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## Nested Machine Learning Models for CTA

Master Thesis Half-Time Talk

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December 16, 2022

E5b Astroparticle Physics

Department of Physics - TU Dortmund

## Overview

Introduction

Scaled Parameters and Feature Selection

Energy Regression

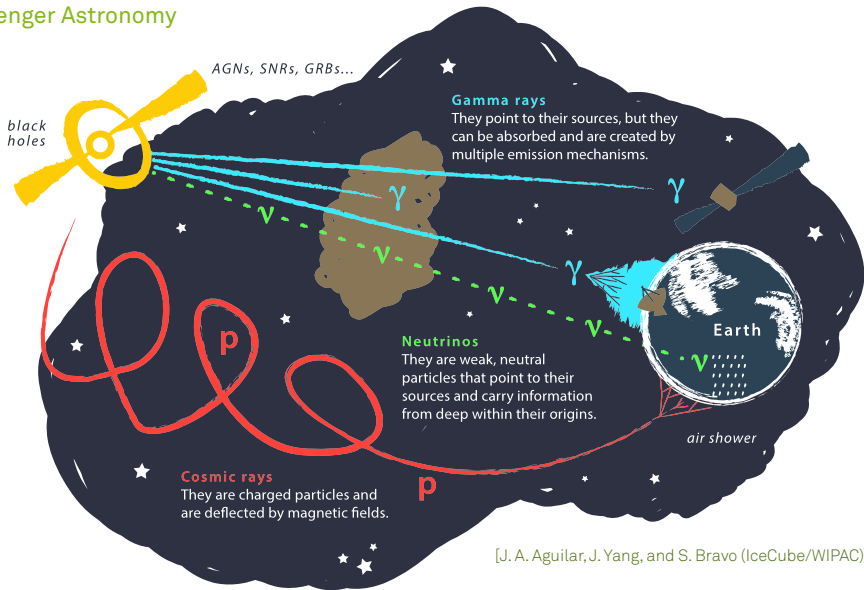
Gamma-Hadron Classification

Origin Reconstruction

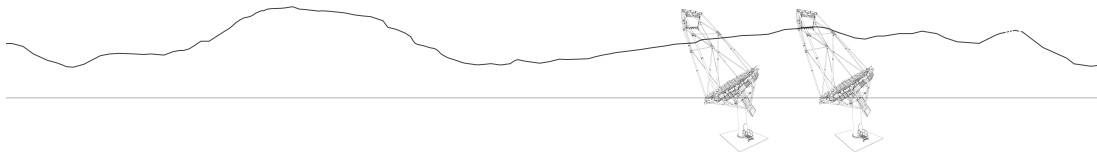
Performance

Outlook

## Multi-Messenger Astronomy



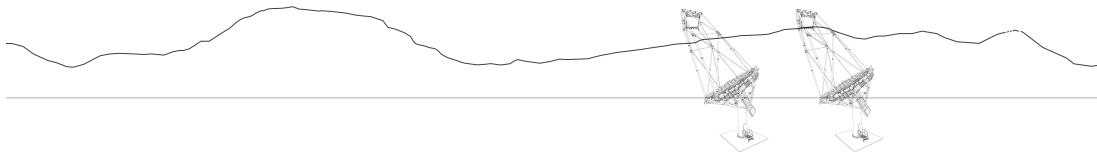
## Imaging Atmospheric Cherenkov Telescopes (IACTs)



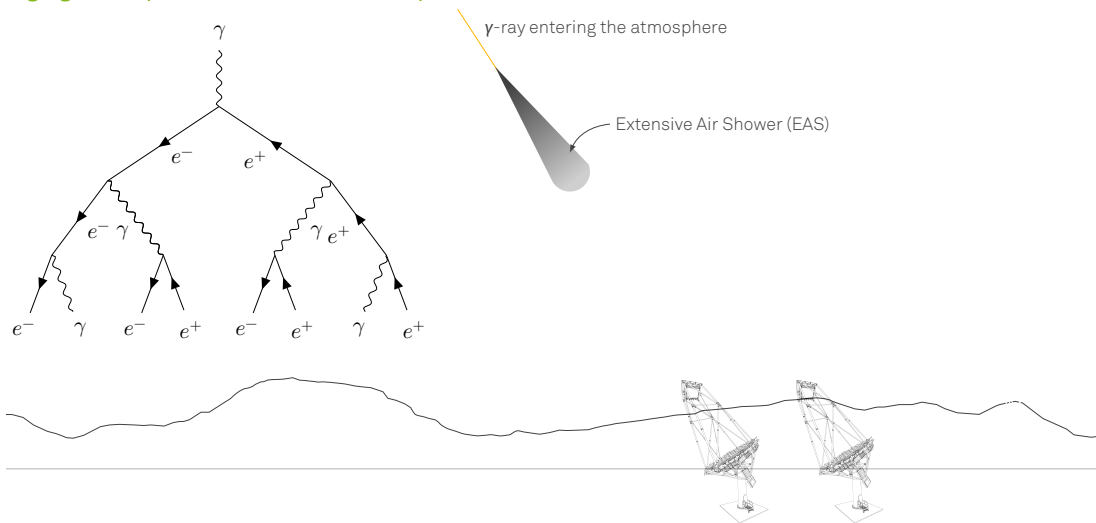


## Imaging Atmospheric Cherenkov Telescopes (IACTs)

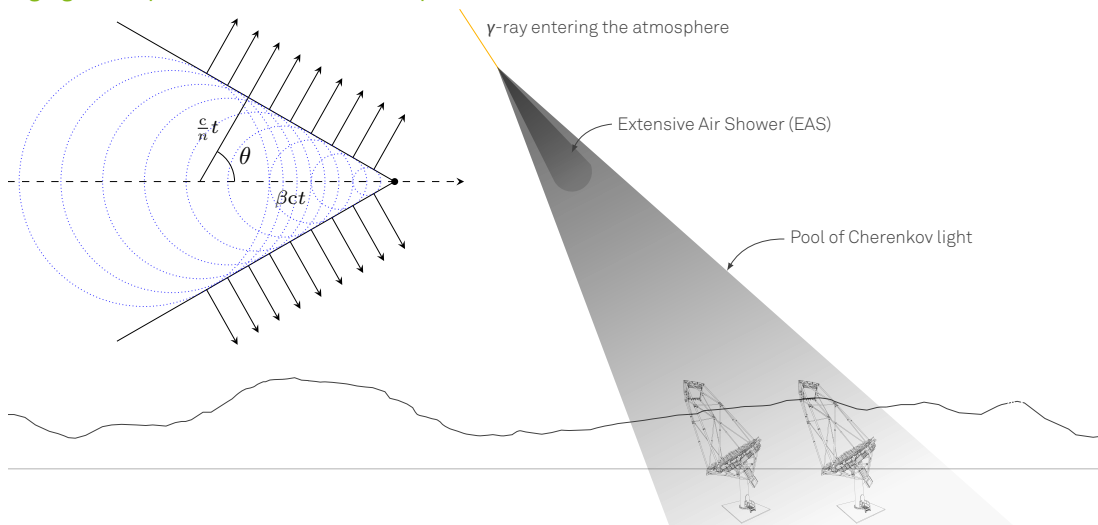
$\gamma$ -ray entering the atmosphere



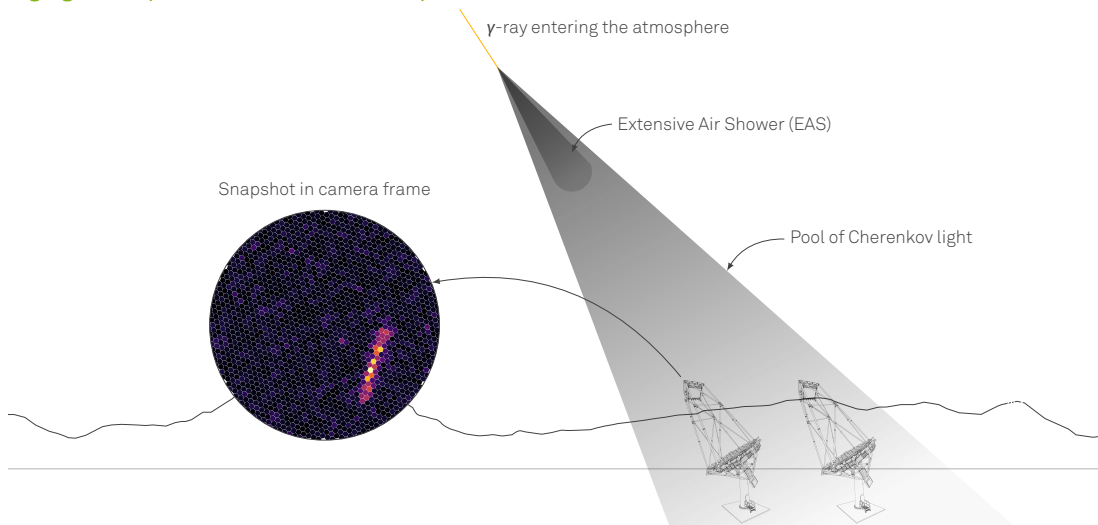
## Imaging Atmospheric Cherenkov Telescopes (IACTs)



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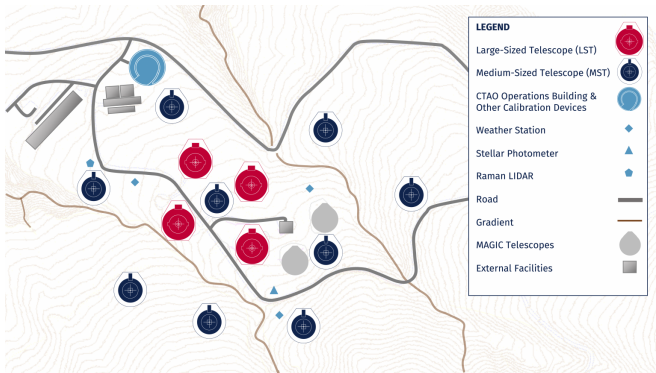


## Imaging Atmospheric Cherenkov Telescopes (IACTs)



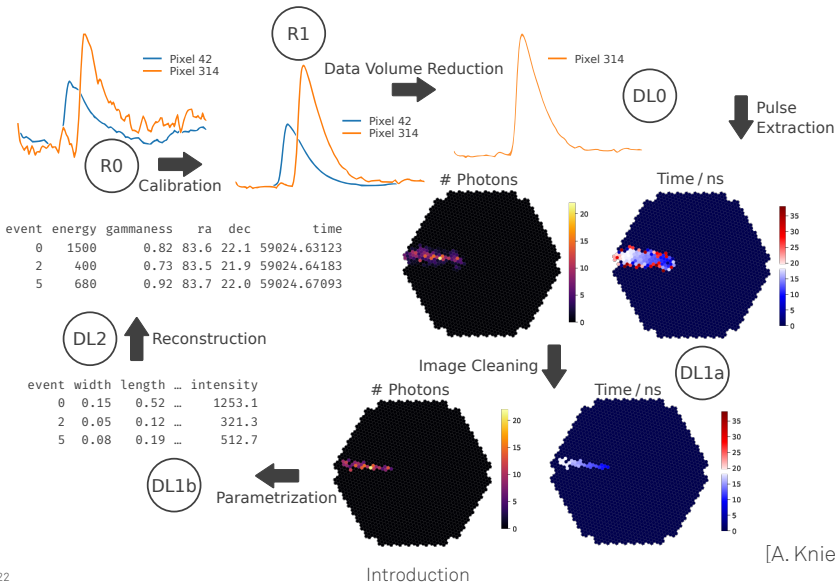
## The Cherenkov Telescope Array

- CTA South (Paranal Observatory, Chile)
- CTA North (La Palma)
  - 4 LSTs + 9 MSTs
- Large-Sized Telescope (LST)
  - 23 m mirror diameter
  - 4.3° FoV
- Medium-Sized Telescope (MST)
  - 11.5 m mirror diameter
  - 7.7° FoV



[CTAO]

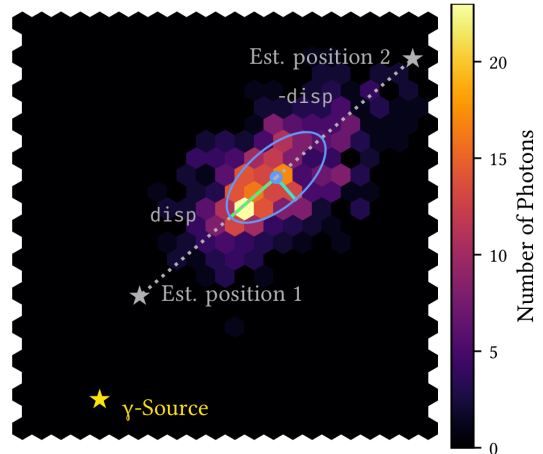
Dataprocessing using **ctapipe**



[A. Knierim, M. Linhoff]

## The disp Method

- Monoscopic origin reconstruction for IACTs
- Assume main shower axis to be correctly reconstructed  $\rightarrow$  source position on axis
- Train regressor to estimate distance from image center of gravity ( $|\text{disp}| / \text{norm}$ )
- Train classifier to decide between remaining two possibilities ( $\text{sign}$ )



[Max Noethe, PhD thesis]

## Scaled Parameters and Feature Selection



## Scaled parameters

Compare image length ( $l$ ) and width ( $w$ ) with expectation value and variance from simulations as function of image charge ( $q$ ), impact distance ( $d$ ), and telescope type ( $t$ ):

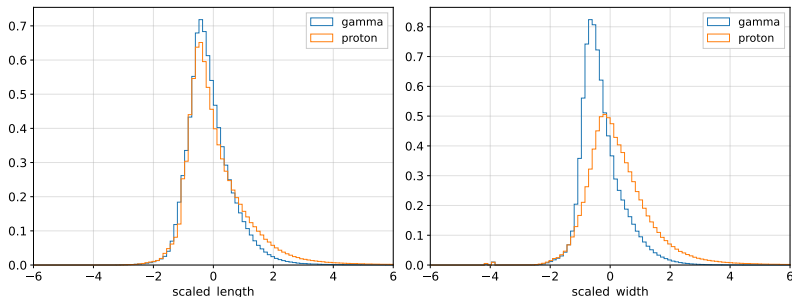
$$SL = \frac{l(q, d, t) - \langle l(q, d, t) \rangle}{\sigma_l(q, d, t)}$$

$$SW = \frac{w(q, d, t) - \langle w(q, d, t) \rangle}{\sigma_w(q, d, t)}$$

Easy combination for stereo observations:

$$MSL = \frac{\sum_{\text{tels}} SL}{\sqrt{n_{\text{tels}}}}$$

$$MSW = \frac{\sum_{\text{tels}} SW}{\sqrt{n_{\text{tels}}}}$$



## MRMR feature selection – Energy

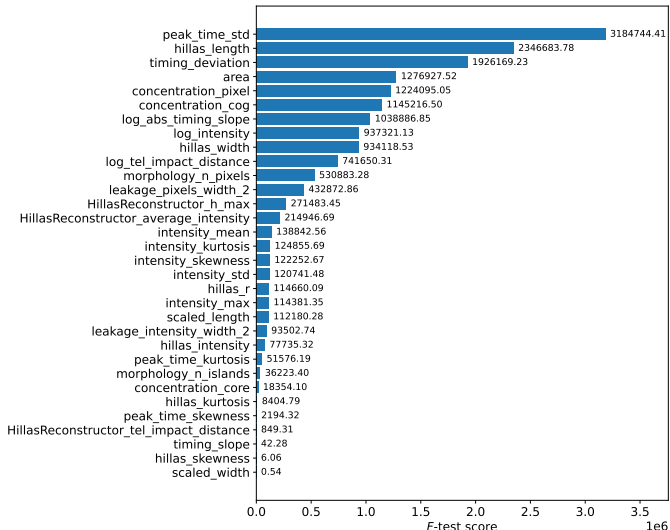
At each iteration  $i$  compute  $score_i$  for all  $f$  not yet selected

$$score_i(f) = \frac{relevance(f | target)}{redundancy(f | f_{\text{already selected}})}$$

and add the feature with the highest score.

### Energy features (15)

- peak\_time\_std
- intensity\_std
- timing\_deviation
- hillas\_length
- concentration\_pixel
- leakage\_intensity\_width\_2
- log\_abs\_timing\_slope
- area
- concentration\_cog
- log\_tel\_impact\_distance
- hillas\_width
- log\_intensity
- morphology\_n\_pixels
- HillasReconstructor\_h\_max
- leakage\_pixels\_width\_2



## MRMR feature selection – Particle Id

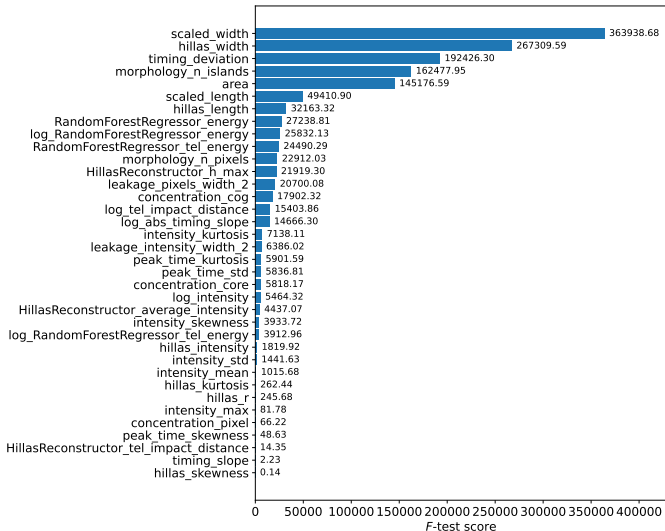
At each iteration  $i$  compute  $score_i$  for all  $f$  not yet selected

$$score_i(f) = \frac{relevance(f | target)}{redundancy(f | f_{\text{already selected}})}$$

and add the feature with the highest score.

### Particle Id features (15)

- scaled\_width
- HillasReconstructor\_h\_max
- log\_tel\_impact\_distance
- hillas\_width
- morphology\_n\_islands
- timing\_deviation
- area
- scaled\_length
- RandomForestRegressor\_energy
- log\_RandomForestRegressor\_energy
- leakage\_pixels\_width\_2
- hillas\_length
- peak\_time\_kurtosis
- RandomForestRegressor\_tel\_energy
- morphology\_n\_pixels



## MRRM feature selection – disp

At each iteration  $i$  compute  $score_i$  for all  $f$  not yet selected

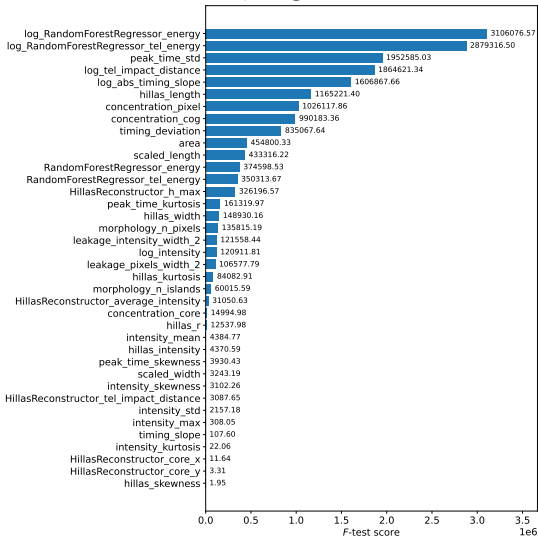
$$score_i(f) = \frac{relevance(f | target)}{redundancy(f | f_{\text{already selected}})}$$

and add the feature with the highest score.

### disp features (19)

- log\_RandomForestRegressor\_energy
- log\_tel\_impact\_distance
- log\_RandomForestRegressor\_tel\_energy
- log\_abs\_timing\_slope
- peak\_time\_std
- concentration\_pixel
- hillas\_length
- concentration\_cog
- timing\_deviation
- scaled\_length
- HillasReconstructor\_h\_max
- RandomForestRegressor\_energy
- area
- peak\_time\_kurtosis
- RandomForestRegressor\_tel\_energy
- timing\_slope
- hillas\_skewness
- HillasReconstructor\_core\_x
- HillasReconstructor\_core\_y

### |disp| regressor



## MRMR feature selection – disp

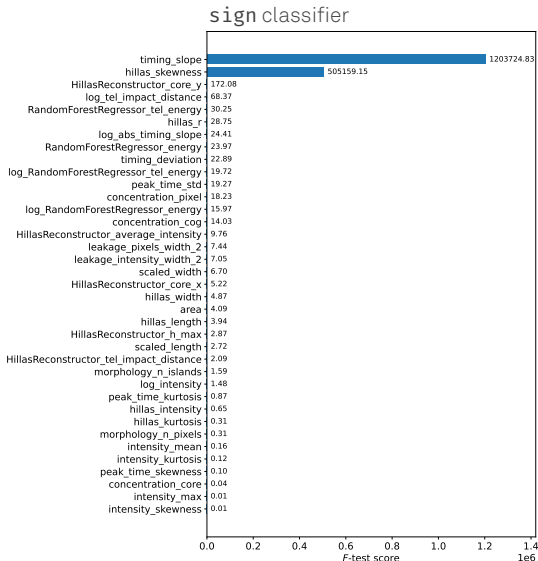
At each iteration  $i$  compute  $score_i$  for all  $f$  not yet selected

$$score_i(f) = \frac{\text{relevance}(f | \text{target})}{\text{redundancy}(f | f_{\text{already selected}})}$$

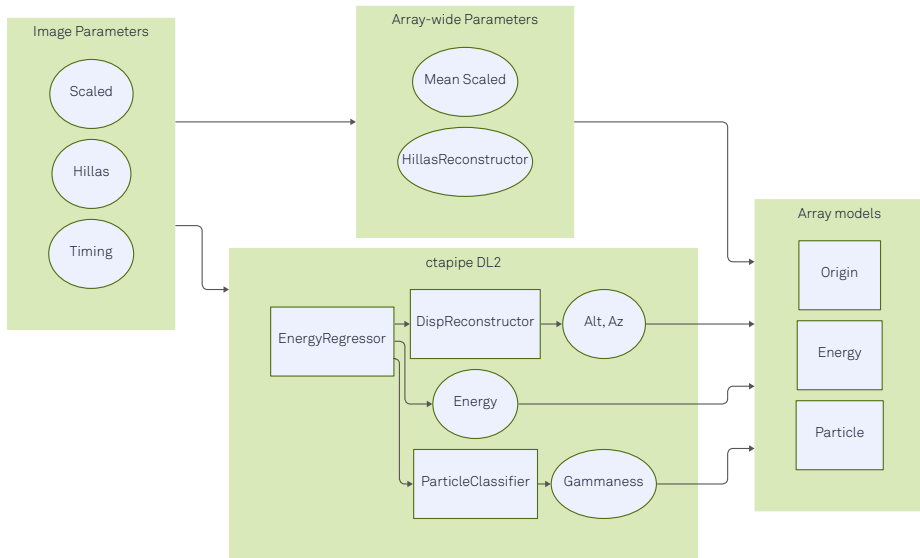
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Concept



Scaled Parameters and Feature Selection

# Energy Regression

## Energy Regression (Telescope)

Randomized hyperparameter optimization yields:

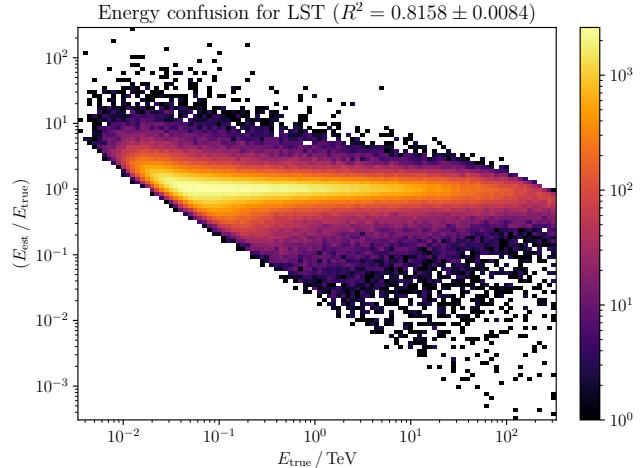
### Configuration energy regressor

```
EnergyRegressor:
  model_cls: RandomForestRegressor
  model_config:
    n_estimators: 69
    max_features: 0.5227
    max_samples: 0.7138
    min_samples_leaf: 0.000013
    n_jobs: 40

  log_target: True
```

5-fold cross-validation:

- 551 635 LST events
- 1 199 782 MST events





## Energy Regression (Telescope)

Randomized hyperparameter optimization yields:

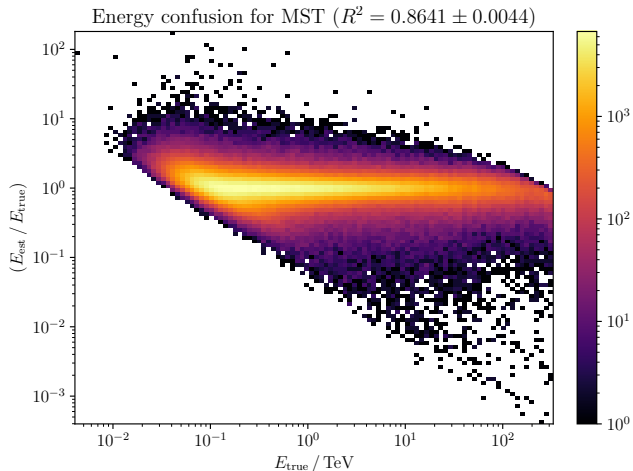
### Configuration energy regressor

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## Energy Regression (Telescope)

Randomized hyperparameter optimization yields:

### Configuration energy regressor

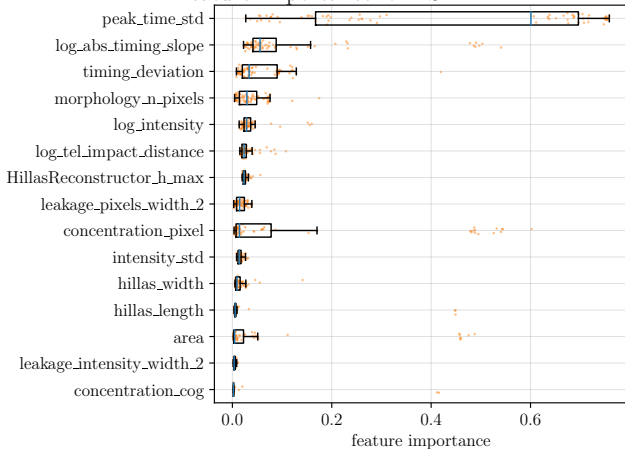
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EnergyRegressor:
model_cls: RandomForestRegressor
model_config:
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### Feature Importance for LST



## Energy Regression (Telescope)

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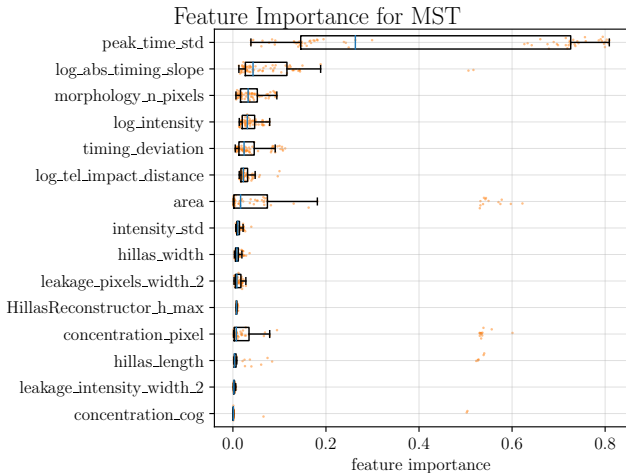
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5-fold cross-validation:

- 551 635 LST events
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## Energy Regression (Array)

- Use (averaged) telescope predictions and array-wide features
- No hyperparameter optimization (yet)
- 5-fold cross-validation on 461 969 events

### Configuration array energy regressor

```

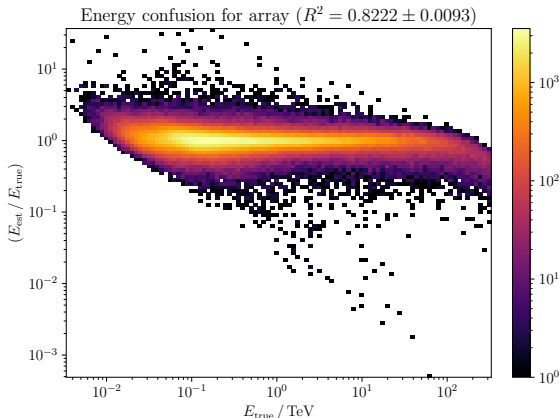
model_cls: RandomForestRegressor
model_config:
  n_estimators: 200
  max_features: "sqrt"
  min_samples_leaf: 0.00001
  n_jobs: 40

log_target: True

features:
  - n_telescopes_HillasReconstructor
  - n_LST_HillasReconstructor
  - n_MST_HillasReconstructor
  - mean_scaled_length
  - mean_scaled_width
  - HillasReconstructor_core_x
  - HillasReconstructor_core_y
  - HillasReconstructor_average_intensity
  - HillasReconstructor_h_max
  - HillasReconstructor_alt
  - HillasReconstructor_az
  - RandomForestClassifier_prediction
  - RandomForestRegressor_energy
    
```

## Energy Regression (Array)

- Use (averaged) telescope predictions and array-wide features
- No hyperparameter optimization (yet)
- 5-fold cross-validation on 461 969 events



### Configuration array energy regressor

```

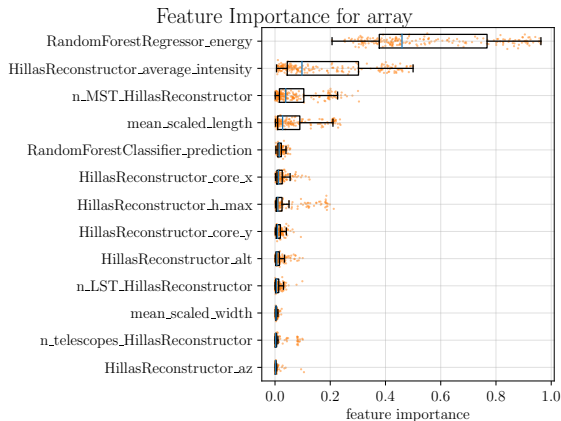
model_cls: RandomForestRegressor
model_config:
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  n_jobs: 40

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- 5-fold cross-validation on **461 969** events



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  min_samples_leaf: 0.00001
  n_jobs: 40
```

```
log_target: True
```

#### features:

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- n\_LST\_HillasReconstructor
- n\_MST\_HillasReconstructor
- mean\_scaled\_length
- mean\_scaled\_width
- HillasReconstructor\_core\_x
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- RandomForestClassifier\_prediction
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## Gamma-Hadron Classification

## Gamma-Hadron Classification (Telescope)

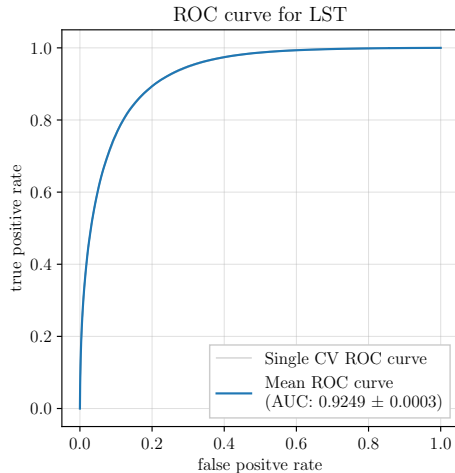
Randomized hyperparameter optimization yields:

Configuration particle classifier

```
ParticleClassifier:
  model_cls: RandomForestClassifier
  model_config:
    n_estimators: 69
    max_features: 0.5227
    max_samples: 0.7138
    min_samples_leaf: 0.000013
    n_jobs: 40
```

5-fold cross-validation:

- LST: 552 754 signal + 561 171 background events
- MST: 1 199 267 signal + 1 122 374 background events





## Gamma-Hadron Classification (Telescope)

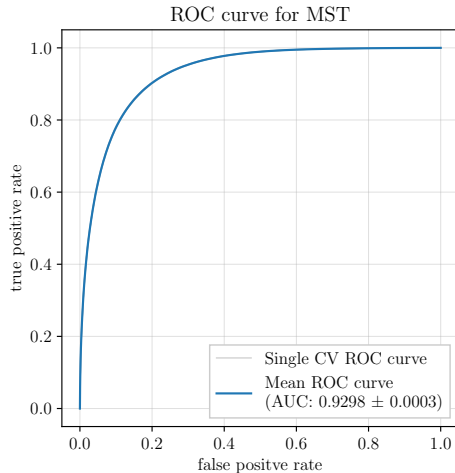
Randomized hyperparameter optimization yields:

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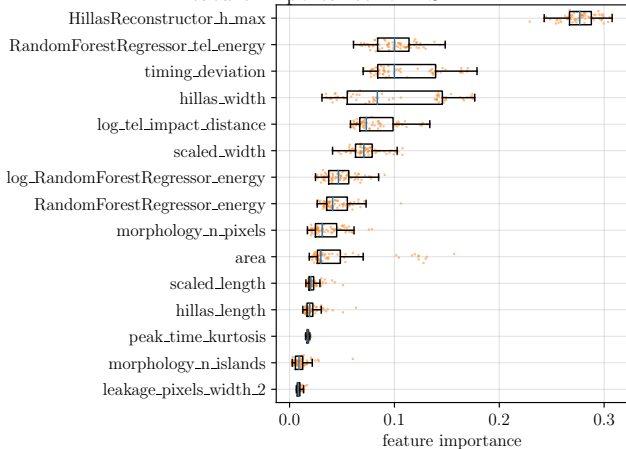
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### Feature Importance for LST



## Gamma-Hadron Classification (Telescope)

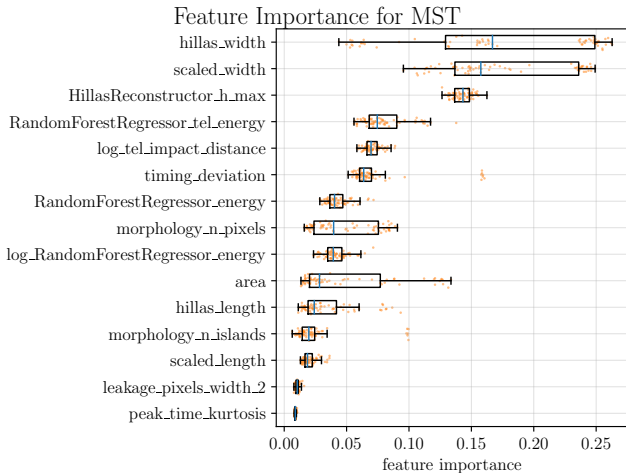
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## Gamma-Hadron Classification (Array)

- Use (averaged) telescope predictions and array-wide features
- No hyperparameter optimization (yet)
- 5-fold cross-validation on 910 387 events

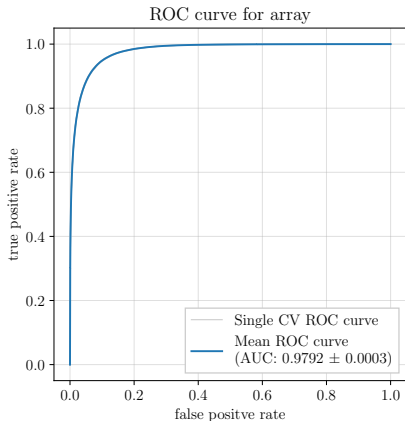
### Configuration array particle classifier

```
model_cls: RandomForestClassifier
model_config:
  n_estimators: 200
  max_features: "sqrt"
  min_samples_leaf: 0.00001
  n_jobs: 40

features:
- n_telescopes_HillasReconstructor
- n_LST_HillasReconstructor
- n_MST_HillasReconstructor
- mean_scaled_length
- mean_scaled_width
- HillasReconstructor_core_x
- HillasReconstructor_core_y
- HillasReconstructor_average_intensity
- HillasReconstructor_h_max
- HillasReconstructor_alt
- HillasReconstructor_az
- RandomForestClassifier_prediction
- RandomForestRegressor_energy
```

## Gamma-Hadron Classification (Array)

- Use (averaged) telescope predictions and array-wide features
- No hyperparameter optimization (yet)
- 5-fold cross-validation on **910 387** events



### Configuration array particle classifier

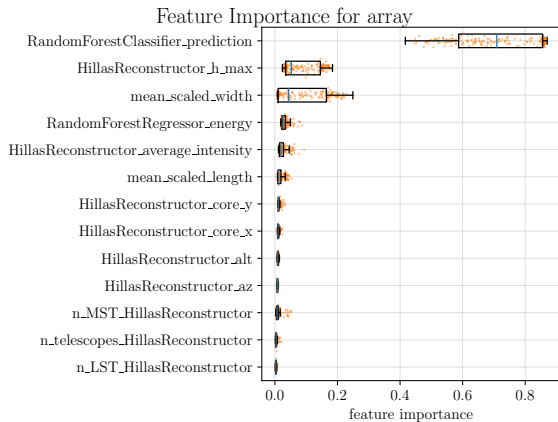
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model_config:
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  max_features: "sqrt"
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  - n_LST_HillasReconstructor
  - n_MST_HillasReconstructor
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  - RandomForestClassifier_prediction
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```

## Gamma-Hadron Classification (Array)

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- 5-fold cross-validation on 910 387 events



### Configuration array particle classifier

```

model_cls: RandomForestClassifier
model_config:
  n_estimators: 200
  max_features: "sqrt"
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  n_jobs: 40
  
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### features:

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- n\_LST\_HillasReconstructor
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- HillasReconstructor\_az
- RandomForestClassifier\_prediction
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## Origin Reconstruction

## Origin Reconstruction using disp

Randomized hyperparameter optimization yields:

### Configuration disp reconstructor

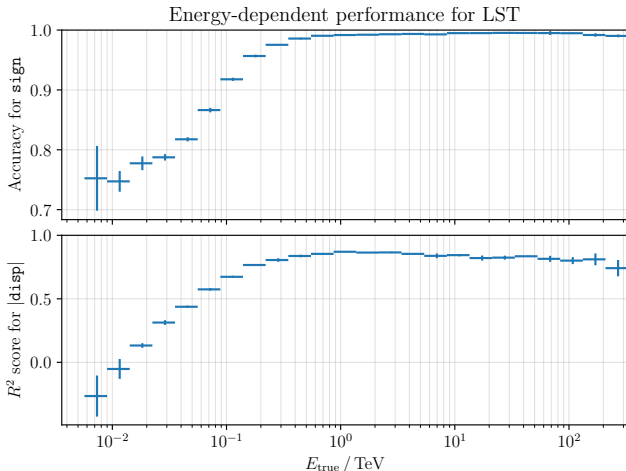
```
norm_cls: RandomForestRegressor
norm_config:
  n_estimators: 69
  max_features: 0.5227
  max_samples: 0.7138
  min_samples_leaf: 0.000013
  n_jobs: 40
```

```
log_target: True
```

```
sign_cls: RandomForestClassifier
sign_config:
  n_estimators: 343
  max_features: 0.6587
  max_samples: 0.5815
  min_samples_leaf: 0.000035
  n_jobs: 40
```

5-fold cross-validation:

- 552 754 LST events
- 1 199 267 MST events





## Origin Reconstruction using disp

Randomized hyperparameter optimization yields:

### Configuration disp reconstructor

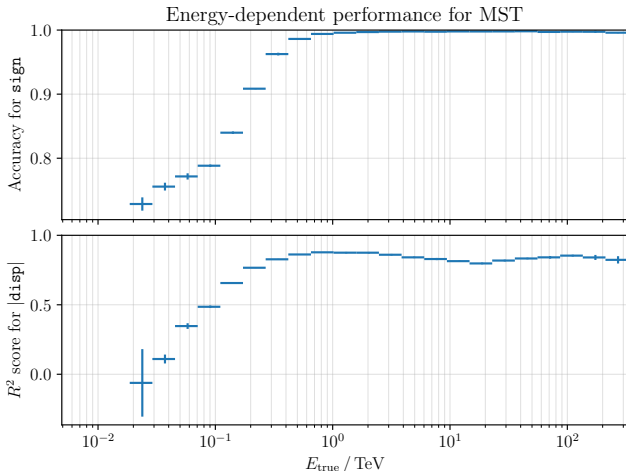
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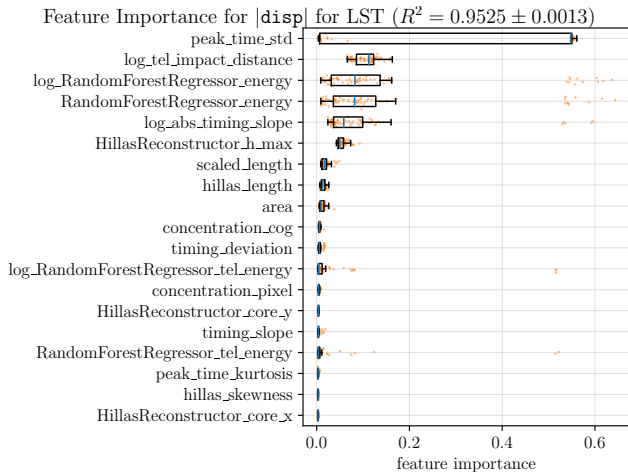
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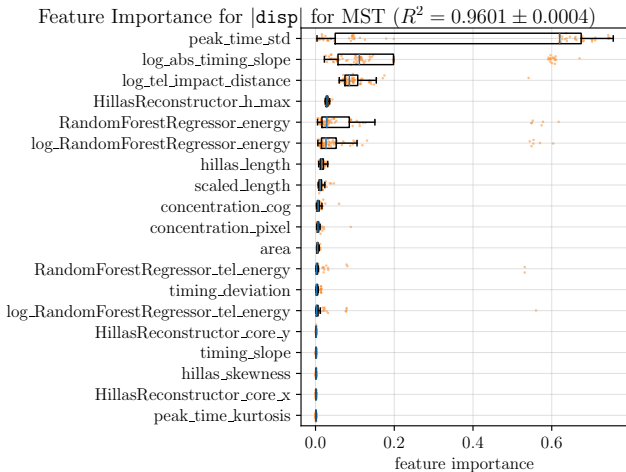
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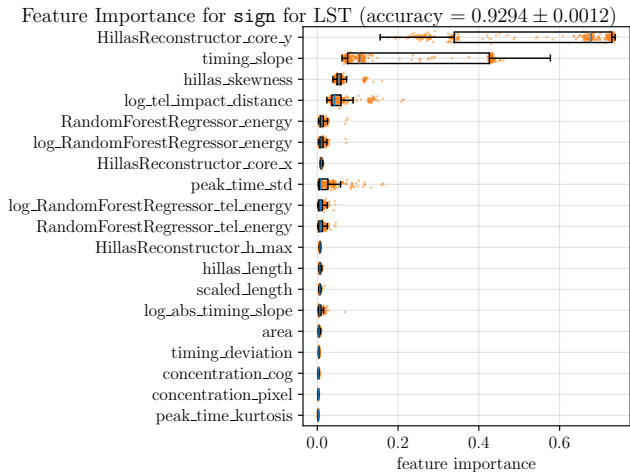
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  n_jobs: 40
```

```
log_target: True
```

```
sign_cls: RandomForestClassifier
sign_config:
  n_estimators: 343
  max_features: 0.6587
  max_samples: 0.5815
  min_samples_leaf: 0.000035
  n_jobs: 40
```

5-fold cross-validation:

■ 552 754 LST events    ■ 1 199 267 MST events



## Origin Reconstruction using disp

Randomized hyperparameter optimization yields:

### Configuration disp reconstructor

`norm_cls: RandomForestRegressor`

`norm_config:`

```
n_estimators: 69
max_features: 0.5227
max_samples: 0.7138
min_samples_leaf: 0.000013
n_jobs: 40
```

`log_target: True`

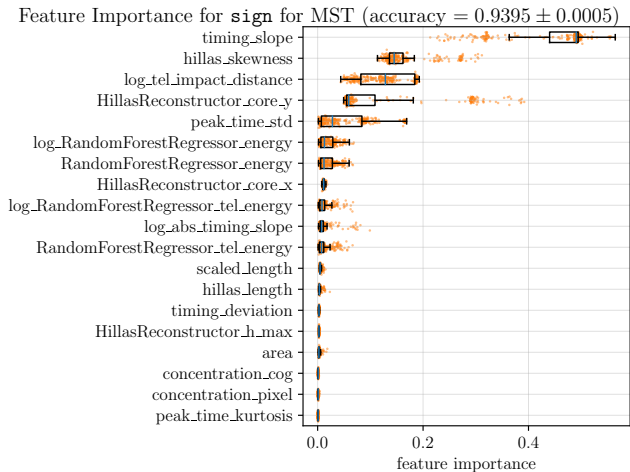
`sign_cls: RandomForestClassifier`

`sign_config:`

```
n_estimators: 343
max_features: 0.6587
max_samples: 0.5815
min_samples_leaf: 0.000035
n_jobs: 40
```

5-fold cross-validation:

■ 552 754 LST events    ■ 1 199 267 MST events



## Origin Reconstruction (Array)

- Predict 3D cartesian position based on unit-sphere (1, *alt*, *az*)
- Use (averaged) telescope predictions and array-wide features
- No hyperparameter optimization (yet)
- 5-fold cross-validation on 461 212 events

### Configuration (every) array origin regressor

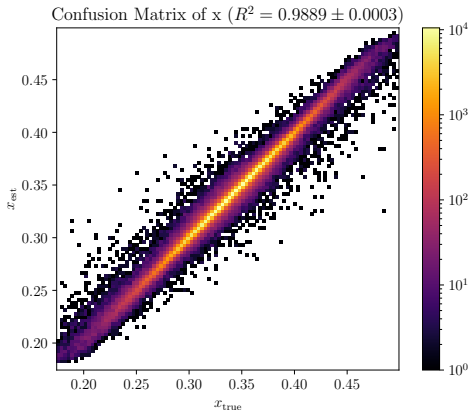
```

model_cls: RandomForestRegressor
model_config:
  n_estimators: 200
  max_features: "sqrt"
  min_samples_leaf: 0.00001
  n_jobs: 40

features:
- n_telescopes_HillasReconstructor
- n_LST_HillasReconstructor
- n_MST_HillasReconstructor
- mean_scaled_length
- mean_scaled_width
- HillasReconstructor_core_x
- HillasReconstructor_core_y
- HillasReconstructor_average_intensity
- HillasReconstructor_h_max
- HillasReconstructor_alt
- HillasReconstructor_az
- disp_alt
- disp_az
- disp_ang_distance_uncert
- RandomForestClassifier_prediction
- RandomForestRegressor_energy
  
```

## Origin Reconstruction (Array)

- Predict 3D cartesian position based on unit-sphere (1, *alt*, *az*)
- Use (averaged) telescope predictions and array-wide features
- No hyperparameter optimization (yet)
- 5-fold cross-validation on 461 212 events



### Configuration (every) array origin regressor

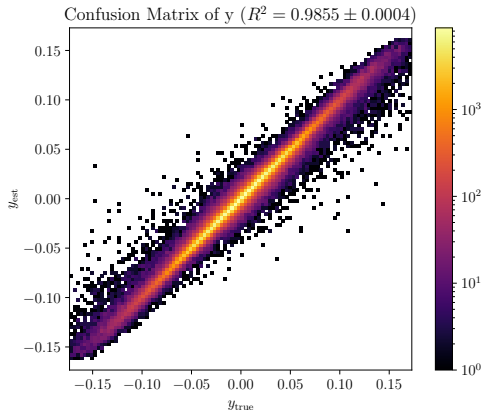
```
model_cls: RandomForestRegressor
model_config:
  n_estimators: 200
  max_features: "sqrt"
  min_samples_leaf: 0.00001
  n_jobs: 40
```

#### features:

- n\_telescopes\_HillasReconstructor
- n\_LST\_HillasReconstructor
- n\_MST\_HillasReconstructor
- mean\_scaled\_length
- mean\_scaled\_width
- HillasReconstructor\_core\_x
- HillasReconstructor\_core\_y
- HillasReconstructor\_average\_intensity
- HillasReconstructor\_h\_max
- HillasReconstructor\_alt
- HillasReconstructor\_az
- disp\_alt
- disp\_az
- disp\_ang\_distance\_uncert
- RandomForestClassifier\_prediction
- RandomForestRegressor\_energy

## Origin Reconstruction (Array)

- Predict 3D cartesian position based on unit-sphere (1, *alt*, *az*)
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### Configuration (every) array origin regressor

```
model_cls: RandomForestRegressor
model_config:
  n_estimators: 200
  max_features: "sqrt"
  min_samples_leaf: 0.00001
  n_jobs: 40
```

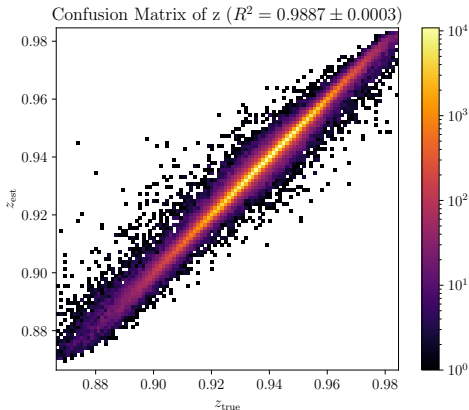
#### features:

- n\_telescopes\_HillasReconstructor
- n\_LST\_HillasReconstructor
- n\_MST\_HillasReconstructor
- mean\_scaled\_length
- mean\_scaled\_width
- HillasReconstructor\_core\_x
- HillasReconstructor\_core\_y
- HillasReconstructor\_average\_intensity
- HillasReconstructor\_h\_max
- HillasReconstructor\_alt
- HillasReconstructor\_az
- disp\_alt
- disp\_az
- disp\_ang\_distance\_uncert
- RandomForestClassifier\_prediction
- RandomForestRegressor\_energy



## Origin Reconstruction (Array)

- Predict 3D cartesian position based on unit-sphere ( $1, alt, az$ )
- Use (averaged) telescope predictions and array-wide features
- No hyperparameter optimization (yet)
- 5-fold cross-validation on 461 212 events



### Configuration (every) array origin regressor

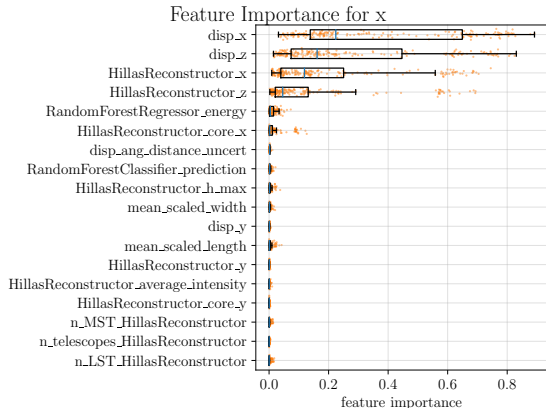
```
model_cls: RandomForestRegressor
model_config:
  n_estimators: 200
  max_features: "sqrt"
  min_samples_leaf: 0.00001
  n_jobs: 40
```

#### features:

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- Predict 3D cartesian position based on unit-sphere (1, *alt*, *az*)
- Use (averaged) telescope predictions and array-wide features
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- 5-fold cross-validation on 461 212 events



### Configuration (every) array origin regressor

```

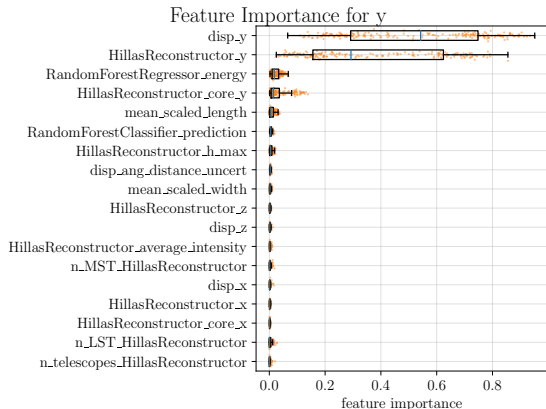
model_cls: RandomForestRegressor
model_config:
  n_estimators: 200
  max_features: "sqrt"
  min_samples_leaf: 0.00001
  n_jobs: 40
  
```

### features:

- n\_telescopes\_HillasReconstructor
- n\_LST\_HillasReconstructor
- n\_MST\_HillasReconstructor
- mean\_scaled\_length
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- HillasReconstructor\_core\_x
- HillasReconstructor\_core\_y
- HillasReconstructor\_average\_intensity
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- RandomForestClassifier\_prediction
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## Origin Reconstruction (Array)

- Predict 3D cartesian position based on unit-sphere (1, *alt*, *az*)
- Use (averaged) telescope predictions and array-wide features
- No hyperparameter optimization (yet)
- 5-fold cross-validation on 461 212 events



### Configuration (every) array origin regressor

```

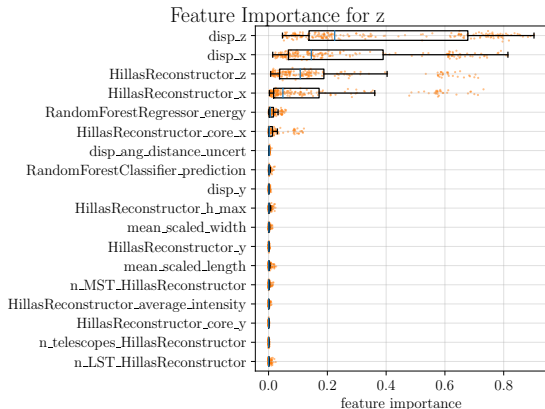
model_cls: RandomForestRegressor
model_config:
  n_estimators: 200
  max_features: "sqrt"
  min_samples_leaf: 0.00001
  n_jobs: 40
  
```

### features:

- n\_telescopes\_HillasReconstructor
- n\_LST\_HillasReconstructor
- n\_MST\_HillasReconstructor
- mean\_scaled\_length
- mean\_scaled\_width
- HillasReconstructor\_core\_x
- HillasReconstructor\_core\_y
- HillasReconstructor\_average\_intensity
- HillasReconstructor\_h\_max
- HillasReconstructor\_alt
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- RandomForestClassifier\_prediction
- RandomForestRegressor\_energy

## Origin Reconstruction (Array)

- Predict 3D cartesian position based on unit-sphere (1, *alt*, *az*)
- Use (averaged) telescope predictions and array-wide features
- No hyperparameter optimization (yet)
- 5-fold cross-validation on 461 212 events



### Configuration (every) array origin regressor

```

model_cls: RandomForestRegressor
model_config:
  n_estimators: 200
  max_features: "sqrt"
  min_samples_leaf: 0.00001
  n_jobs: 40
  
```

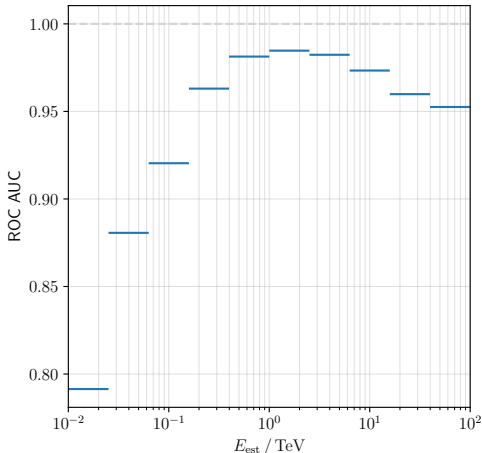
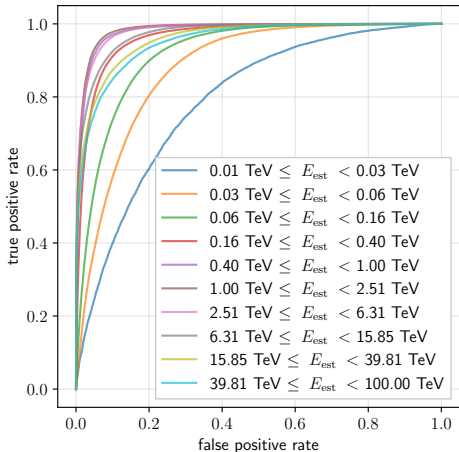
### features:

- n\_telescopes\_HillasReconstructor
- n\_LST\_HillasReconstructor
- n\_MST\_HillasReconstructor
- mean\_scaled\_length
- mean\_scaled\_width
- HillasReconstructor\_core\_x
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- HillasReconstructor\_alt
- HillasReconstructor\_az
- disp\_alt
- disp\_az
- disp\_ang\_distance\_uncert
- RandomForestClassifier\_prediction
- RandomForestRegressor\_energy

## Performance

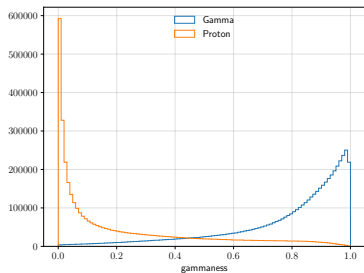
Gamma-Hadron Performance (Energy-Dependent)

Array classifier

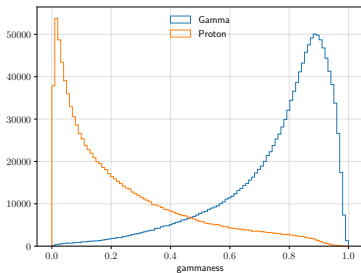


## Gamma-Hadron Scores

Single telescope predictions

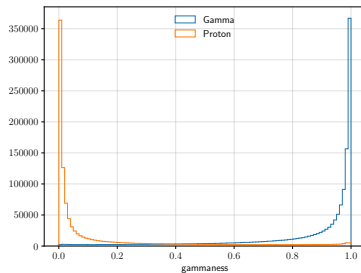


Averaged telescope predictions



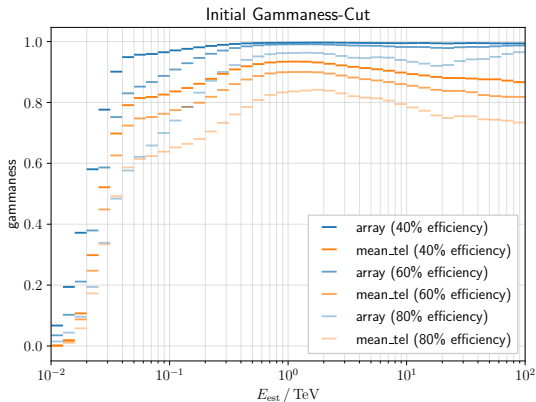
ROC AUC = 0.9442

Array classifier predictions



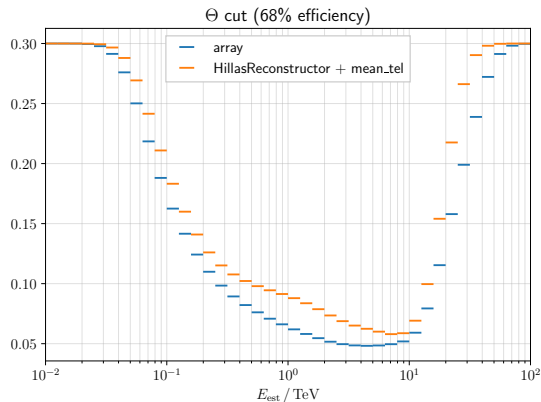
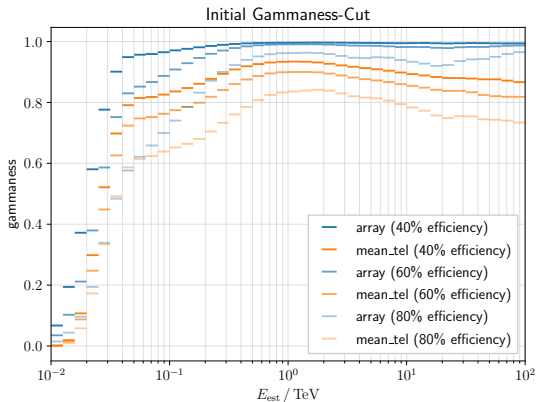
ROC AUC = 0.9538

## Gammaness and $\theta$ Cuts





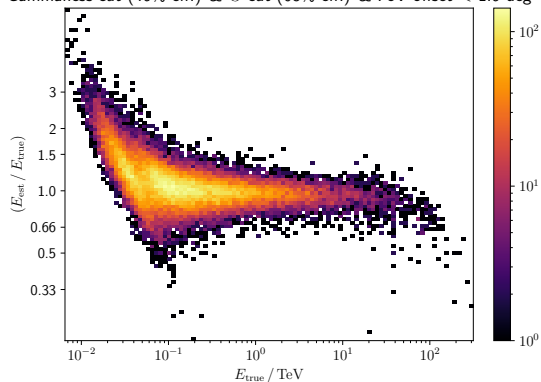
## Gammaness and $\theta$ Cuts



## Energy Migration

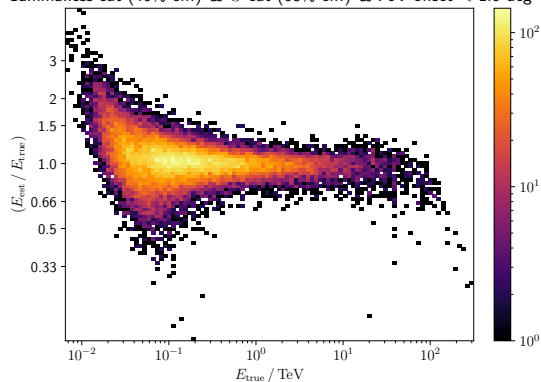
Mean telescope predictions

Gammaness cut (40% eff.) &  $\Theta$  cut (68% eff.) & FoV offset < 1.0 deg



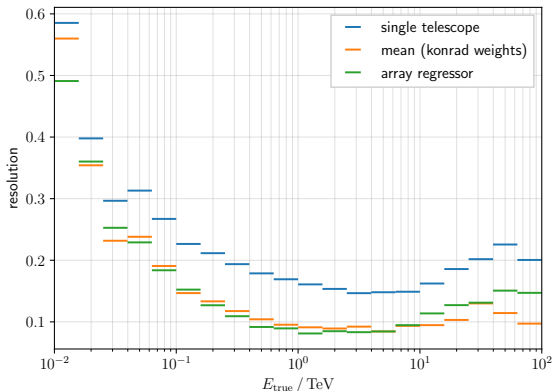
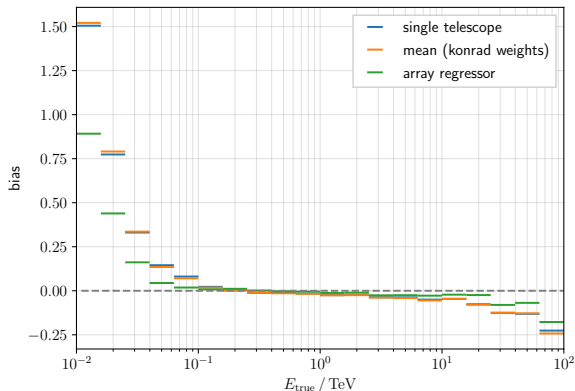
Array regressor

Gammaness cut (40% eff.) &  $\Theta$  cut (68% eff.) & FoV offset < 1.0 deg



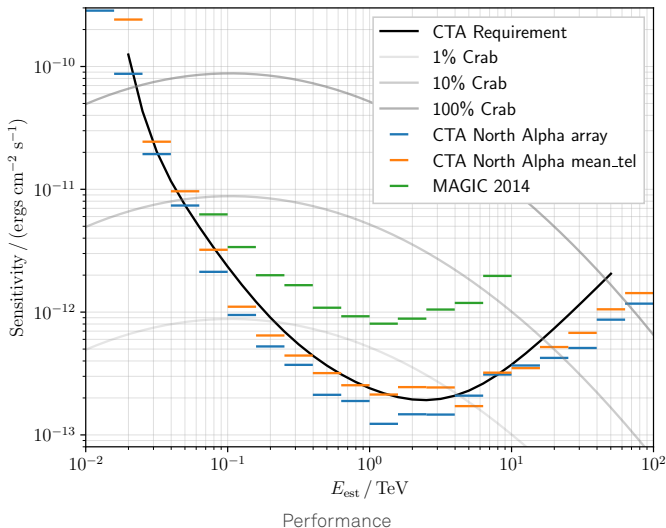
## Energy – Bias and Resolution

Gammaness cut (40% eff.) &  $\Theta$  cut (68% eff.) & FoV offset < 1.0 deg



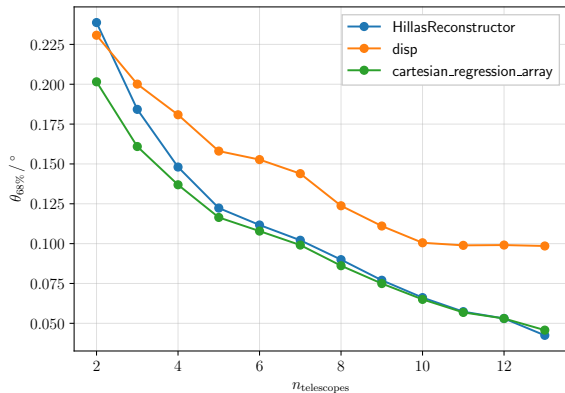
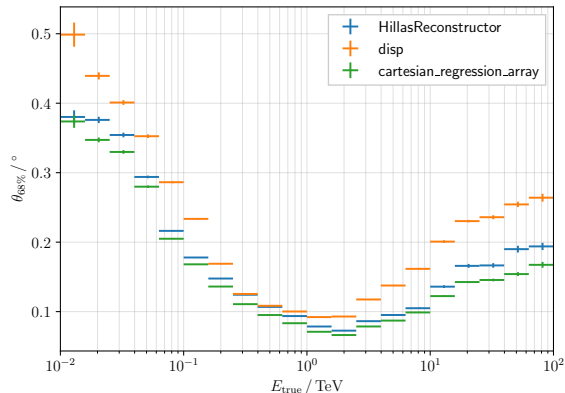
## Sensitivity

⇒ This and all following plots use gammaness cuts optimized for maximum sensitivity!



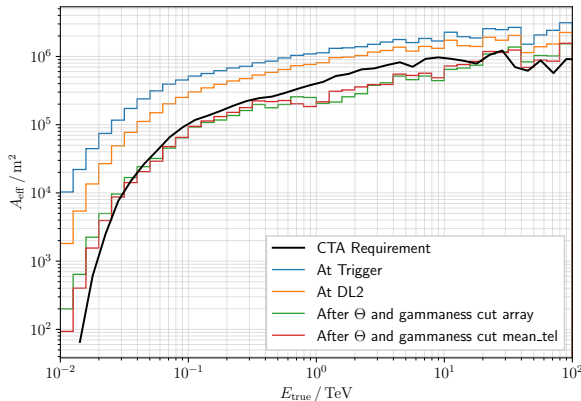
## Angular Resolution

Optimized gammaness cut

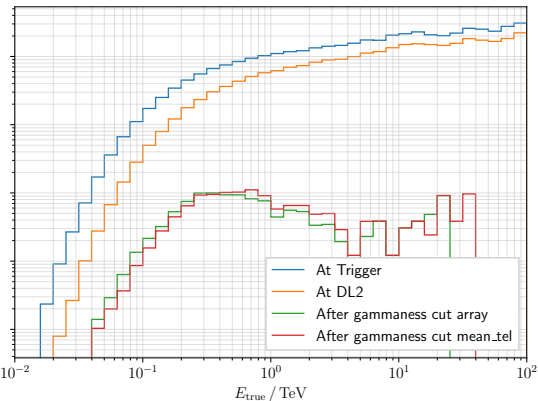


Effective Area

Effective Area for Gammas



Effective Area for Protons



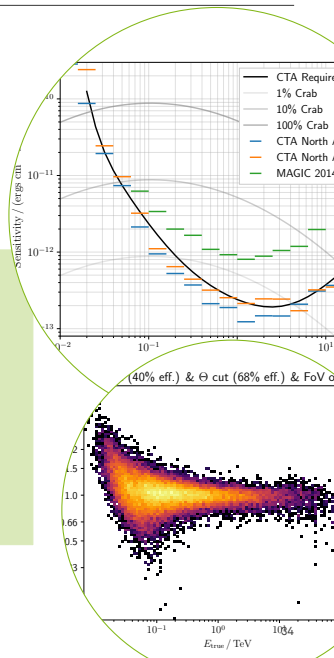
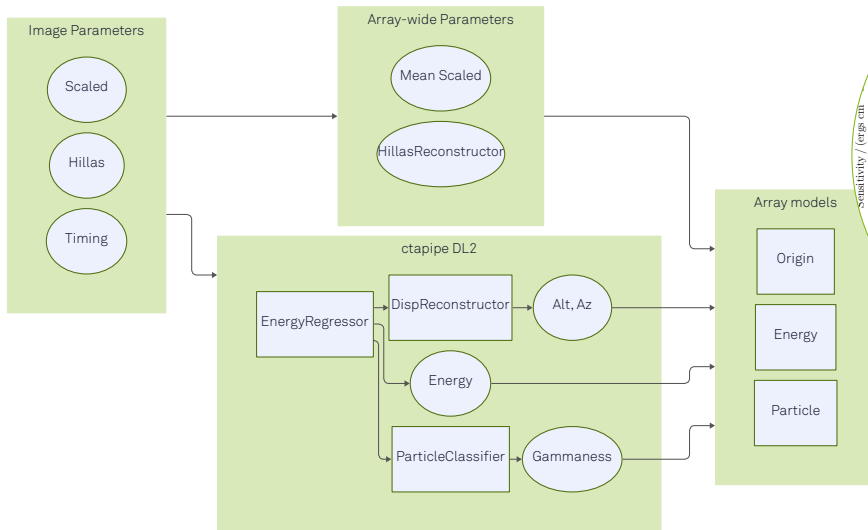
## Outlook

## TODO

- Separate dataset for array models → optimize hyperparameters
- Try other methods for averaging disp predictions (→ Lukas' master thesis)
- Telescope models using only mono features → include “mono” events
- Try other ML algorithms (e.g. boosted decision trees) incl. hyperparameter optimization

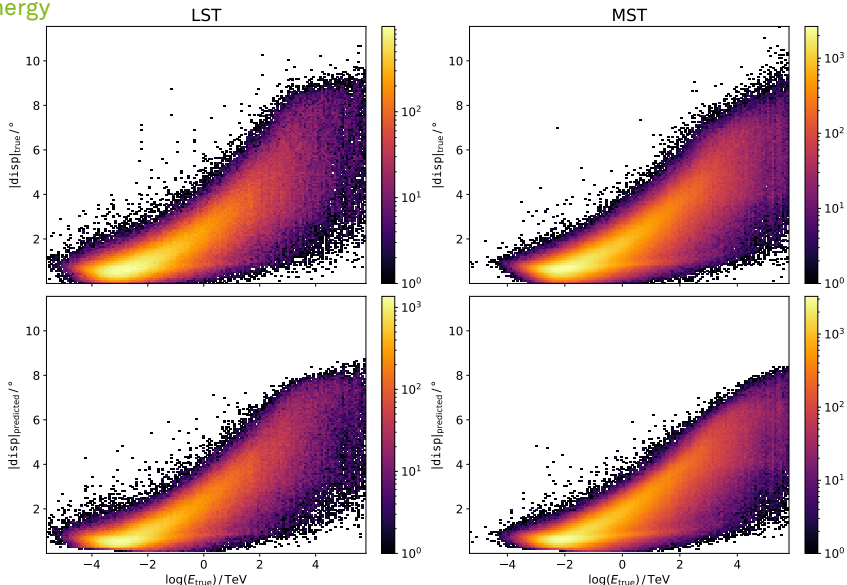


## Summary

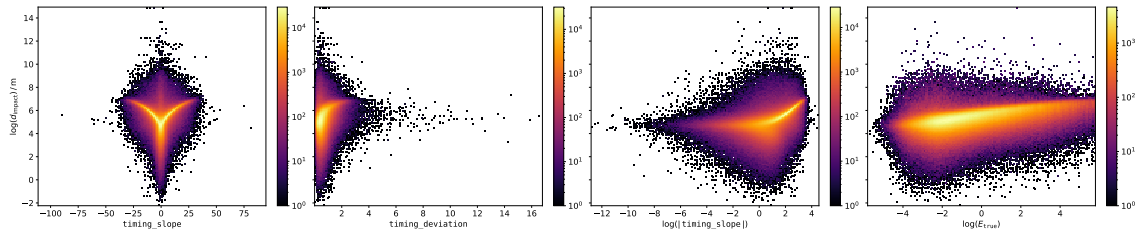


## Backup

**|disp| vs Energy**



## Timing Parameters vs Impact Distance



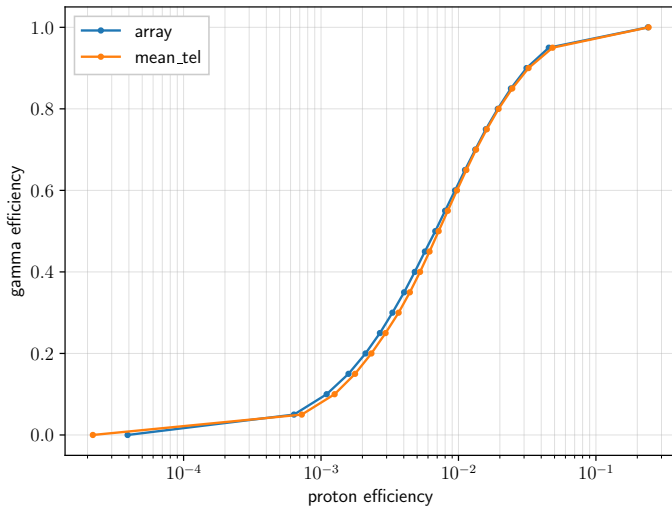
## Quality Cuts

### QualityQuery

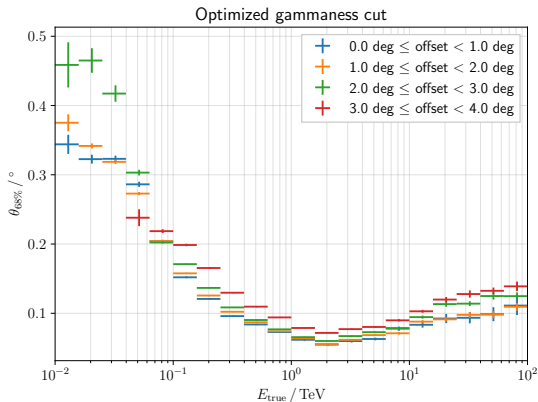
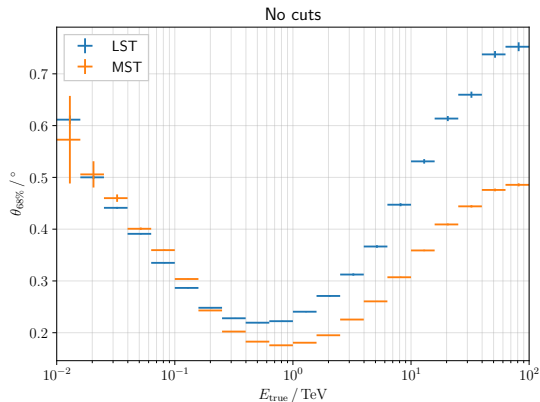
#### quality\_criteria:

- ["enough intensity", "hillas\_intensity > 50"]
- ["Positive width", "hillas\_width > 0"]
- ["enough pixels", "morphology\_n\_pixels > 3"]
- ["not clipped", "leakage\_intensity\_width\_2 < 0.5"]
- ["HillasValid", "HillasReconstructor\_is\_valid"]

## Background Rejection

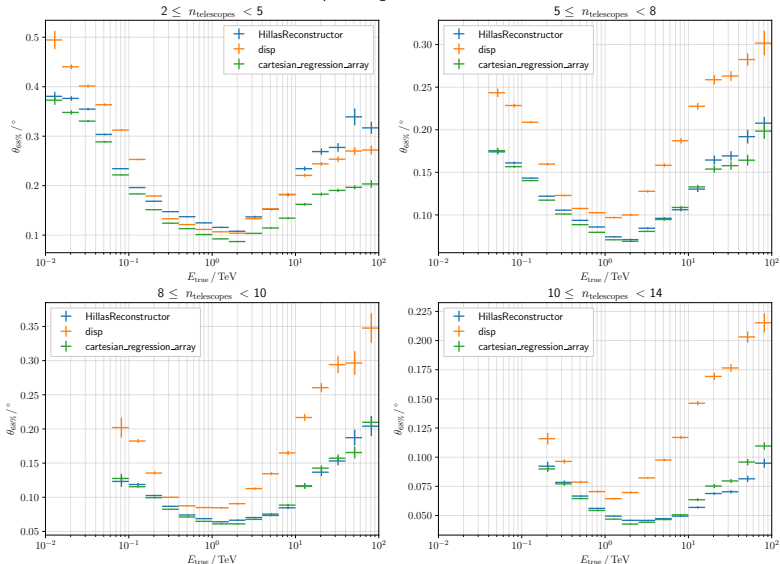


## Angular Resolution – More Plots



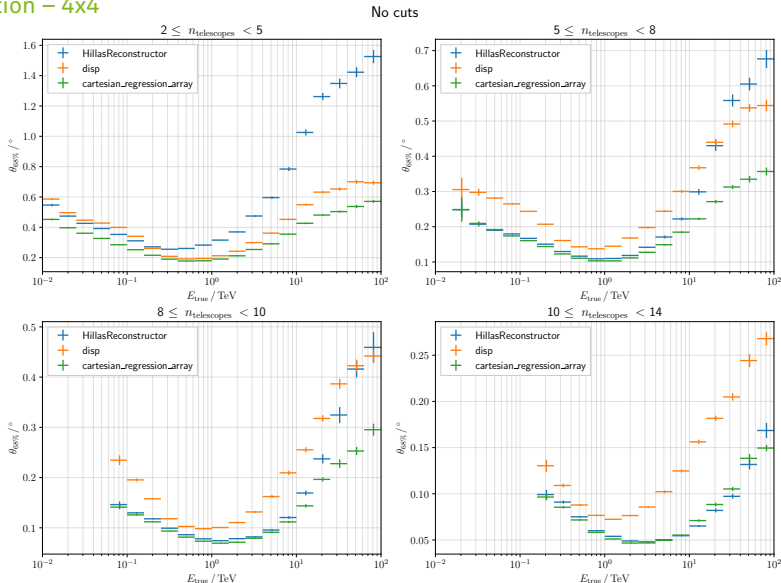
Angular Resolution – 4x4

Optimized gammaness cut





## Angular Resolution – 4x4



Outlook

Error of Mean disp Predicitons

