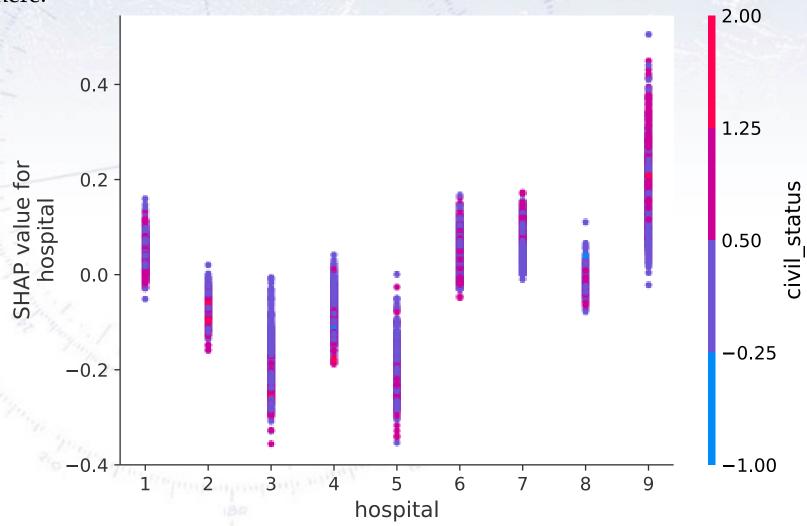
Hospital is not great to see so high in the list! (\*)

Also good is to see "snore" and the likes low in the list.



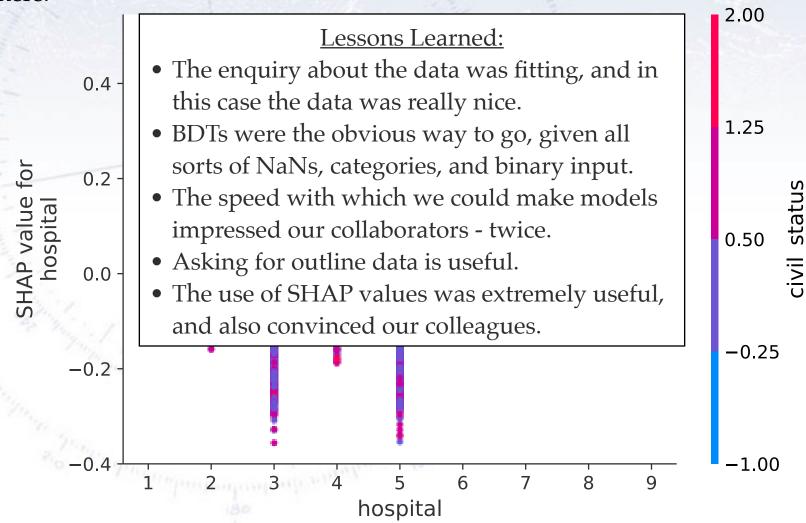
## Further improvements

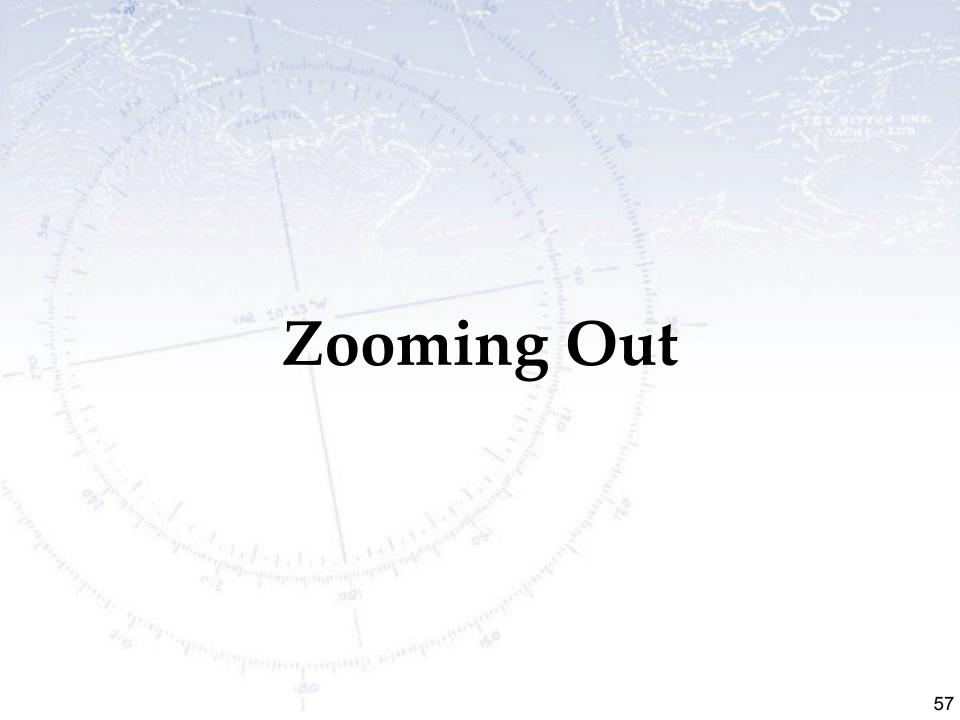
We don't know which is "Hospital=9", but we don't want to send Mathias there!



## Further improvements

We don't know which is "Hospital=9", but we don't want to send Mathias there!





Machine Learning is a great new tool, but of course comes with caveats:

Remember the context and goal:
 You might do something great... to no avail!

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- Start with a simple model, and then expand.
   Maybe the simple model is best/enough.

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   You might do something great... to no avail!
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- Ensure **reproducibility**:
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- Beware of domain shifts:
   Simulated and real data are never the same.
- All the **old rules apply**: Inspect, Check, and Question data and output.

Machine Learning is a sharpening of our scientific senses - not a substitution

