Machine Learning: Lecture II

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SLAC

CERN Academic Training Lectures

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Lecture Topics

- <u>Recap of last time</u>
  - What is Machine Learning
  - Linear Regression
  - Logistic Regression
  - Over fitting and Regularization
  - Training procedures and cross validation
  - Gradient descent

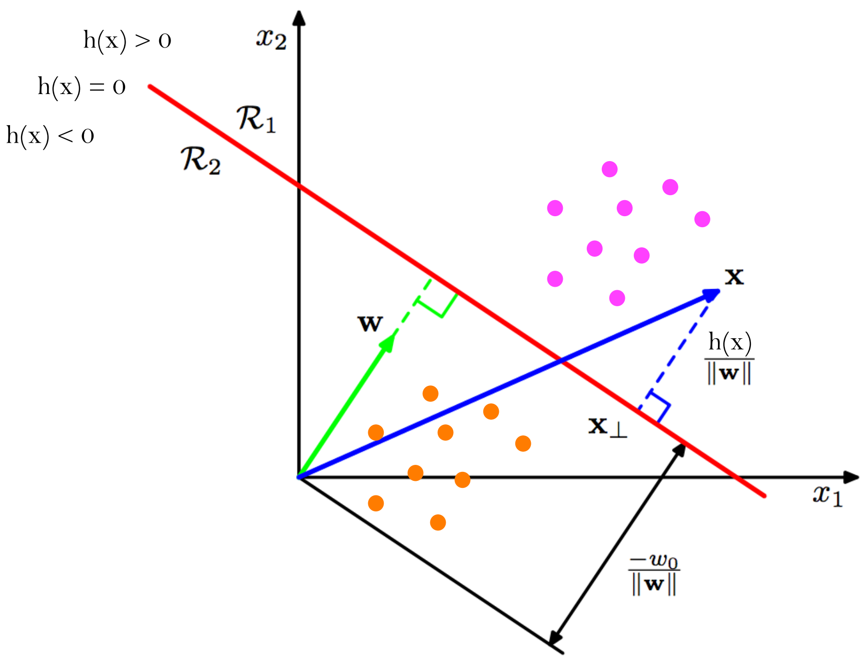
- <u>This Lecture</u>
  - Neural Networks → Just an intro, more on this tomorrow!
  - Decision Trees and Ensemble Methods
  - Unsupervised Learning
    - Dimensionality reduction
    - Clustering
  - No Free Lunch and Practical Advice

Neural Networks

Reminder of Logistic Regression

- Input output pairs $\{x_i, y_i\}$, with
  - $\mathbf{x}_i \in \mathbb{R}^m$
  - $y_i \in \{0,1\}$

- Linear decision boundary $$h(\mathbf{x}; \mathbf{w}) = \mathbf{w}^T \mathbf{x}$$



[Bishop]

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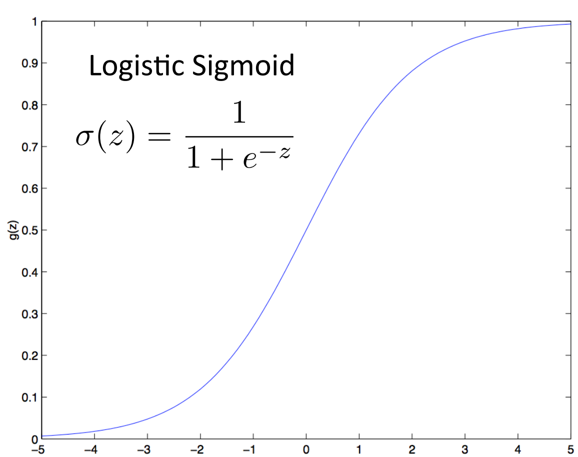
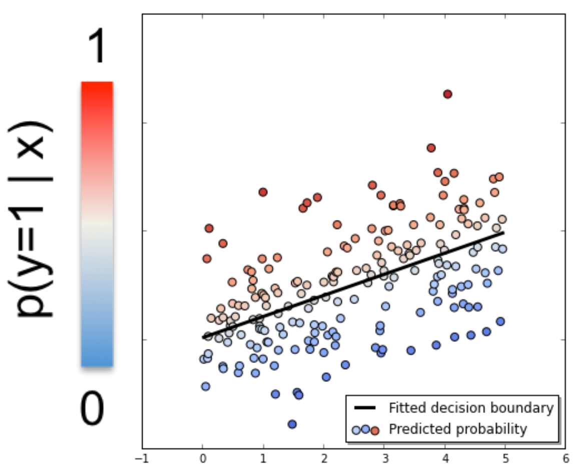
- Linear decision boundary

$$h(\mathbf{x};\mathbf{w}) = \mathbf{w}^T\mathbf{x}$$

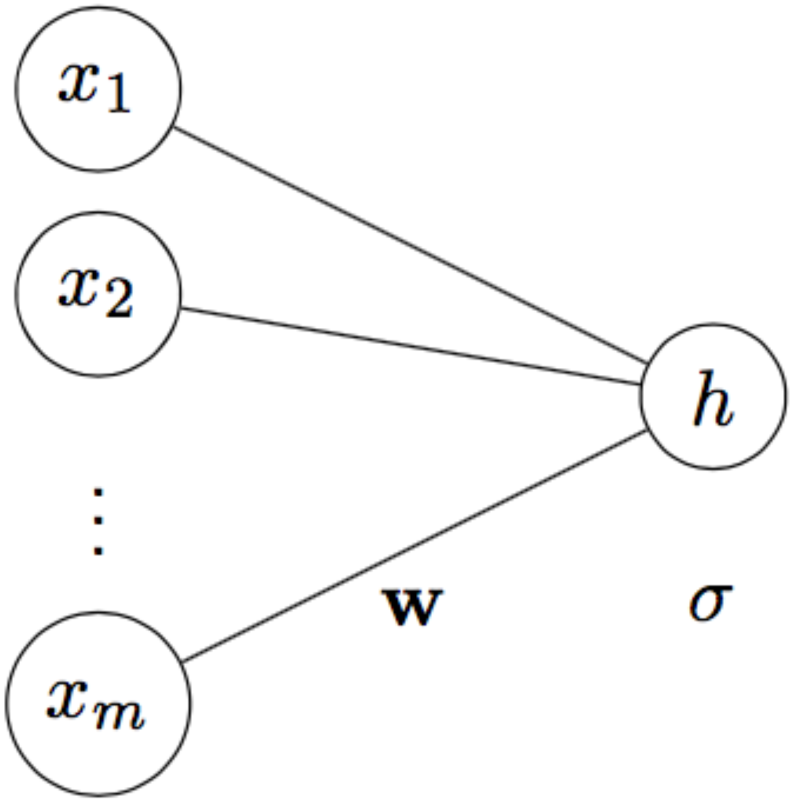
- Distance from decision boundary is converted to class probability using logistic sigmoid function

$$p(y=1|\mathbf{x}) = \sigma(h(\mathbf{x},\mathbf{w})) = \frac{1}{1+e^{-\mathbf{w}^T\mathbf{x}}}$$





Logistic Regression



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Adding non-linearity

- What if we want a non-linear decision boundary?

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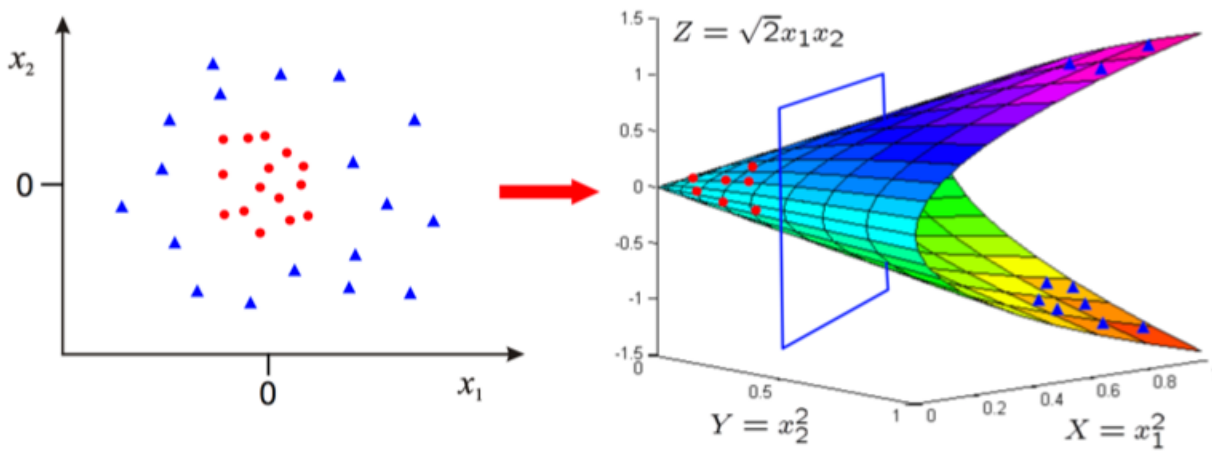
  - Choose basis functions, e.g: $\phi(x) \sim \{x^2, \sin(x), \log(x), \ldots\}$

$$p(y = 1|\mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w}^T \phi(\mathbf{x})}}$$

$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \to \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1 x_2 \end{pmatrix} \qquad \mathbb{R}^2 \to \mathbb{R}^3$$



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- What if we don't know what basis functions we want?

- Learn the basis functions directly from data

$$\phi(\mathbf{x}; \mathbf{u}) \qquad \mathbb{R}^m \longrightarrow \mathbb{R}^d$$

  - Where $\mathbf{u}$ is a set of parameters for the transformation

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  - Combines basis selection and learning
  - Several different approaches, focus here on neural networks
  - Complicates the optimization

Neural Networks

- Define the basis functions j = {1…d}

$$\phi_j(\mathbf{x};\, \mathbf{u}) = \sigma(\mathbf{u}_j^T \mathbf{x})$$

Neural Networks

- Define the basis functions $j = \{1 \ldots d\}$

$$\phi_j(\mathbf{x};\, \mathbf{u}) = \sigma(\mathbf{u}_j{}^T \mathbf{x})$$

- Put all $\mathbf{u}_j \in \mathbb{R}^{1\text{xm}}$ vectors into matrix $\mathbf{U}$

$$\phi(\mathbf{x};\, \mathbf{U}) = \sigma(\mathbf{U}\mathbf{x}) = \begin{bmatrix} \sigma(\mathbf{u_1}^T\mathbf{x}) \\ \sigma(\mathbf{u_2}^T\mathbf{x}) \\ \cdots \\ \sigma(\mathbf{u_d}^T\mathbf{x}) \end{bmatrix} \in \mathbb{R}^d$$

  – σ is a pointwise sigmoid acting on each vector element

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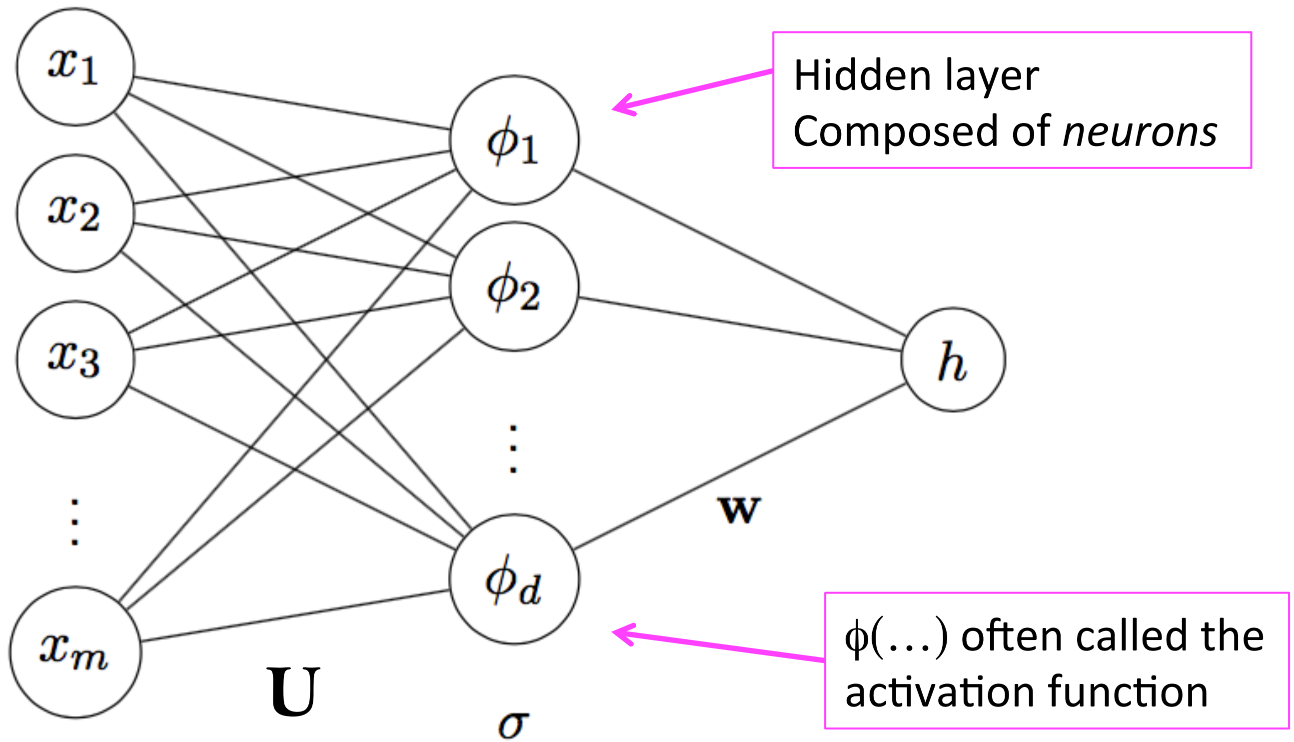
- Full model becomes

$$h(\mathbf{x}; \mathbf{w}, \mathbf{U}) = \mathbf{w}^T \phi(\mathbf{x}; \mathbf{U})$$

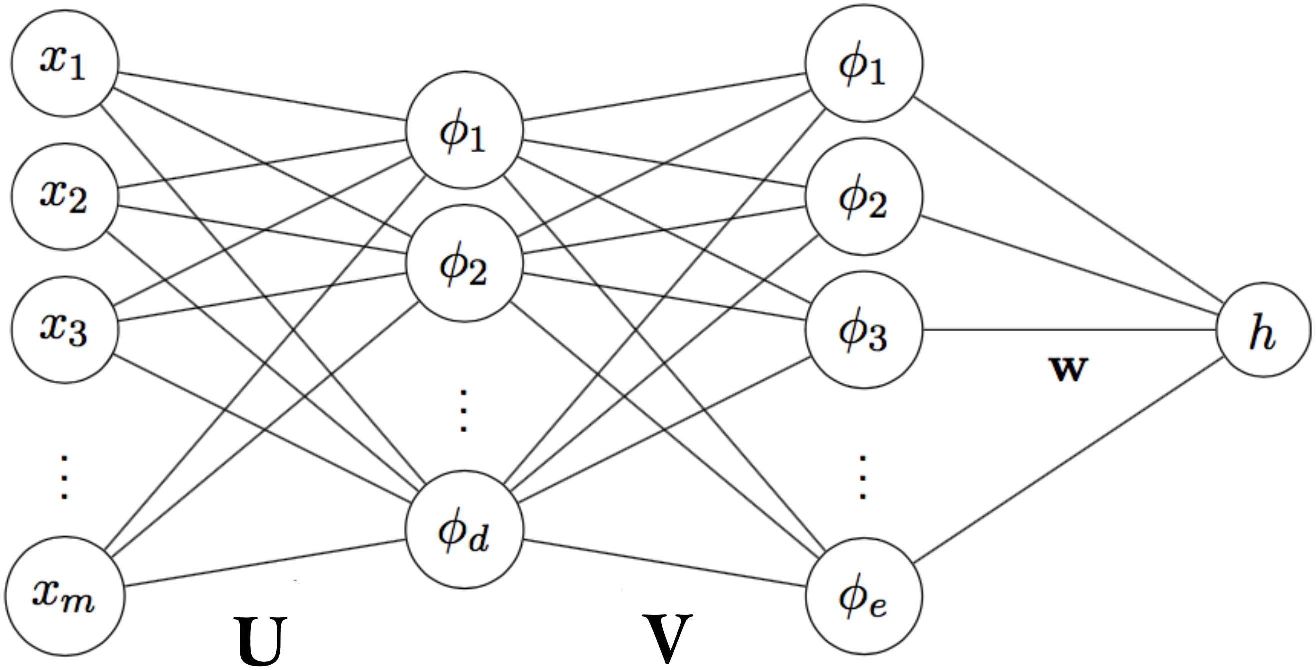
Feed Forward Neural Network



$$\phi(\mathbf{x}) = \sigma(\mathbf{U}\mathbf{x})$$

$$h(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x})$$

Multi-layer Neural Network



- Multilayer NN
  - Each layer adapts basis based on previous layer

Universal approximation theorem

- Feed-forward neural network with a single hidden layer containing a finite number of neurons can approximate continuous functions arbitrarily well on a compact space of $\mathbb{R}^n$
  - Only mild assumptions on non-linear activation function needed. Sigmoid functions work, as do others

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- But no information on how many neurons needed, or how much data!
- How to find the parameters, given a dataset, to perform this approximation?

Neural Network Optimization Problem

- Neural Network Model: $h(\mathbf{x}) = \mathbf{w}^T \sigma(\mathbf{U}\mathbf{x})$

- **Classification**: Cross-entropy loss function

$$p_i = p(y_i = 1 | \mathbf{x}_i) = \sigma(h(\mathbf{x}_i))$$

$$L(\mathbf{w}, \mathbf{U}) = -\sum_i y_i \ln(p_i) + (1 - y_i) \ln(1 - p_i)$$

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- **Regression**: Square error loss function

$$L(\mathbf{w}, \mathbf{U}) = \frac{1}{2} \sum_i (y_i - h(\mathbf{x}_i))^2$$

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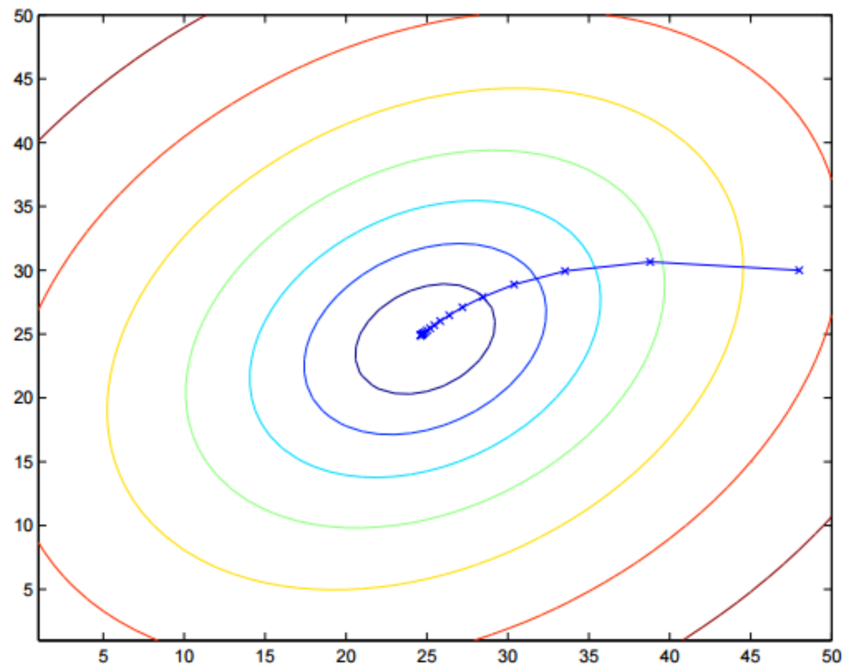
- **Regression**: Square error loss function

$$L(\mathbf{w}, \mathbf{U}) = \frac{1}{2} \sum_i (y_i - h(\mathbf{x}_i))^2$$

- Minimize loss with respect to weights **w**, **U**

Gradient Descent

- Minimize loss by repeated gradient steps
  - Compute gradient w.r.t. parameters: $\frac{\partial L(\mathbf{w})}{\partial \mathbf{w}}$
  - Update parameters: $\mathbf{w}' \leftarrow \mathbf{w} - \eta \frac{\partial L(\mathbf{w})}{\partial \mathbf{w}}$



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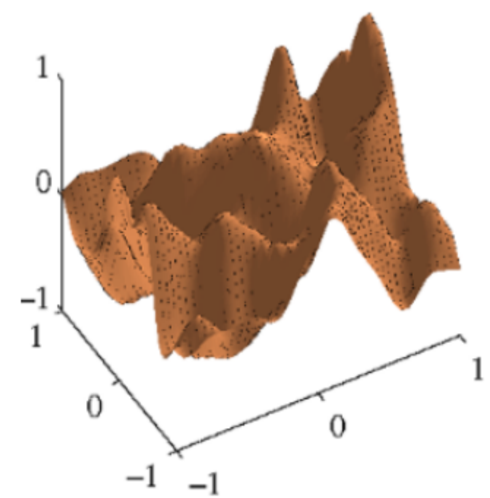
  - Update parameters: $\mathbf{w}' \leftarrow \mathbf{w} - \eta \frac{\partial L(\mathbf{w})}{\partial \mathbf{w}}$
- Now we need gradients w.r.t. **w** and **U**
- Gradients will depend on loss and network architecture
- Loss function is non-convex (many local minimum / saddle points)
  - Gradient descent may not find global minimum
  - Can be a major issue!
  - Variants of stachastic gradient descent can be helpful!



Chain Rule

$$L(\mathbf{w}, \mathbf{U}) = -\sum_i y_i \ln(\sigma(h(\mathbf{x}_i))) + (1 - y_i) \ln(1 - \sigma(h(\mathbf{x}_i)))$$

- Derivative of sigmoid: $\frac{\partial \sigma(x)}{\partial x} = \sigma(x)(1 - \sigma(x))$
- Chain rule to compute gradient w.r.t. **w**

$$\frac{\partial L}{\partial \mathbf{w}} = \frac{\partial L}{\partial h} \frac{\partial h}{\partial \mathbf{w}} = \sum_i y_i (1 - \sigma(h(\mathbf{x}_i)))\sigma(\mathbf{U}\mathbf{x}) + (1 - y_i)\sigma(h(\mathbf{x}))\sigma(\mathbf{U}\mathbf{x}_i)$$

- Chain rule to compute gradient w.r.t. $\mathbf{u}_j$

$$\frac{\partial L}{\partial \mathbf{u}_j} = \frac{\partial L}{\partial h} \frac{\partial h}{\partial \sigma} \frac{\partial \sigma}{\partial \mathbf{u}_j} =$$

$$= \sum_i y_i (1 - \sigma(h(\mathbf{x}_i))) w_j \sigma(\mathbf{u}_j \mathbf{x}_i)(1 - \sigma(\mathbf{u}_j \mathbf{x}_i))\mathbf{x}_i$$

$$+ (1 - y_i)\sigma(h(\mathbf{x}_i)) w_j \sigma(\mathbf{u}_j \mathbf{x}_i)(1 - \sigma(\mathbf{u}_j \mathbf{x}_i))\mathbf{x}_i$$

Backpropagation

- Loss function composed of layers of nonlinearity

$$L(\phi^a(\ldots\phi^1(\mathbf{x})))$$

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- Forward step (f-prop)
  - Compute and save intermediate computations

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- Backward step (b-prop) $\dfrac{\partial L}{\partial \phi^a} = \sum_j \dfrac{\partial \phi_j^{(a+1)}}{\partial \phi_j^a} \dfrac{\partial L}{\partial \phi_j^{(a+1)}}$

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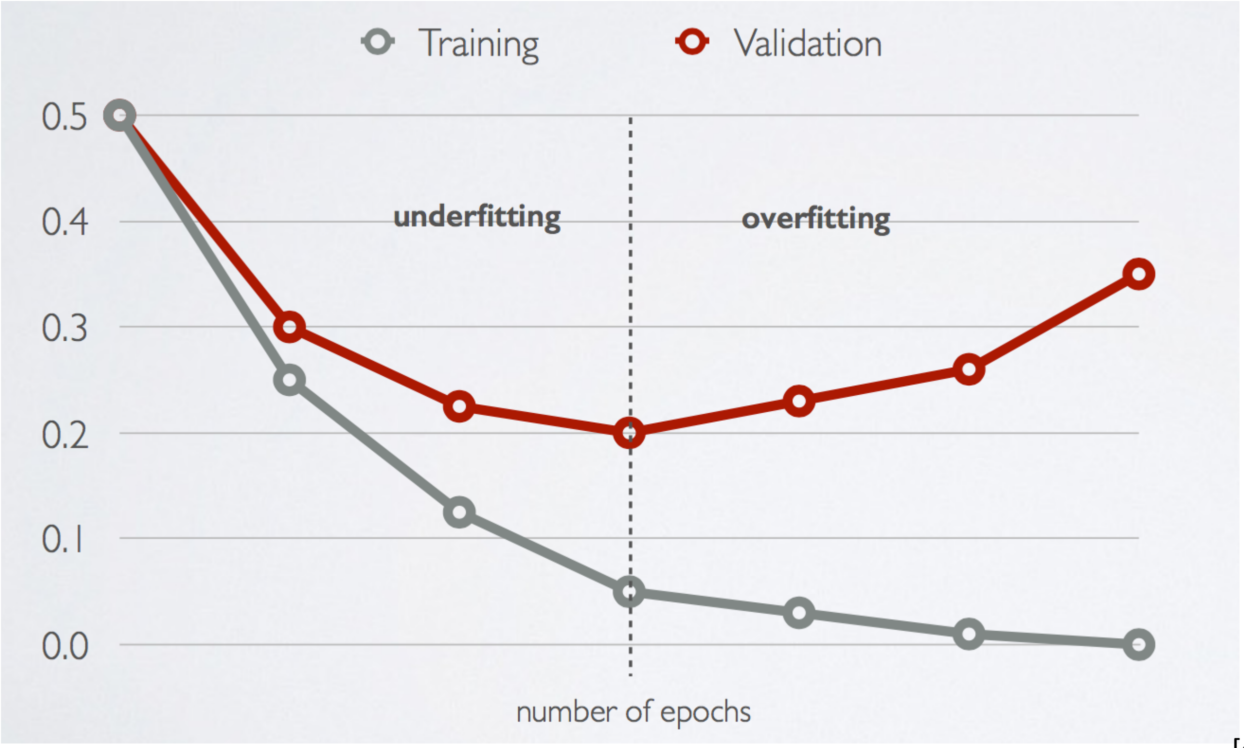
- Compute parameter gradients $$\frac{\partial L}{\partial \mathbf{w}^a} = \sum_j \frac{\partial \phi_j^a}{\partial \mathbf{w}^a} \frac{\partial L}{\partial \phi_j^a}$$

Training

- Repeat gradient update of weights reduce loss
  - Each iteration through dataset is called an epoch

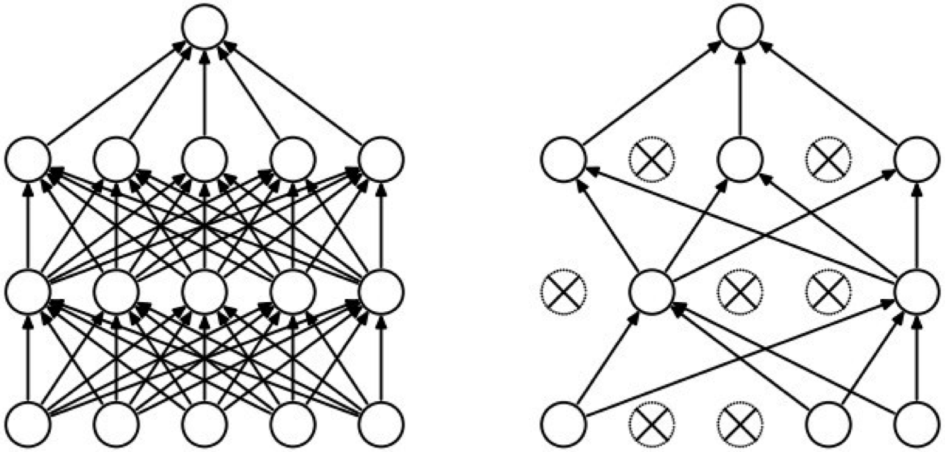
- Use validation set to examine for overtraining, and determine when to stop training



[graphic from H. Larochelle]

Regularization

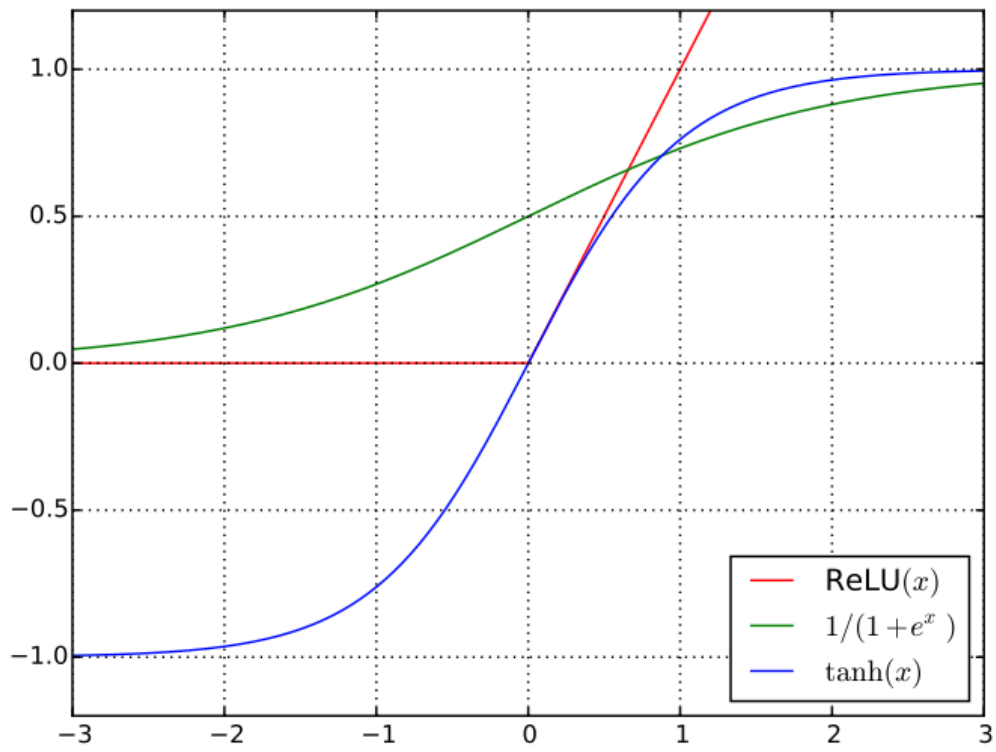
- L2 regularization: add $\Omega(\mathbf{w}) = ||\mathbf{w}||^2$ to loss
  - Also called "weight decay"
  - Gaussian prior on weights, keep weights from getting too large and saturating activation function
- Regularization inside network, example: **Dropout**
  - Randomly remove nodes during training
  - Avoid co-adaptation of nodes
  - Essentially a large model averaging procedure



(a) Standard Neural Net (b) After applying dropout.

arXiv:1207.0580

Activation Functions



- **Vanishing gradient problem**
  - Derivative of sigmoid:

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)(1-\sigma(x))$$

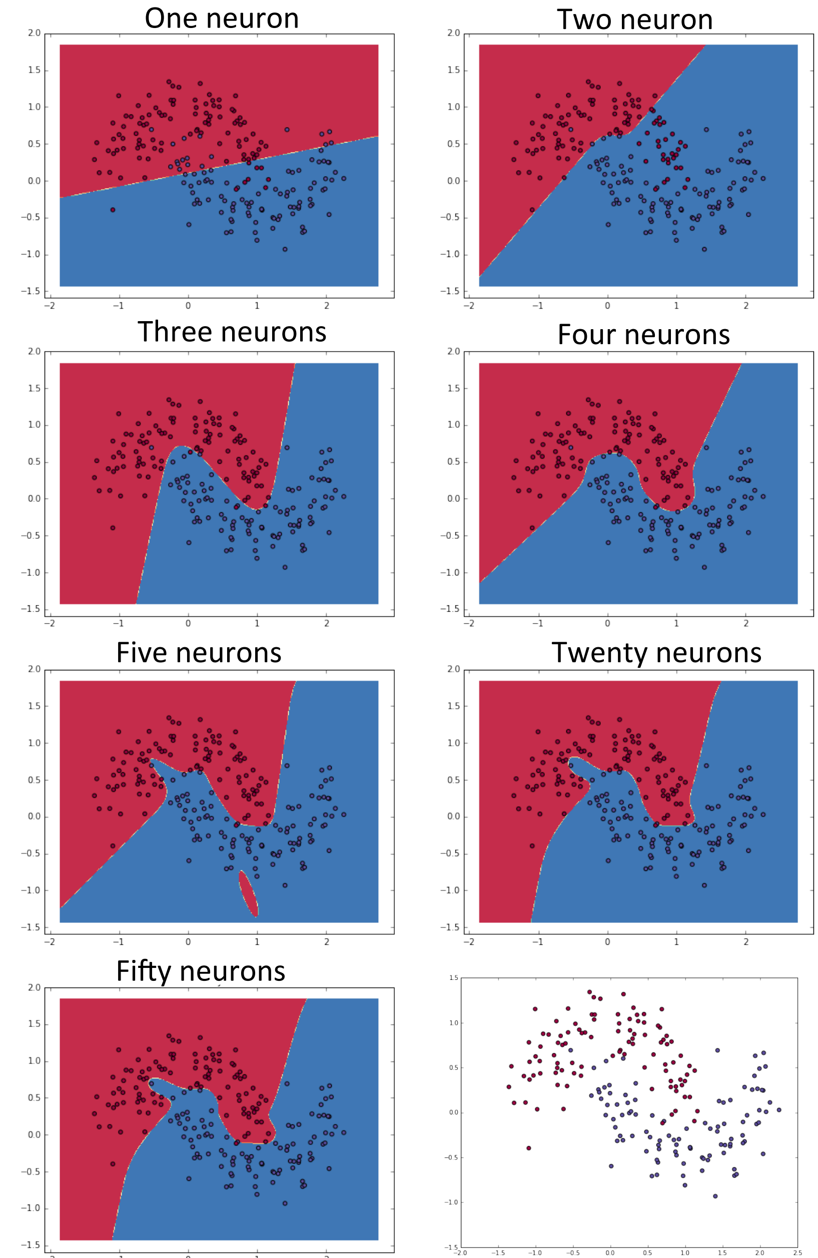
  - Nearly 0 when x is far from 0!
  - Gradient descent difficult!

- **Rectified Linear Unit (ReLU)**
  - ReLU(x) = max{0, x}
  - Derivative is constant!

$$\frac{\partial \mathrm{Re}LU(x)}{\partial x} = \begin{cases} 1 & \textit{when } x > 0 \\ 0 & \textit{otherwise} \end{cases}$$

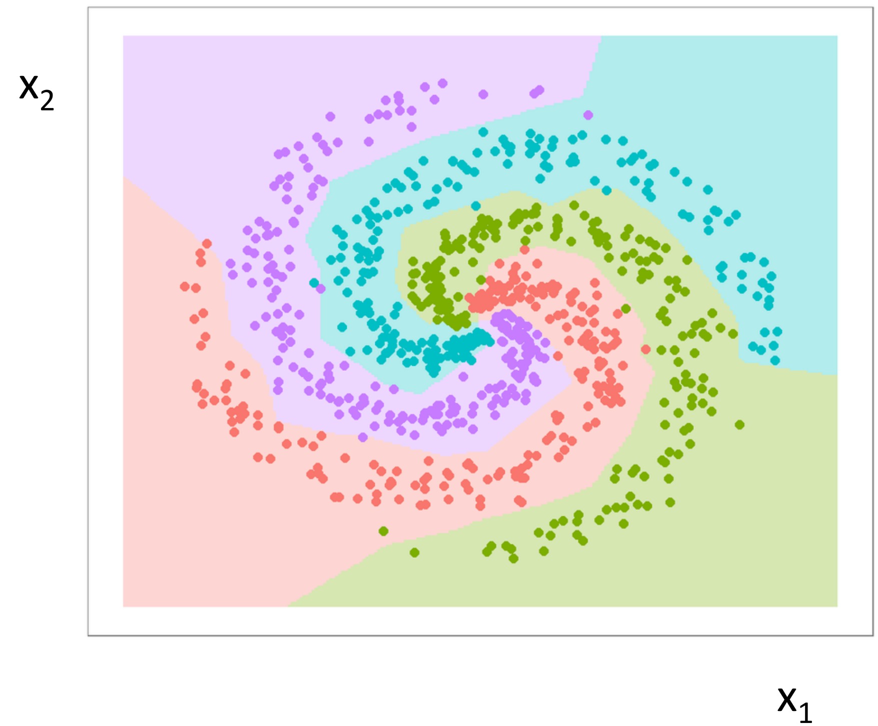
  - ReLU gradient doesn't vanish

Neural Network Decision Boundaries



2-class classification
1-hidden layer NN
L2 norm regularization

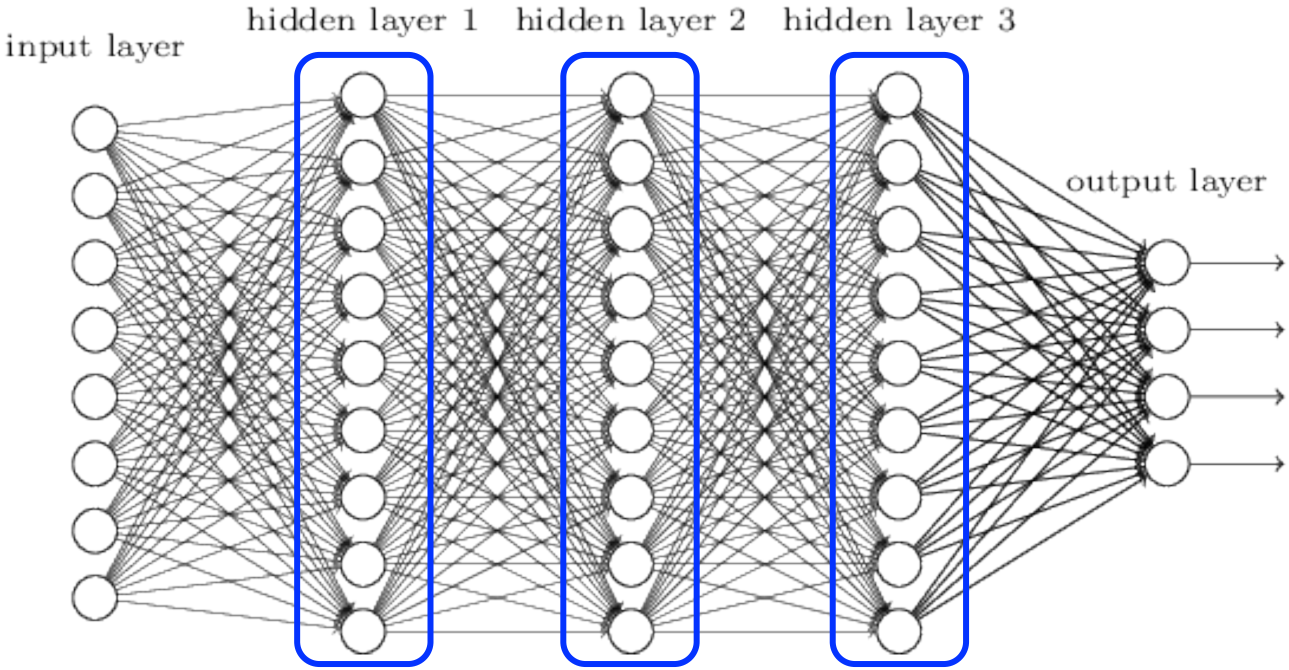
4-class classification
2-hidden layer NN
ReLU activations
L2 norm regularization



http://www.wildml.com/2015/09/implementing-a-neural-network-from-scratch/

http://junma5.weebly.com/data-blog/build-your-own-neural-network-classifier-in-r

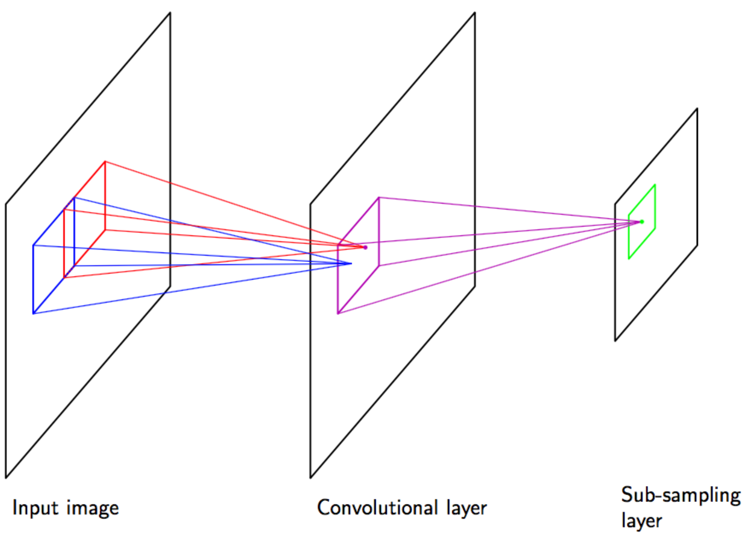
Deep Neural Networks



- As data complexity grows, need exponentially large number of neurons in a single-hidden-layer network to capture all the structure in the data
- Deep neural networks have many hidden layers
  - Factorize the learning of structure in the data across many layers
- Difficult to train, only recently possible with large datasets, fast computing (GPU) and new training procedures / network structures (like dropout) → More next time

Neural Network Architectures

- Structure of the networks, and the node connectivity can be adapted for problem at hand
- **Convolutions**: shared weights of neurons, but each neuron only takes subset of inputs



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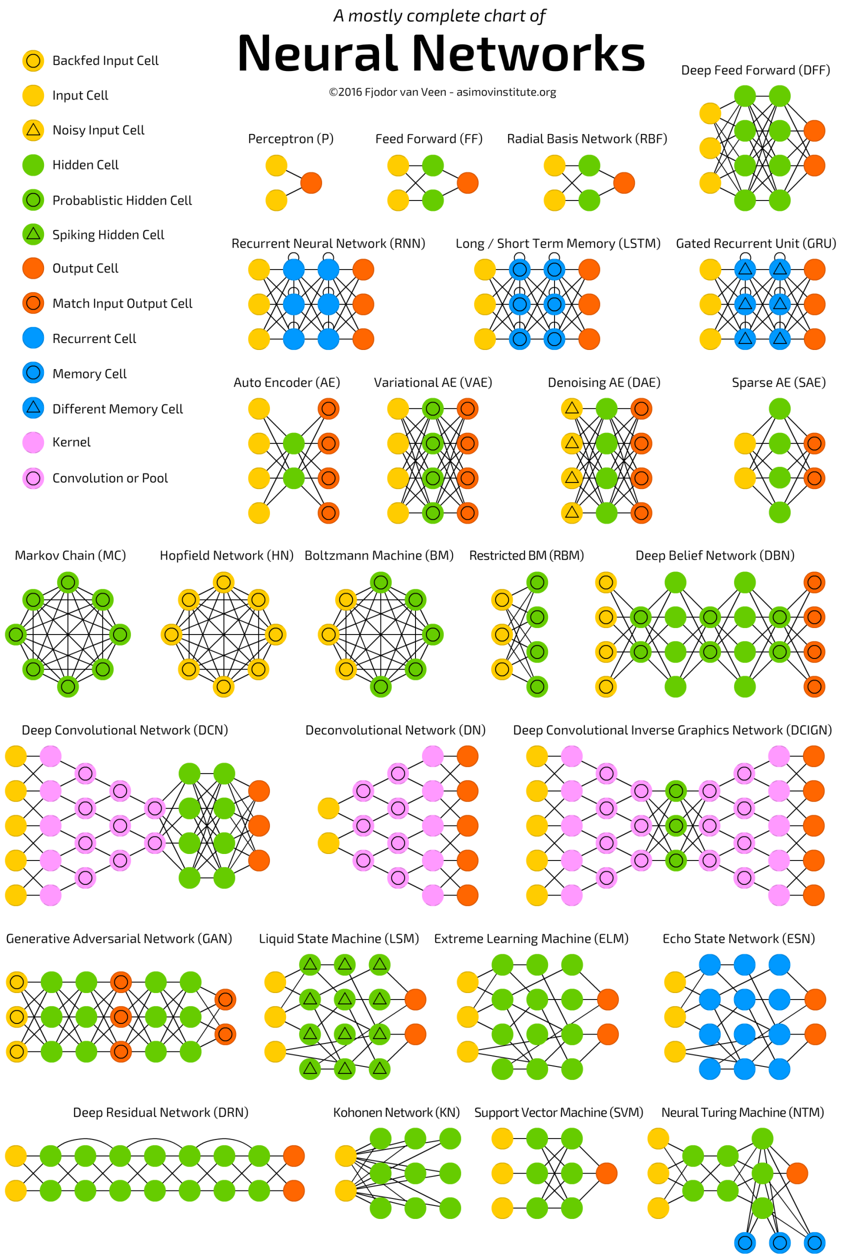
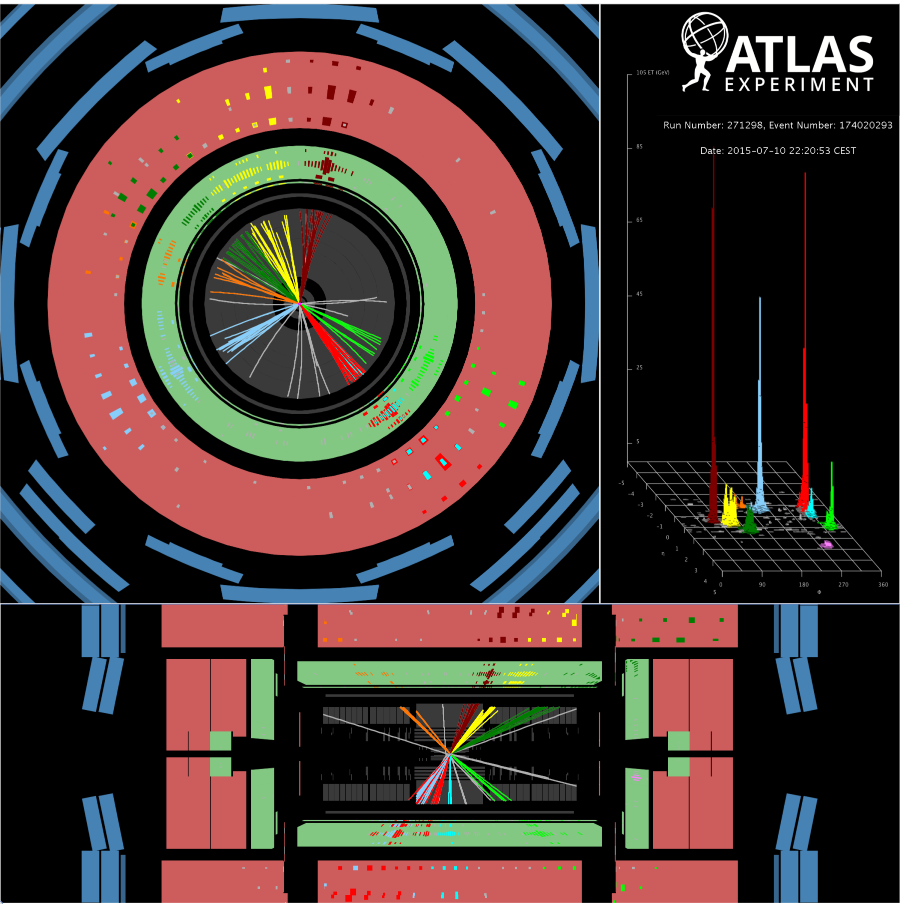


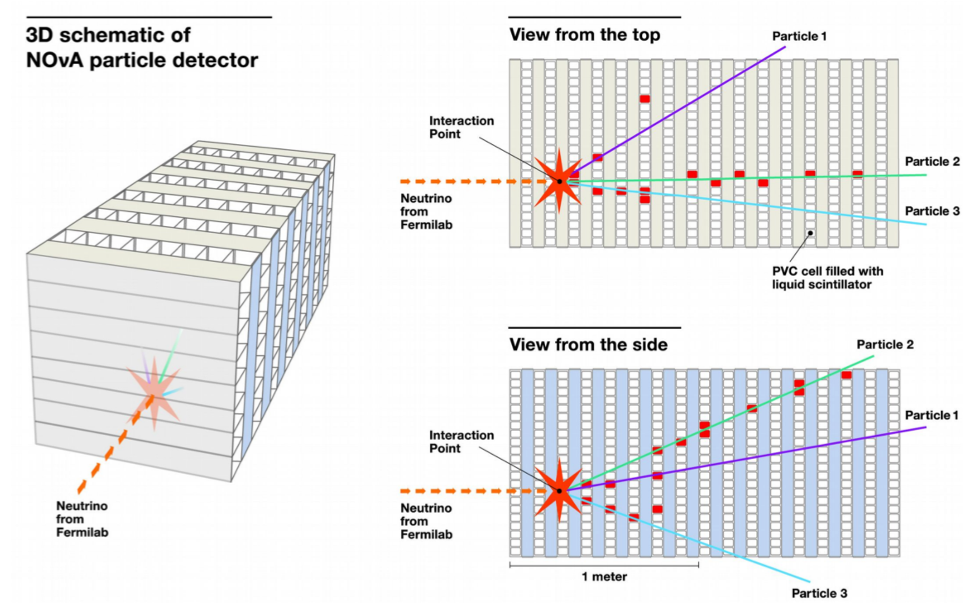
http://www.asimovinstitute.org/neural-network-zoo/

Neural Networks in HEP

Jets at the LHC



Neutrino identification
Example: NOνA



What do neural networks learn?

- Can visualize weights: neutrino decay classification

arXiv:1604.01444

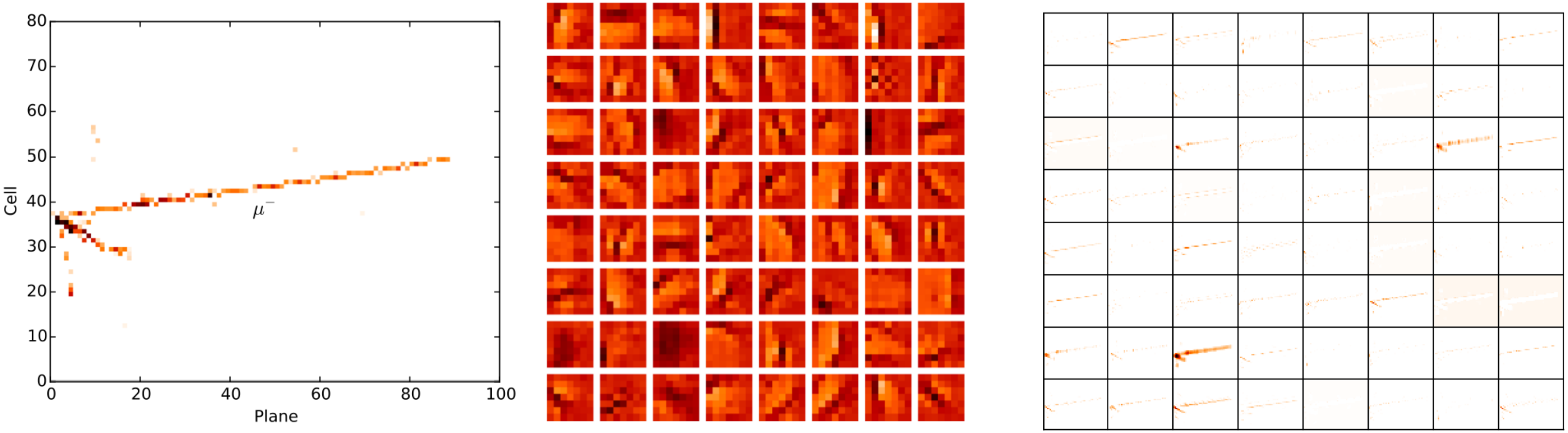
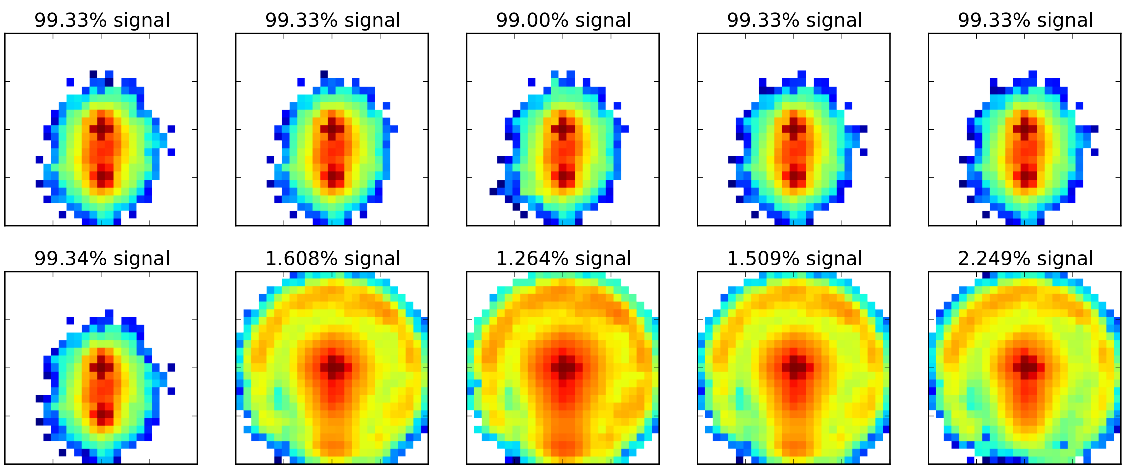


Image Y-view → Weights of First layer → Output of convolution

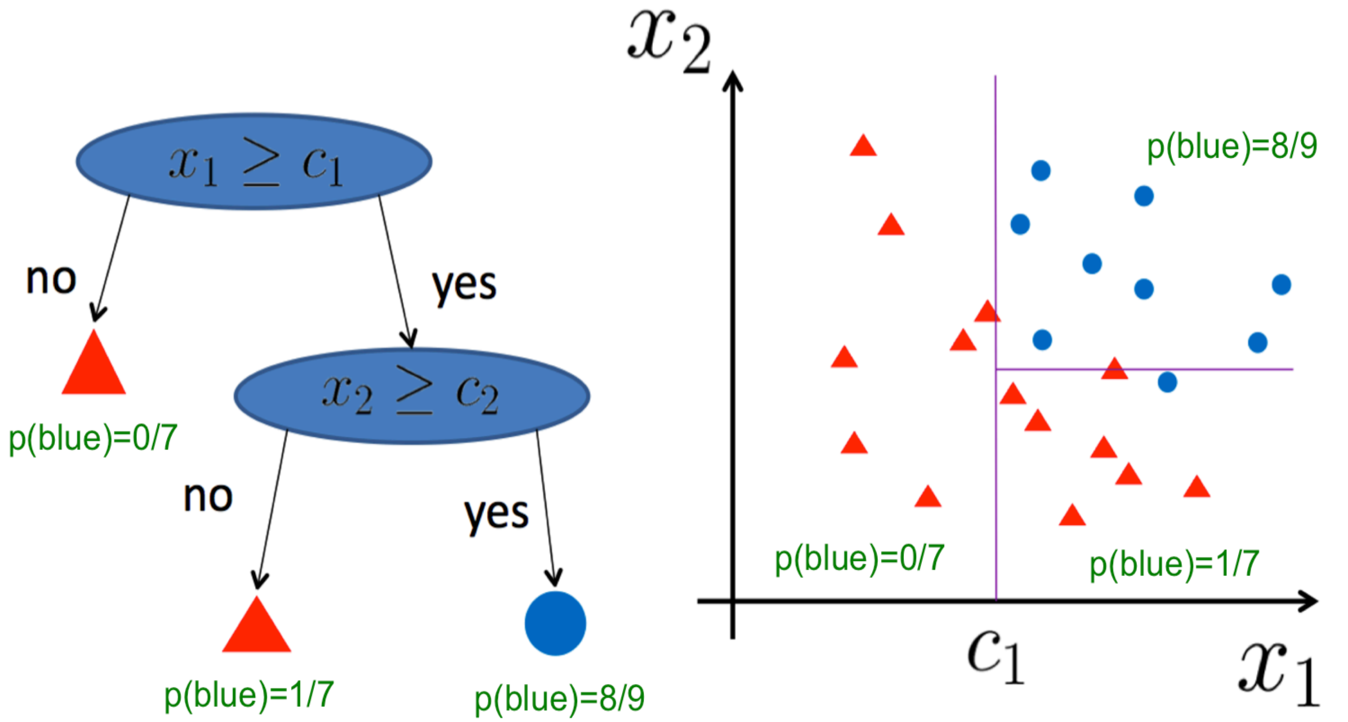
- Find inputs that most activate a neuron:
  – Separating boosted W-jets from quark/gluon jets

https://arxiv.org/abs/1511.05190



Decision Tree Models

Decision Trees



- Partition data based on a sequence of thresholds

- In a given partition, estimate the class probability from N_m examples in partition *m* and N_k of the examples in partition from class *k*:

$$p_{mk} = \frac{N_k}{N_m}$$

Single Decision Trees: Pros and Cons

- Pros:
  - Simple to understand, can visualize a tree
  - Requires little data preparation, and can use continuous and categorical inputs

- Cons:
  - Can create complex models that overfit data
  - Can be unstable to small variations in data
  - Training a tree is an NP-complete problem
    - Hard to find a global optimum of all data partitionings
    - Have to use heuristics like *greedy optimization* where locally optimal decisions are made

- We will discuss the ways to overcome these Cons, including early stopping of training, and ensembles

Greedy Training of a Decision Tree

- **Greedy Training**: instead of optimizing all splittings at the same time, optimize them one-by-one, then move onto next splitting

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- Given N_m examples in a node, for a candidate splitting $\theta=(x_j, t_m)$ for feature x_j and threshold t_m
- If data partitioned into subsets Q_{left} and Q_{right}, compute:

$$G(Q,\theta) = \frac{n_{\text{left}}}{N_m} H(Q_{\text{left}}(\theta)) + \frac{n_{\text{right}}}{N_m} H(Q_{\text{right}}(\theta))$$

  – Where *H()* is an impurity function

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  – Where *H()* is an impurity function

- Choose splitting θ using: $\theta^* = \arg\min_{\theta} G(Q,\theta)$

Impurity Functions

- Classification
  - Proportion of class k in node m: $p_{mk} = \frac{N_k}{N_m}$
  - Gini: $H(X_m) = \sum_k p_{mk}(1 - p_{mk})$
  - Cross entropy: $H(X_m) = -\sum_k p_{mk} \log(p_{mk})$
  - Miss-classification: $H(X_m) = 1 - \max_k(p_{mk})$
- Regression
  - Continuous target y, in region estimate: $c_m = \frac{1}{N_m} \sum_{i \in N_m} y_i$
  - Square error: $H(X_m) = \frac{1}{N_m} \sum_{i \in N_m} (y_i - c_m)^2$

When to stop splitting?

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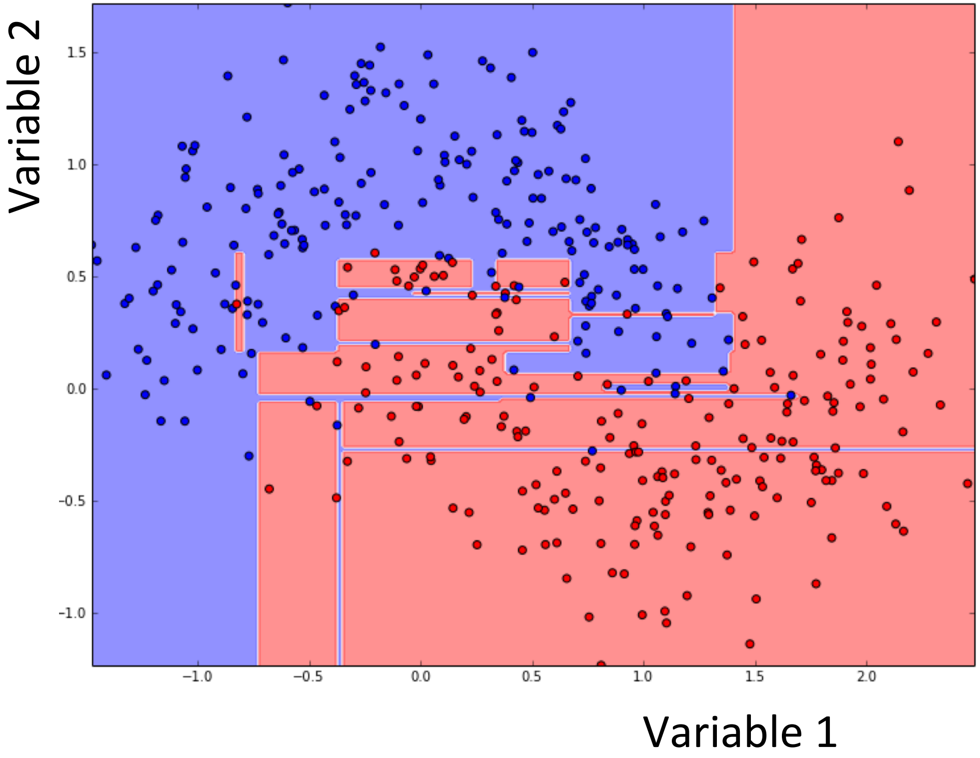


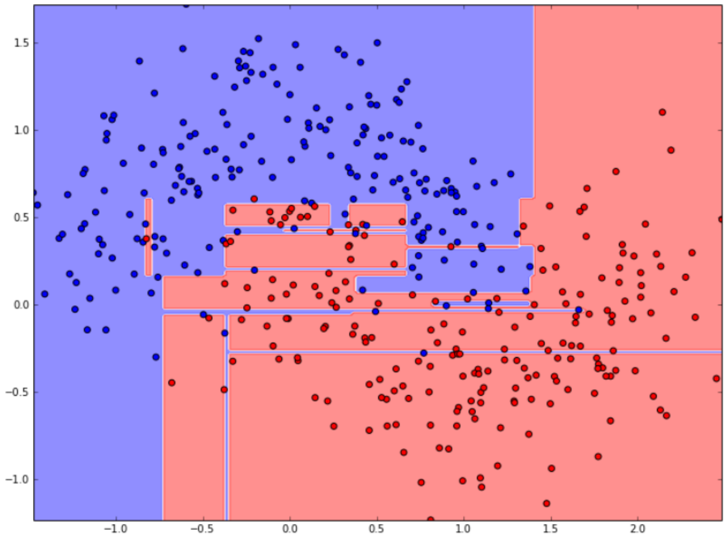
[Rogozhnikov]

- Single decision trees can quickly overfit
- Especially when increasing the depth of the tree

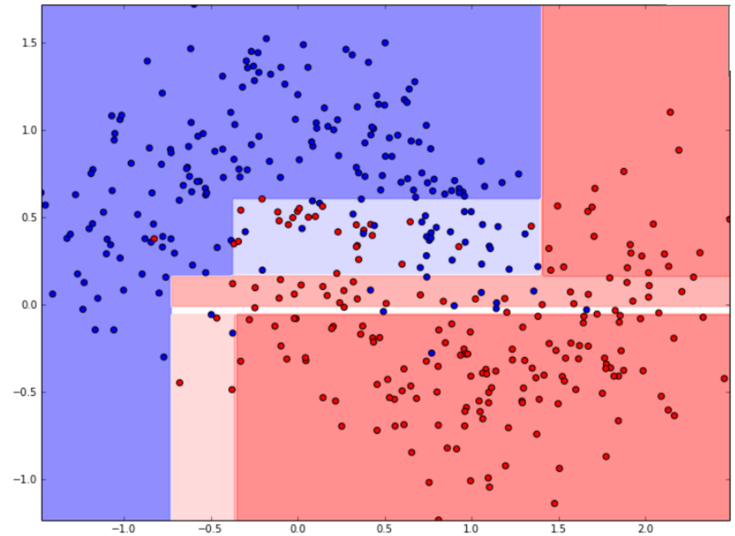
When to stop splitting?

- In principle, can keep splitting until every event is properly classified…
- Can stop splitting early. Many criteria:
  - Fixed tree depth
  - Information gain is not enough
  - Fix minimum samples needed in node
  - Fix minimum number of samples needed to split node
  - Combinations of these rules work as well

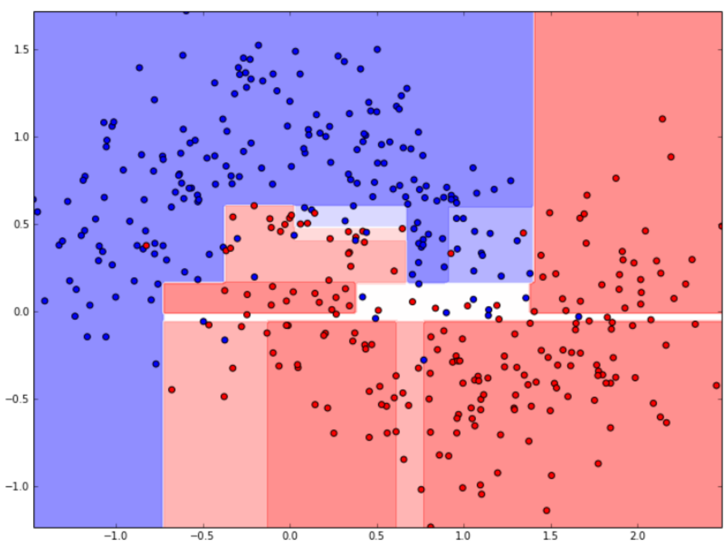
Mitigating Overfitting



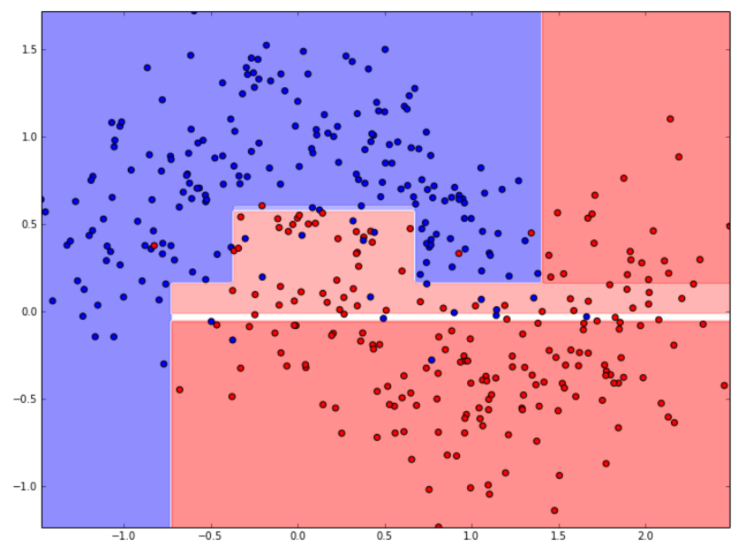
no pre-stopping



max_depth



min # of samples in leaf



maximal number of leaves

[Rogozhnikov]

Ensemble Methods

- Can we reduce the variance of a model without increasing the bias?

Ensemble Methods

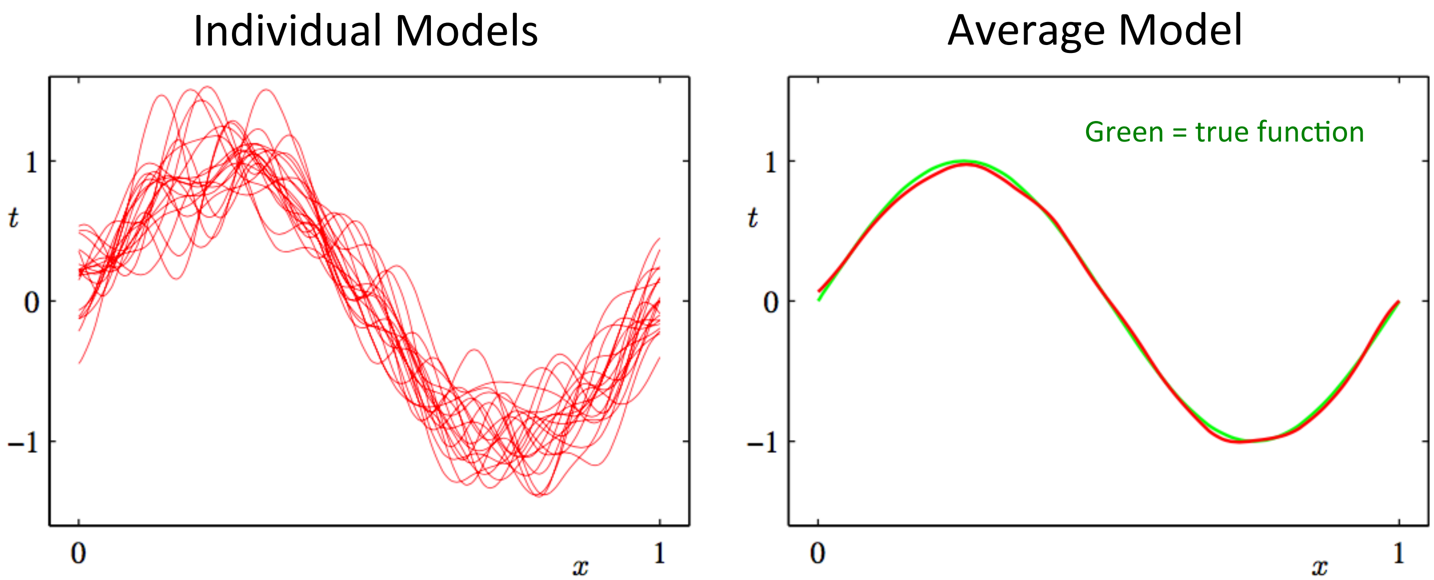
- Can we reduce the variance of a model without increasing the bias?

- Yes! By training several slightly different models and taking majority vote (classification) or average (regression) prediction

  - Bias does not largely increase because the average ensemble performance is equal to the average of its members

  - Variance decreases because a spurious pattern picked up by one model may not be picked up by other

Ensemble Methods



[Bishop]

- Combining several weak learners (only small correlation with target value) with high variance can be extremely powerful
- Can be used with decision trees to overcome their problems of overfitting!

Bagging and Boosting

- **Bootstrap Aggregating (Bagging)**:
  - Sample dataset D with replacement N-times, and train a separate model on each derived training set
  - Classify example with majority vote, or compute average output from each tree as model output

$$h(\mathbf{x}) = \frac{1}{N_{trees}} \sum_{i=1}^{N_{trees}} h_i(\mathbf{x})$$

- **Boosting**:
  - Train N models in sequence, giving more weight to examples not correctly classified by previous models
  - Take weighted vote to classify examples

$$h(\mathbf{x}) = \frac{\sum_{i=1}^{N_{trees}} \alpha_i h_i(\mathbf{x})}{\sum_{i=1}^{N_{trees}} \alpha_i}$$

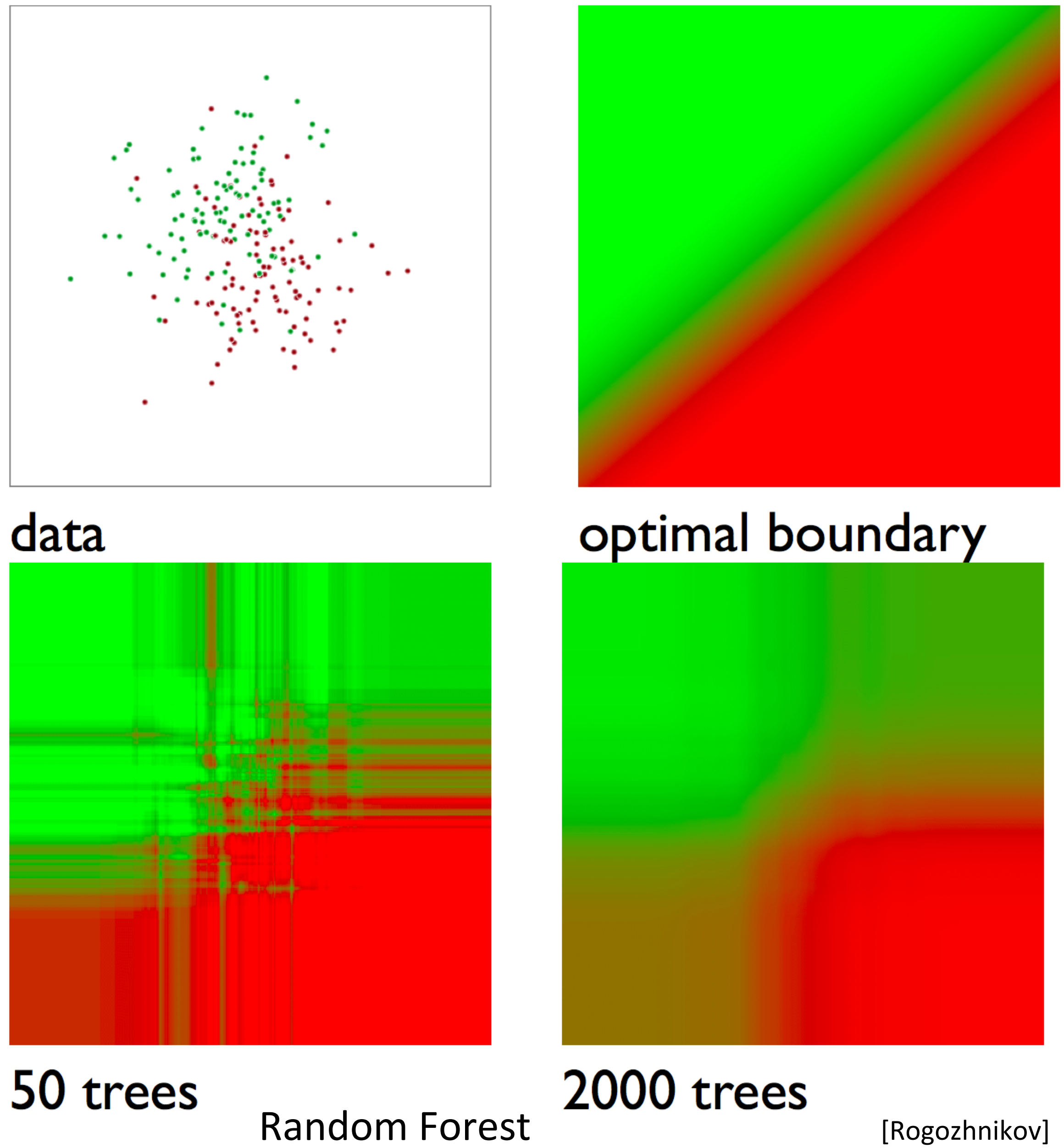
  - Boosting algorithms include: AdaBoost, Gradient boost, XGBoost

Random Forest

- One of the most commonly used algorithms in industry is the **Random Forest**
  - Use bagging to select random example subset
  - Train a tree, but only use random subset of features ($\sqrt{m}$ features) at each split. This increases the variance

Ensembles of Trees

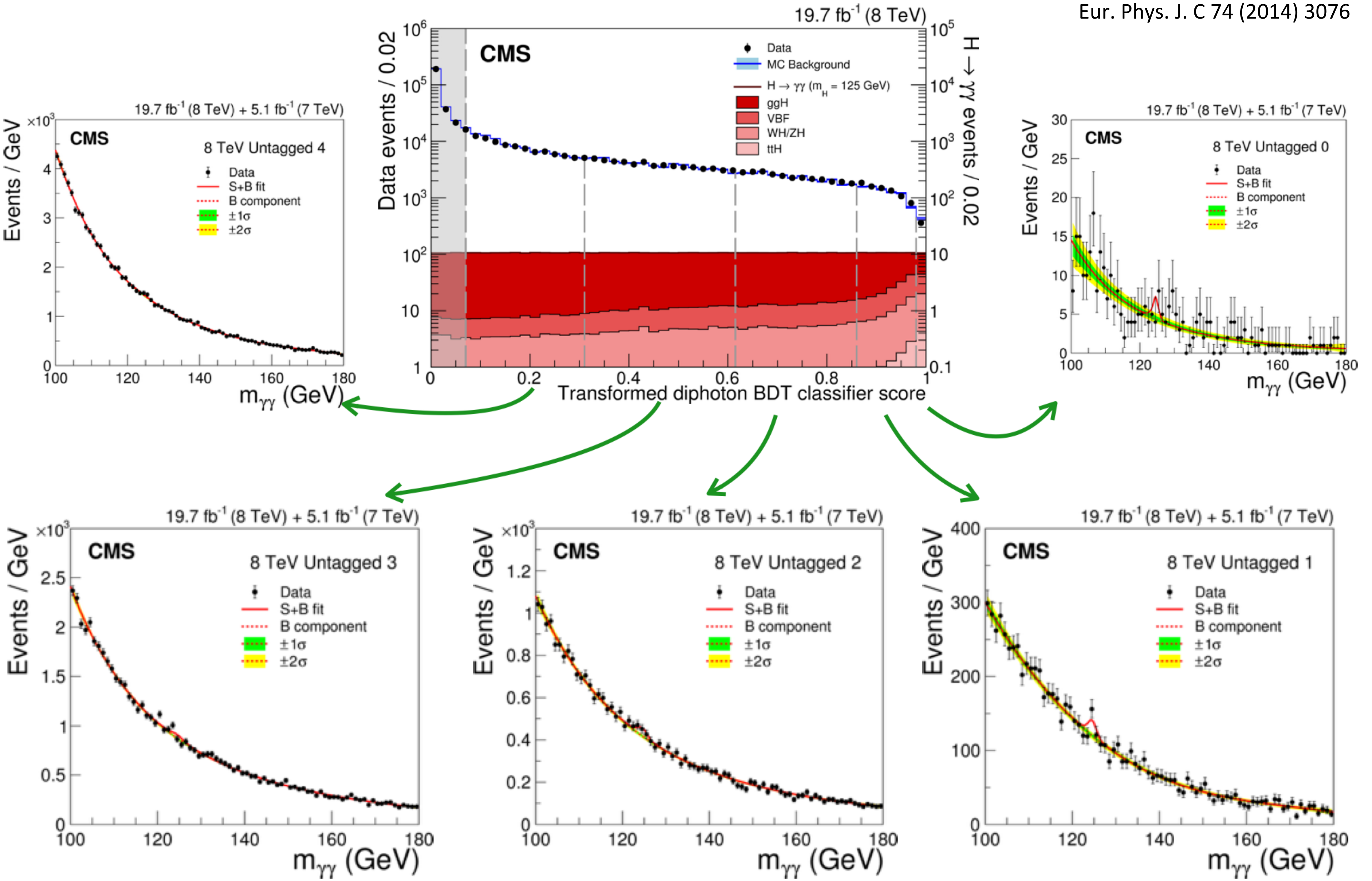
- Tree Ensembles tend to work well
  - Relatively simple
  - Relatively easy to train
  - Tend not to overfit (especially random forests)
  - Work with different feature types: continuous, categorical, etc.



[Rogozhnikov]

CMS h→γγ (8 TeV) – Boosted decision tree

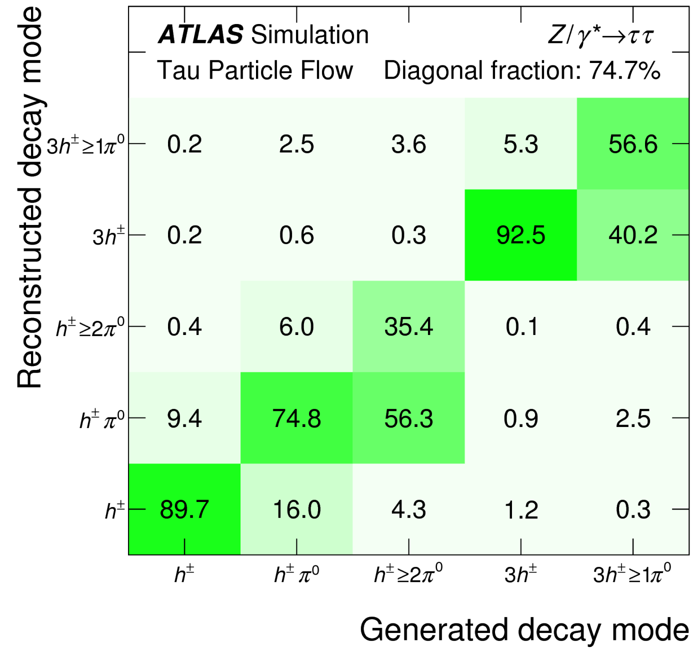
Eur. Phys. J. C 74 (2014) 3076

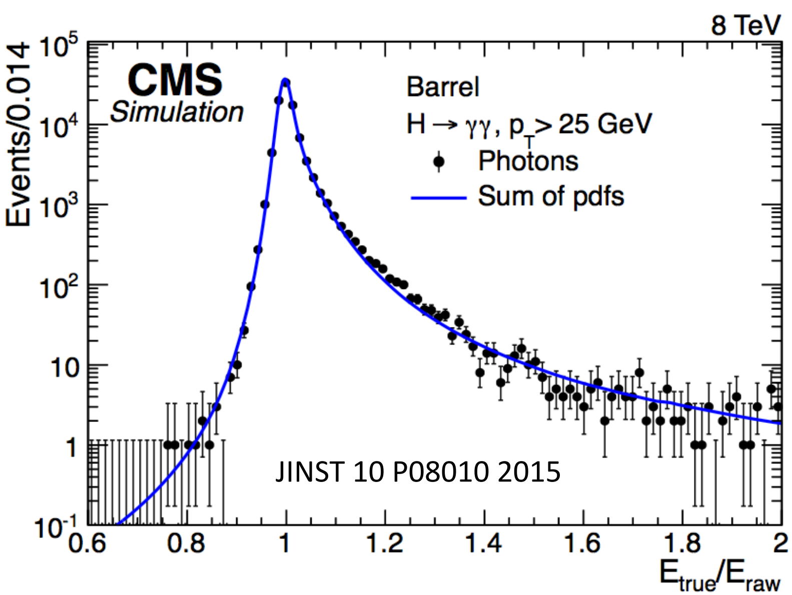


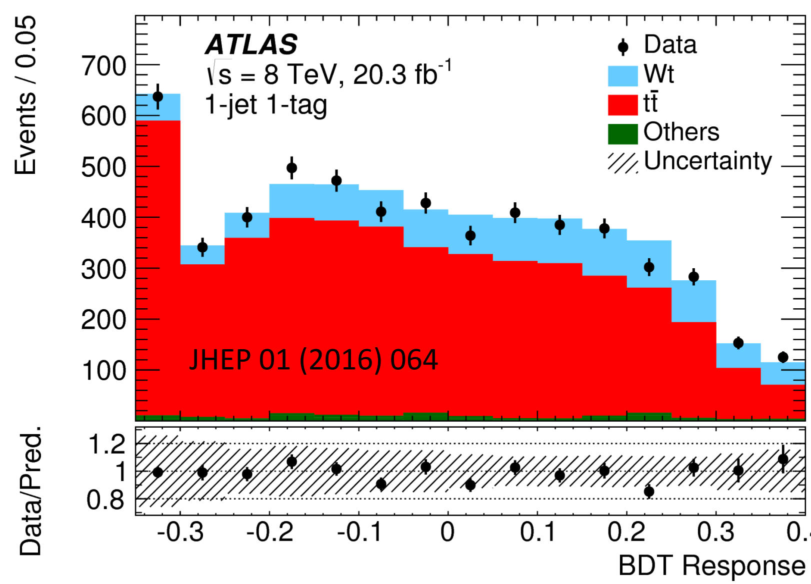
Decision Tree Ensembles in HEP

- Decision tree ensembles, especially with boosting, are used very widely in HEP!

https://arxiv.org/abs/1512.05955







Unsupervised Learning

- Learning without targets/labels, find structure in data

Dimensionality Reduction

- Find a low dimensional (less complex) representation of the data with a mapping $Z=h(X)$

Principle Components Analysis

- Given data $\{\mathbf{x}_i\}_{i=1\ldots N}$ can we find a directions in features space that explain most variation of data?

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- Let $\mathbf{u}_1$ be the projected direction, we can solve:

Variance of projected data

Unit length vector constraint

$$\mathbf{u}_1^* = \arg\max_{\mathbf{u}_1} \underbrace{\mathbf{u}_1^T \mathbf{S} \mathbf{u}_1}_{\text{Variance of projected data}} + \lambda\underbrace{(1 - \mathbf{u}_1^T \mathbf{u}_1)}_{\text{Unit length vector constraint}}$$

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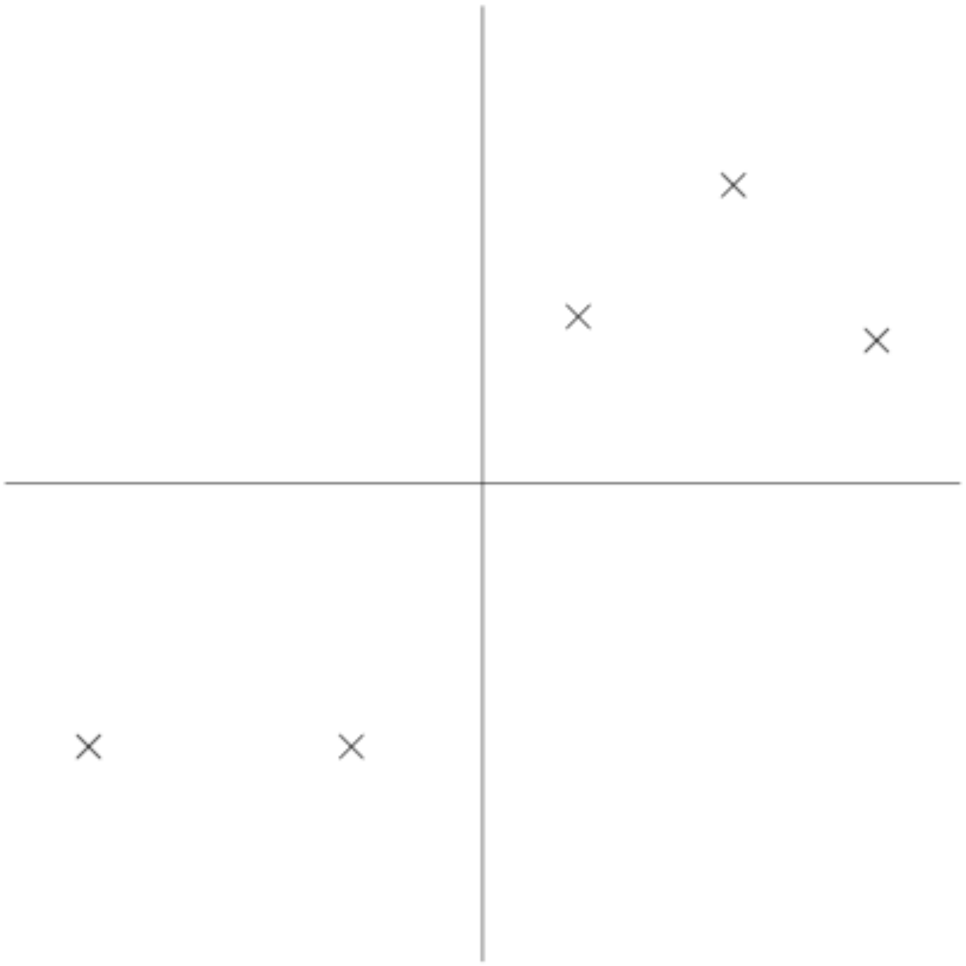
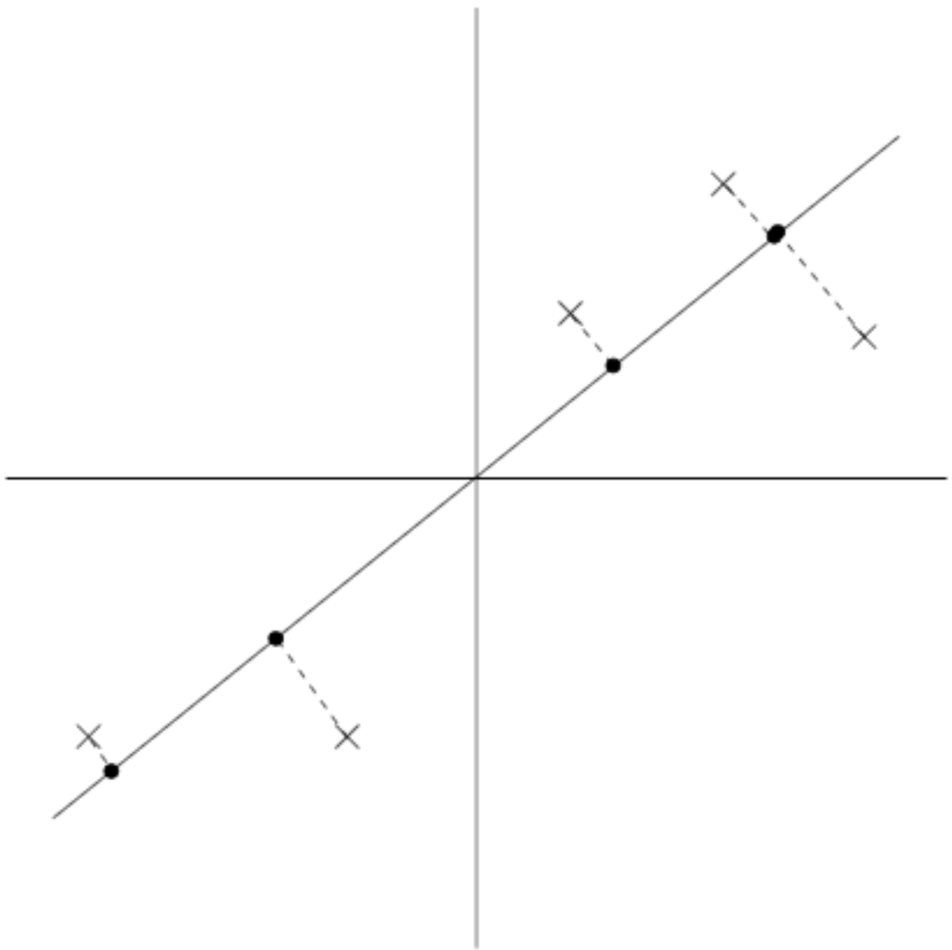
- *Principle components* are the eigenvectors of the data covariance matrix!
  - Eigenvalues are the variance explained by that component

PCA Example



[Ng]

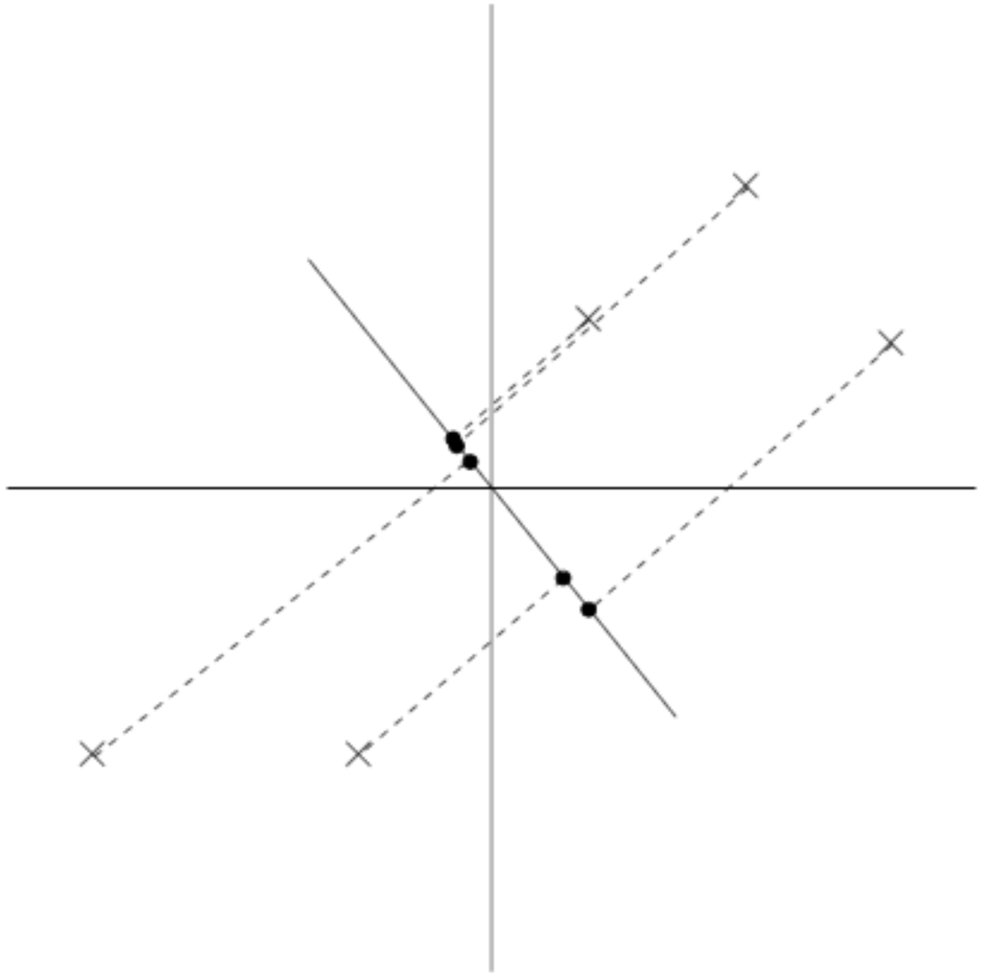
PCA Example



First principle component, projects on to this axis have large variance

[Ng]

PCA Example



Second principle component, projects have small variance

[Ng]

Fisher Discriminant

- Suppose our $\{\mathbf{x}_i, \mathbf{y}_i\}_{i=1\ldots N}$ is separated in two classes, we want a projection to maximize the separation between the two classes.

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$$\mathbf{S}_B = (\mathbf{m}_2 - \mathbf{m}_1)^T(\mathbf{m}_2 - \mathbf{m}_1)$$

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$$\mathbf{S}_W = \sum_{i \in C_1} (\mathbf{x}_i - \mathbf{m}_1)^T(\mathbf{x}_i - \mathbf{m}_1) + \sum_{i \in C_2} (\mathbf{x}_i - \mathbf{m}_2)^T(\mathbf{x}_i - \mathbf{m}_2)$$

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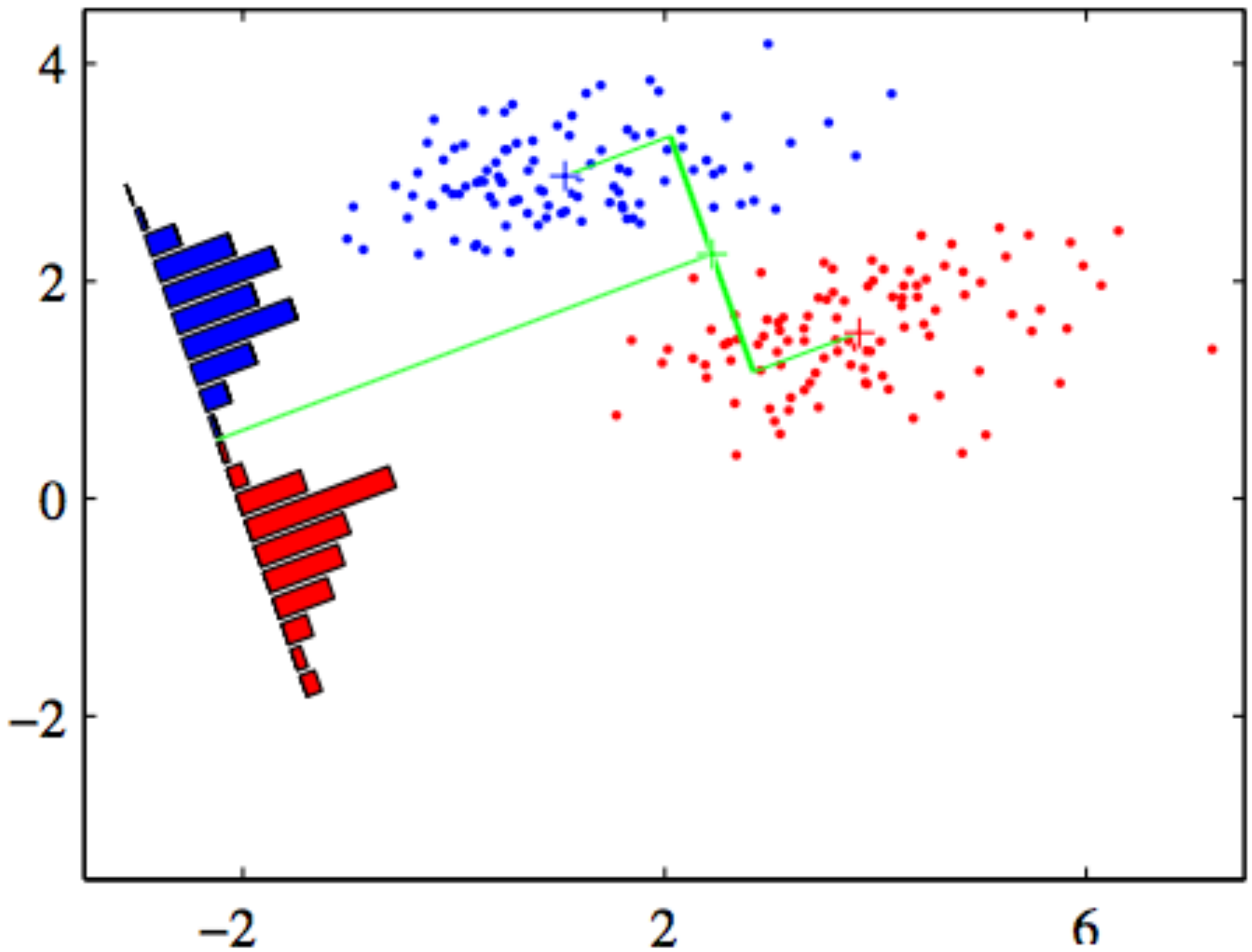
- Maximize Fisher criteria

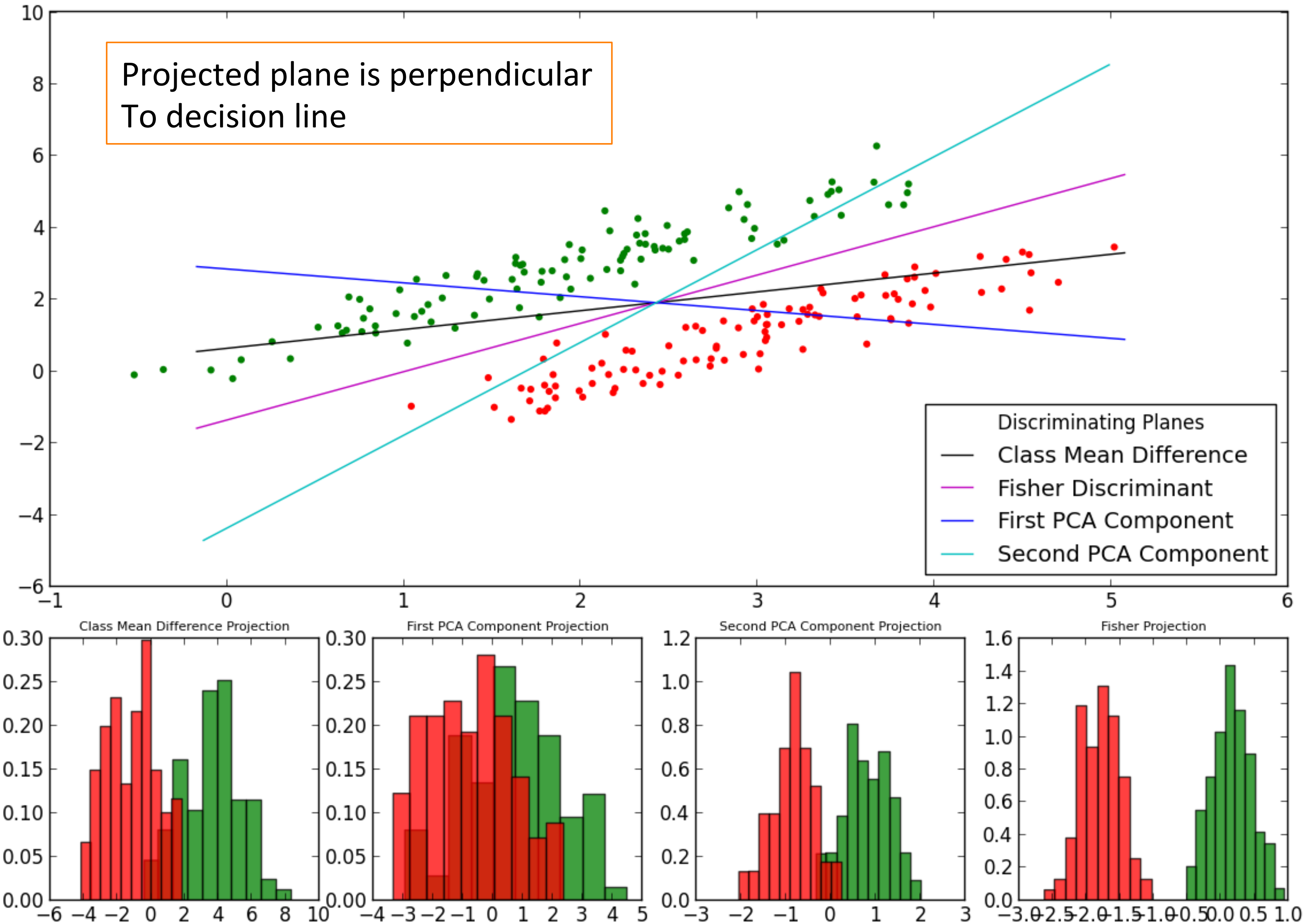
$$J(\mathbf{w}) = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}} \quad \rightarrow \quad \boxed{\mathbf{w} \propto \mathbf{S}_W (\mathbf{m}_2 - \mathbf{m}_1)}$$

Fisher Discriminant



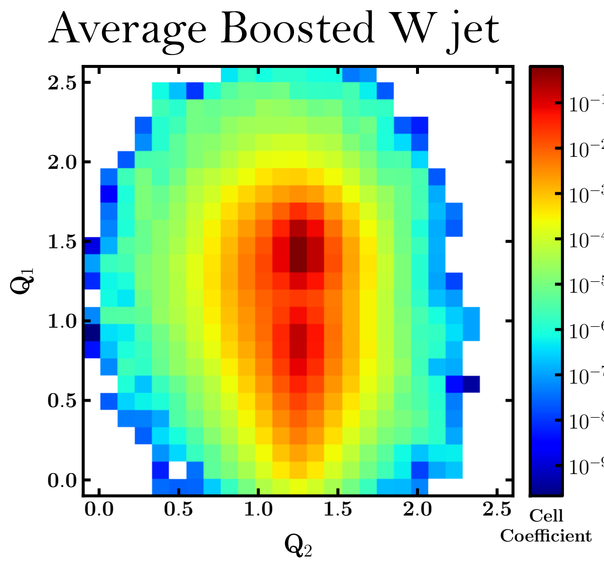
[Bishop]

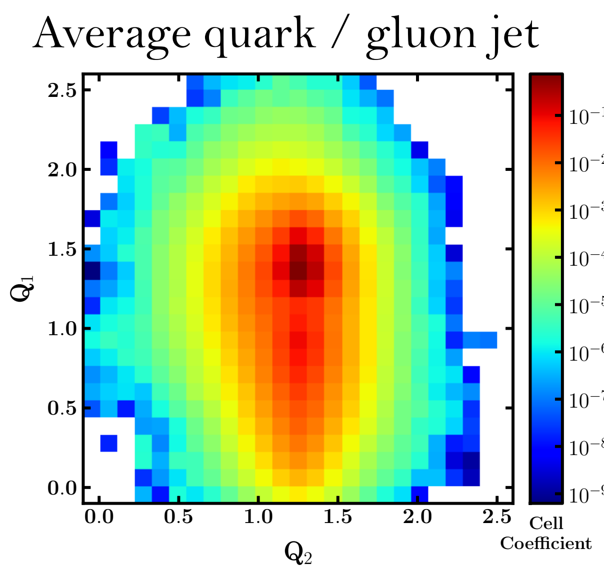
Comparing Techniques

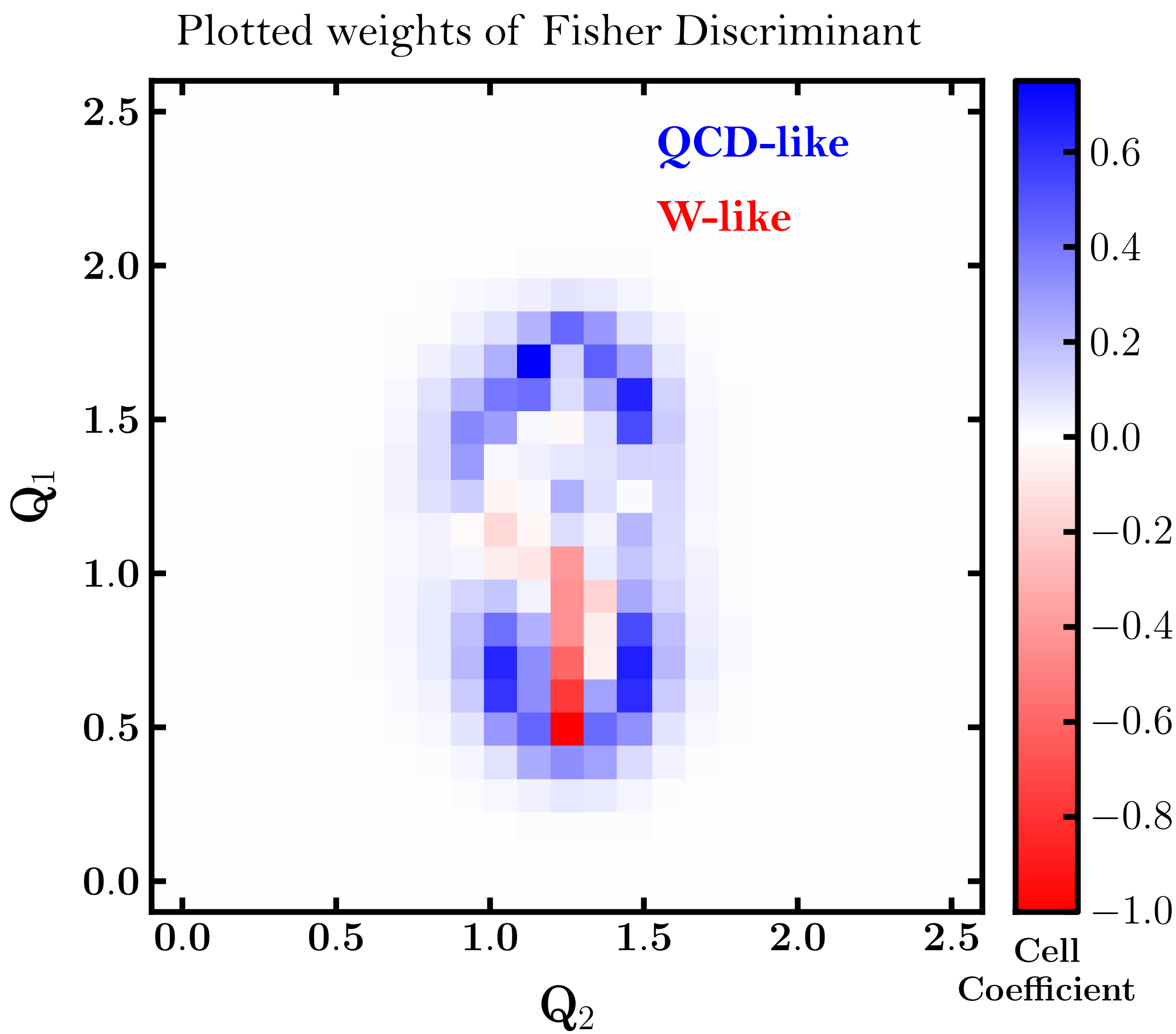


Fisher Discriminant

http://arxiv.org/abs/1407.5675







Clustering

- Partition the data into groups $D = \{D_1 \cup D_2 \ \ldots \cup D_k\}$

- *What is a good clustering*?
  - One where examples within a cluster are more "similar" than to examples in other clusters

  - What does similar mean? Use distance metric, e.g.

$$d(\mathbf{x}, \mathbf{x}') = \sqrt{\sum_i (x_i - x_i')^2}$$

K-means

- Data $\mathbf{x}_i \in \mathbb{R}^m$ which you want placed in K clusters

- Associate each example to a cluster by minimizing within-class variance

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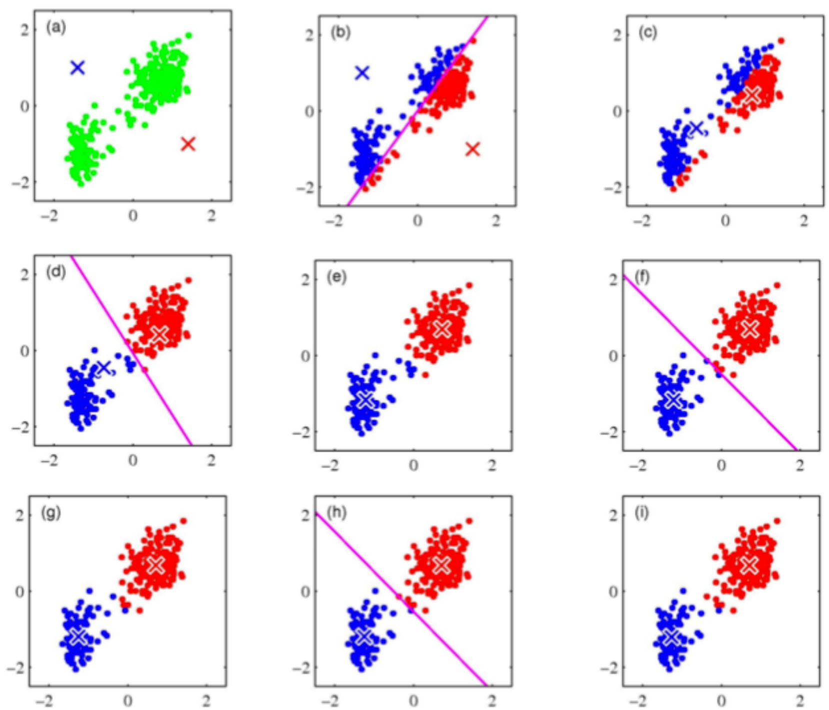
  - Find prototypes and assignments to minimize

$$L(S,\mu) = \sum_{k=1}^{K} \sum_{i \in S_k} \sqrt{(\mathbf{x}_i - \mu_k)^2}$$

    - This is an NP-hard problem, with many local minimum!

K-means algorithm

- Initialize the μ_k at random (typically using K-means++ initialization)
- **Repeat until convergence**:
  - Assign each example to closest prototype $\min_{k \in \{1 \dots K\}} \sqrt{(\mathbf{x}_i - \mu_k)^2}$
  - Update prototypes $\mu_k = \frac{1}{n_k} \sum_{i \in S_k} \mathbf{x}_i$



[Bishop]

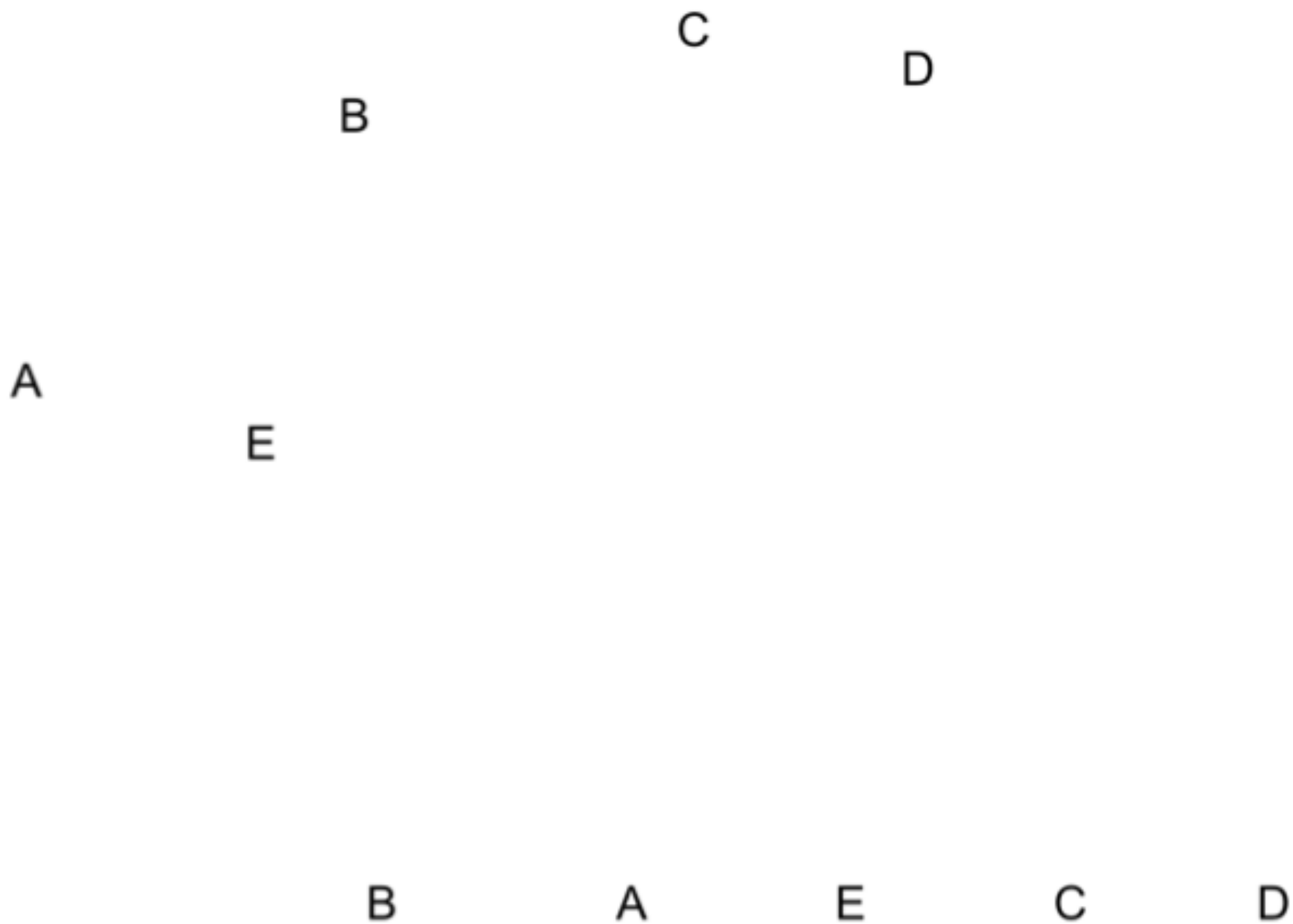
Hierarchical Agglomerative Clustering

- **Algorithm**
  - Start with each example $\mathbf{x}_i$ as its own cluster
  - Take pairwise distance between examples
  - Merge closest pair into a new cluster
  - Repeat until one cluster

- Doesn't require choice of number of clusters
- Clusters can have arbitrary shape
- Clusters have intrinsic heirarchy
- No random initialization

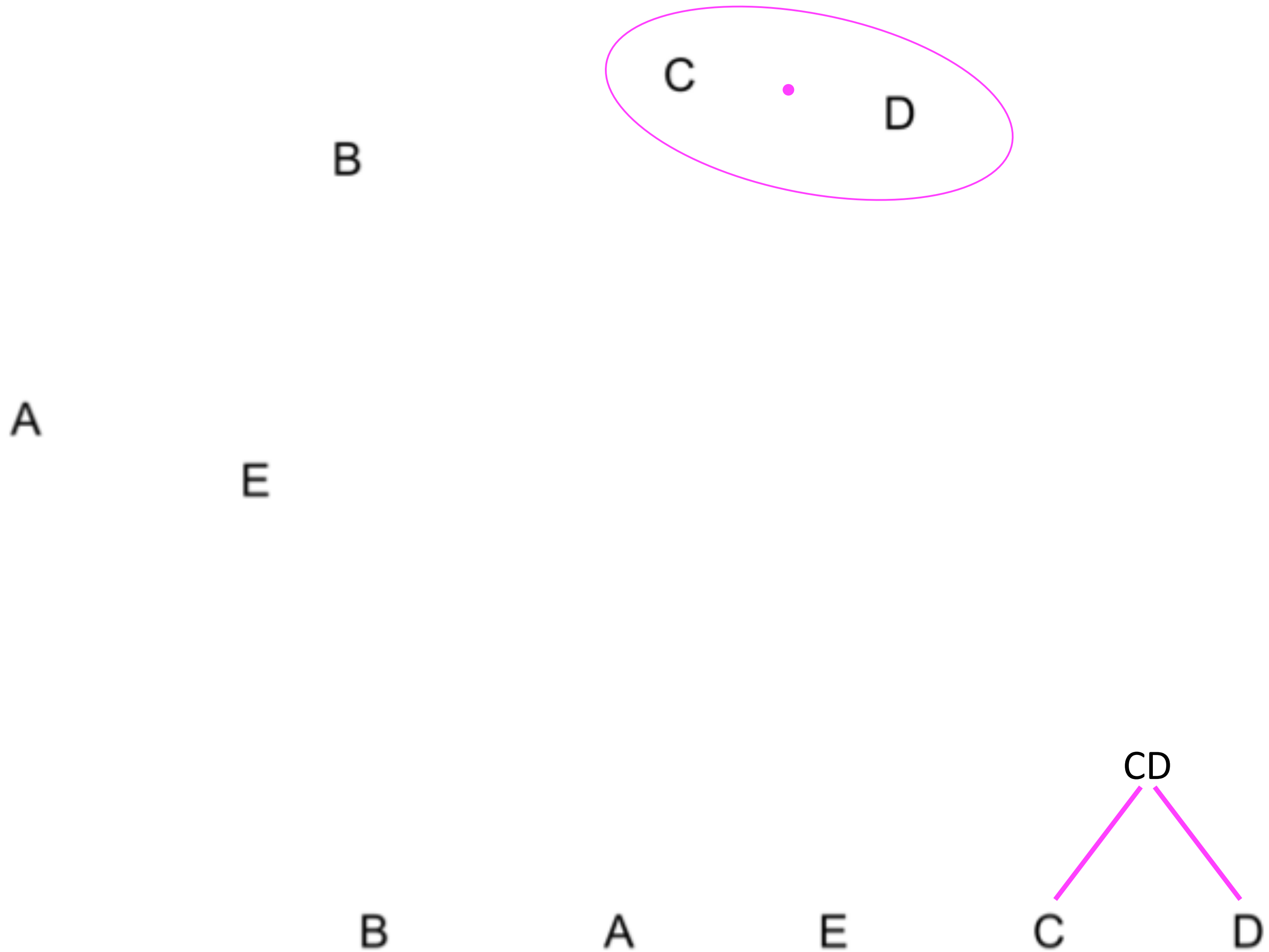
- What distance metric to use?
  - Here use Euclidean distance between cluster centroid (average of examples in cluster)

Hierarchical Agglomerative Clustering



[Parkes]

Hierarchical Agglomerative Clustering



[Parkes]

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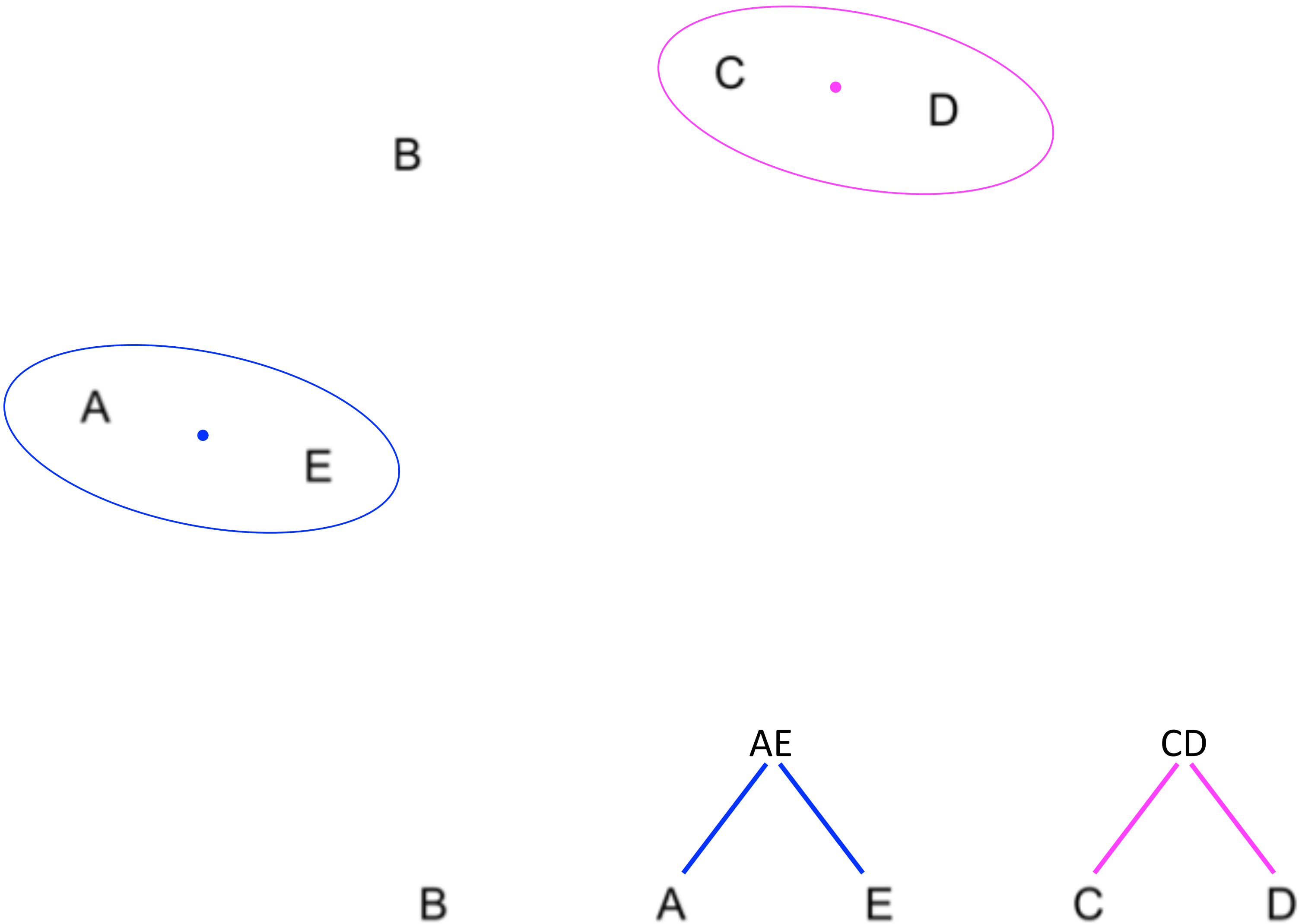

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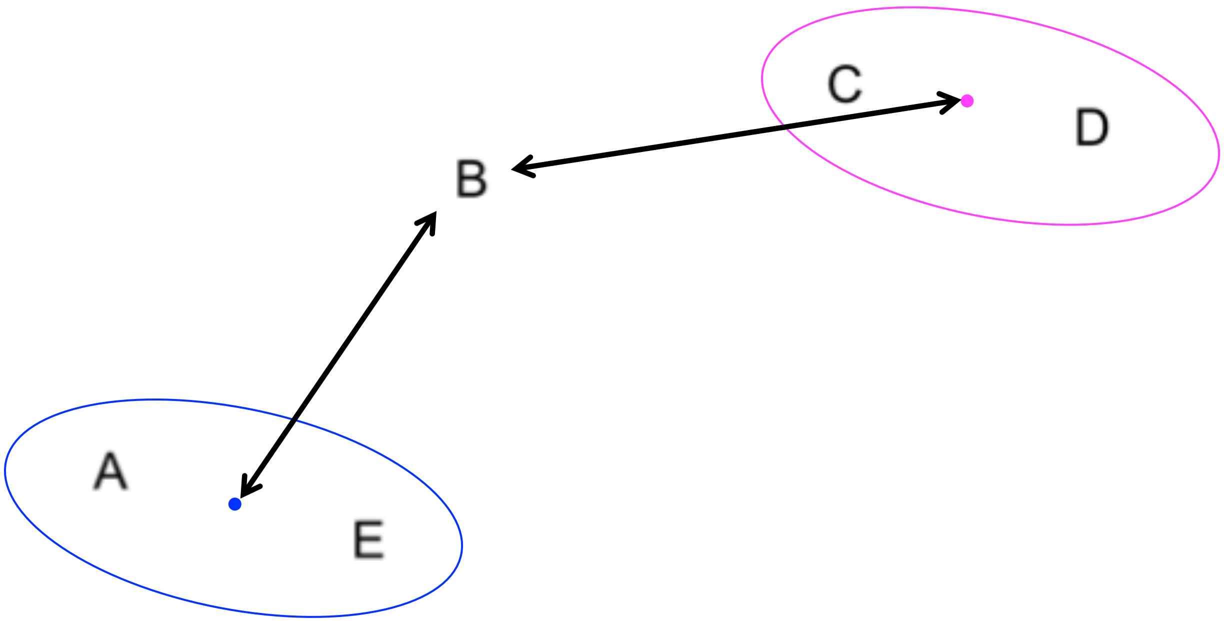

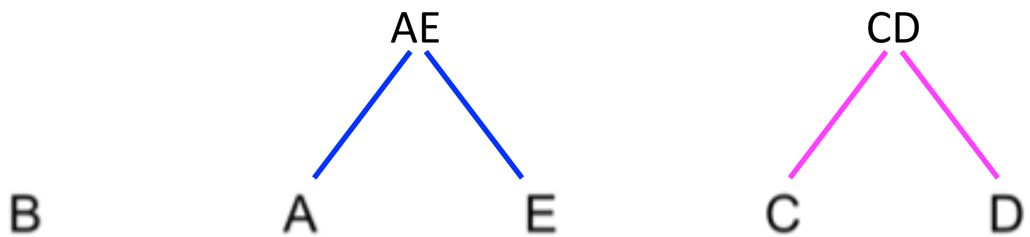

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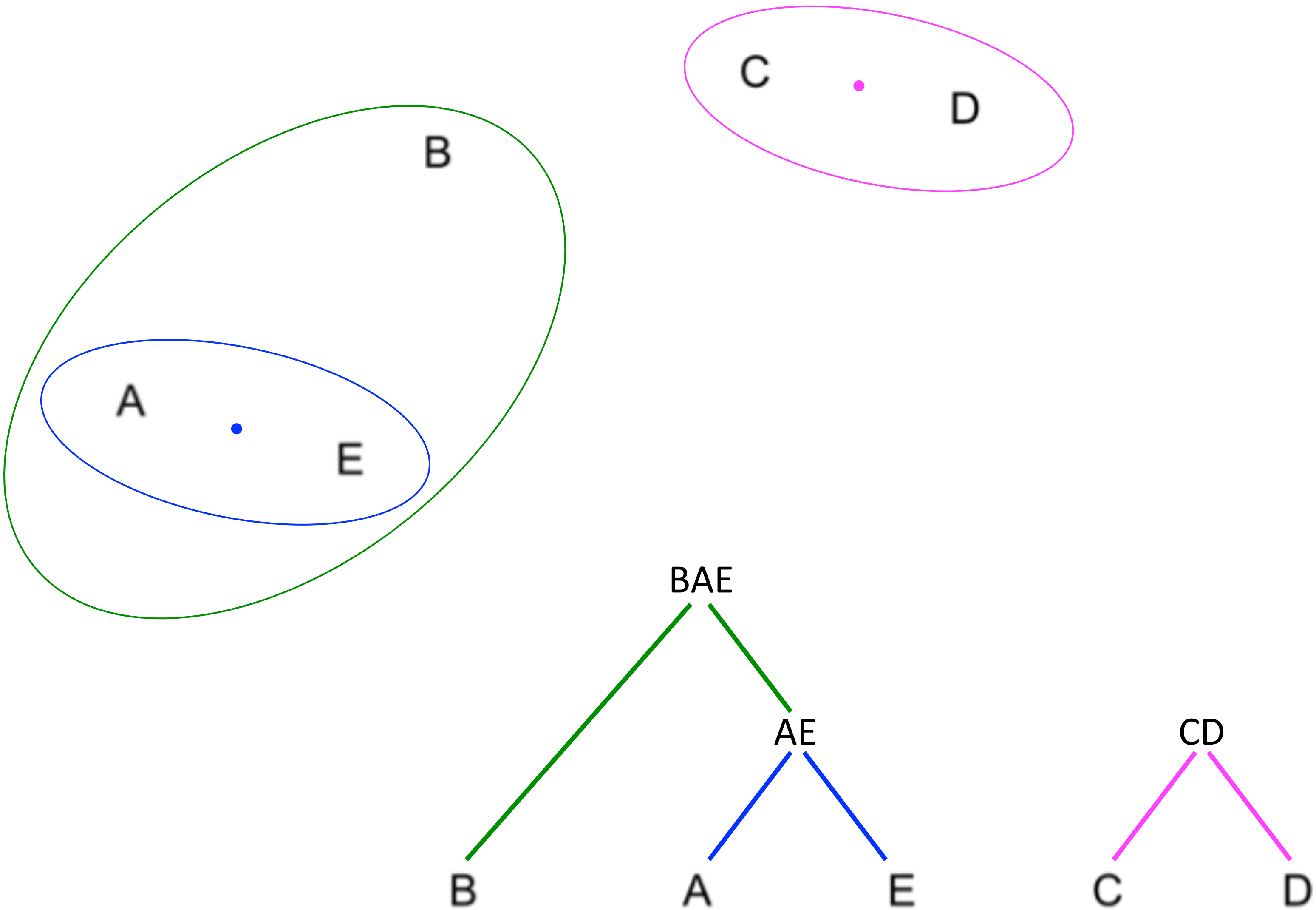

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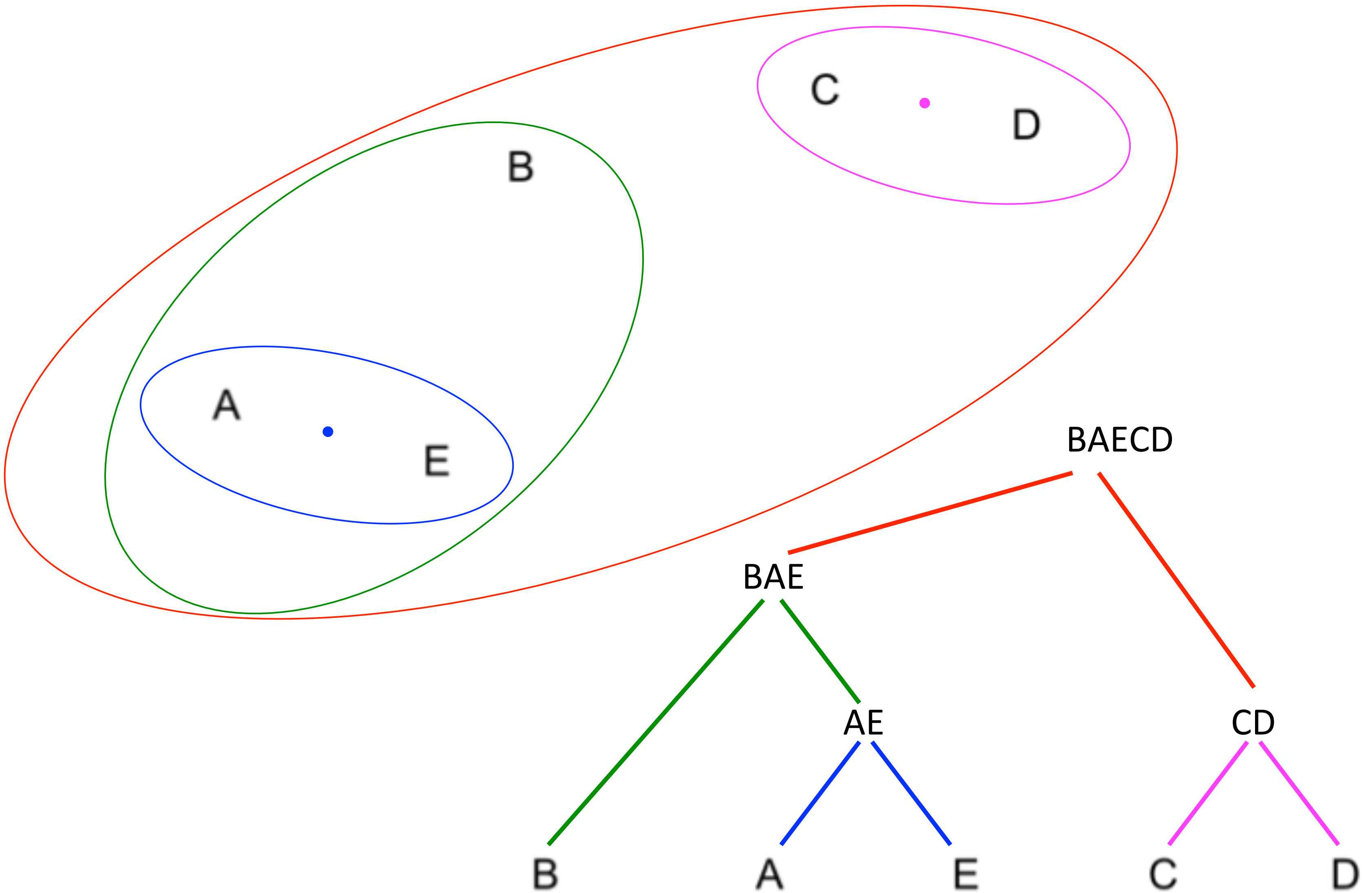
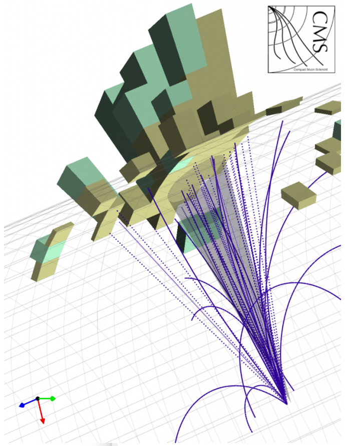


[Parkes]

Jet Algorithms



- Sequential pairwise jet clustering algorithms are hierarchical clustering, and are a form of unsupervised learning

- Compute distance between pseudojets i and j

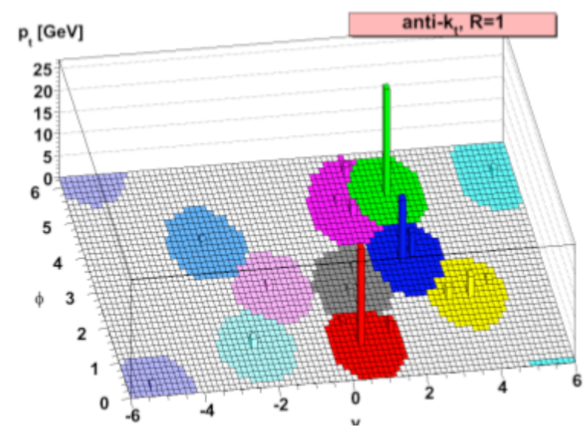
$$d_{ij} = \min\left(k_{\mathrm{T}i}^{2p}, k_{\mathrm{T}j}^{2p}\right) \frac{\Delta_{ij}}{D}$$

$$\Delta_{ij}^2 = (y_i - y_j)^2 + (\phi_i - \phi_j)^2$$

- Distance between pseudojet and beam

$$d_{iB} = k_{\mathrm{T}i}^{2p}$$

- Find smallest distance between pseudojets d_{ij} or d_{iB}
  - Combine (sum 4-momentum) of two pseudojets if d_{ij} smallest
  - If d_{iB} is smallest, remove pseudojet i, call it a jet
  - Repeat until all pseudojets are jets



Practical Advice

What To Use? So Many Choices

- Once you know what you want to do…

  WHAT algorithm should you use?
  - Linear model
  - Nearest Neighbors
  - (Deep?) Neural network
  - Decision tree ensemble
  - Support vector machine
  - Gaussian processes
  - … and so many more …

No Free Lunch - Wolpert (1996)

- In the absence of prior knowledge, there is no a priori distinction between algorithms, no algorithm that will work best for every supervised learning problem
  - You can not say algorithm X will be better without knowing about the system
  - A model may work really well on one problem, and really poorly on another
  - This is why data scientists have to try lots of algorithms!
- But there are some empirical heuristics that have been observed…

Practical Advice – Empirical Analysis

- Test 179 classifiers (no deep neural networks) on 121 datasets
  http://jmlr.csail.mit.edu/papers/volume15/delgado14a/delgado14a.pdf
  - *The classifiers most likely to be the bests are the random forest (RF) versions, the best of which (...) achieves 94.1% of the maximum accuracy overcoming 90% in the 84.3% of the data sets*

From Kaggle

- For Structured data: "High level" features that have meaning
  - Winning algorithms have been lots of feature engineering + random forests, or more recently XGBoost (also a decision tree based algorithm)
- Unstructured data: "Low level" features, no individual meaning
  - Winning algorithms have been deep learning based, Convolutional NN for image classification, and Recurrent NN for text and speech

More general advice

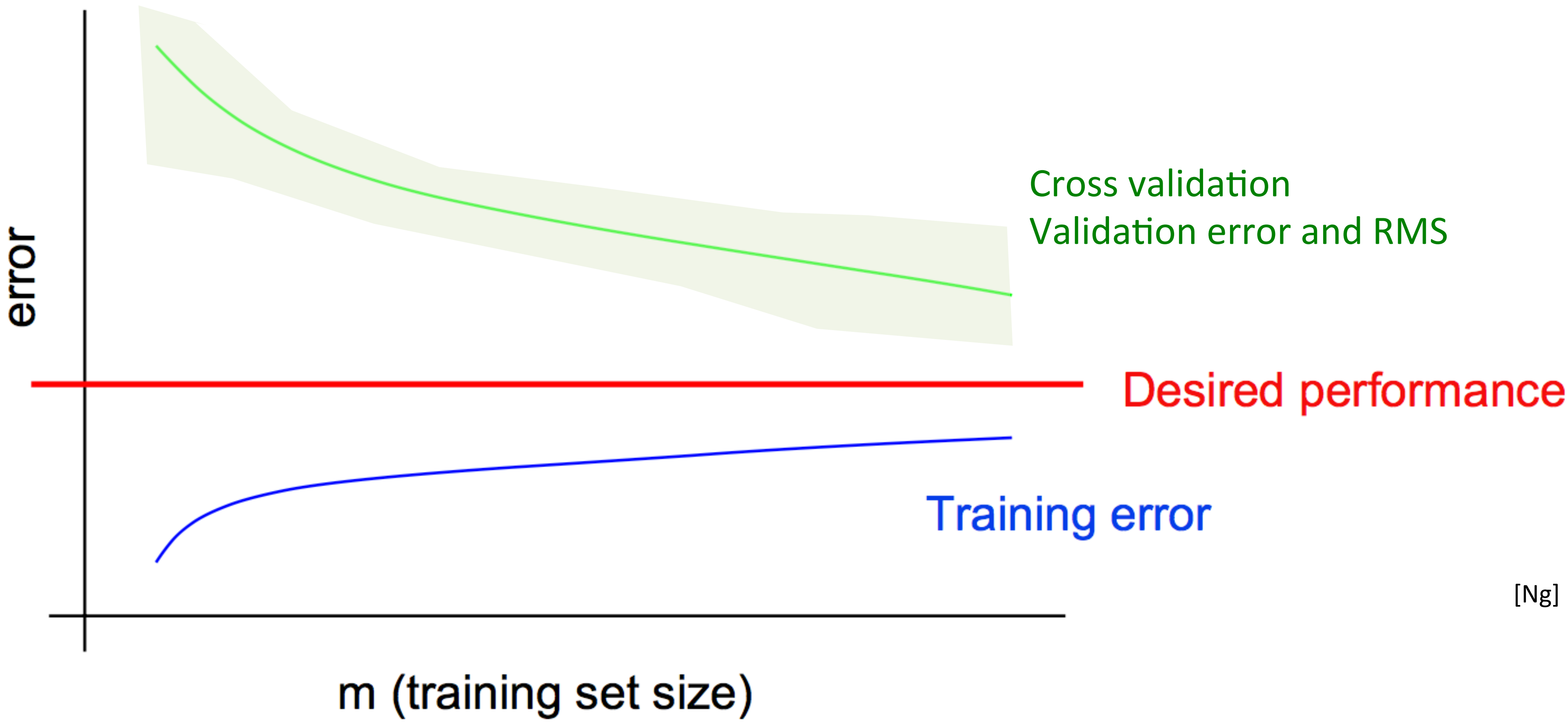
- You will likely need to try many algorithms…
  - Start with something simple!
  - Use more complex algorithms as needed
  - Use cross validation to check for overcomplexity / overtraining
- Check the literature
  - If you can cast your (HEP) problem as something in the ML / data science domain, there may be guidance on how to proceed
- Hyperparameters can be hard to tune
  - Use cross validation to compare models with different hyperparameter values!
- Use a training / validation / testing split of your data
  - Don't use training or validation set to determine final performance
  - And use cross validation as well!

Debugging Learning Algorithms

- Is my model working properly?
  - Where do I stand with respect to bias and variance?
  - Has my training converged?
  - Did I choose the right model / objective?
  - Where is the error in my algorithm coming from?

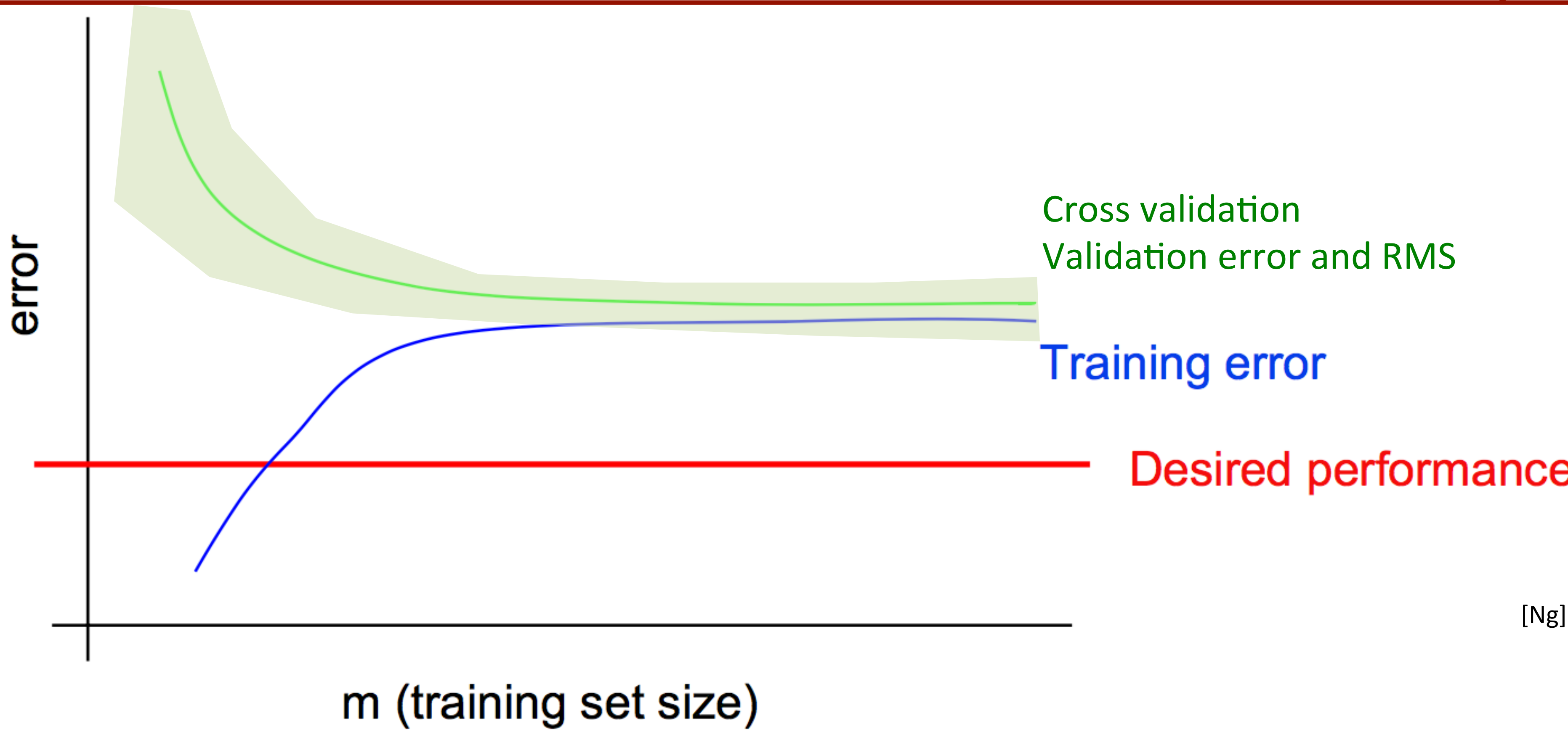
Section derived from [Ng]

Typical learning curve for high variance



- Performance is not reaching desired level
- Error still decreasing with training set size
  - suggests to use more data in training
- Large gap between training and validtaion error
  - Some gap is expected (inherint bias towards training set)
- Better: Large Cross-validation RMS, large performance variation in trainings

Typical learning curve for high bias



- Training error is unacceptably high
- Small gap between training and validation error
- Cross validation RMS is small

Potential Fixes

- Fixes to try:
  - Get more training data — Fixes high variance
  - Try smaller feature set size — Fixes high variance
  - Try larger feature set size — Fixes high bias
  - Try different features — Fixes high bias

- Did the training converge?
  - Run gradient descent a few more iterations — Fixes optimization algorithm
    - or adjust learning rate
  - Try different optimization algorithm — Fixes optimization algorithm

- Is it the correct model / objective for the problem?
  - Try different regularization parameter value — Fixes optimization objective
  - Try different model — Fixes optimization objective

- You will often need to come up with your own diagnostics to understand what is happening to your algorithm

[Ng]

Conclusions

- Machine learning uses mathematical and statistical models learned from data to characterize patterns and relations between inputs, and use this for inference / prediction

- Machine learning provides a powerful toolkit to analyze data
  - Linear methods can help greatly in understanding data

  - Complex models like NN and decision trees can model intricate patterns
    - Care needed to train them and ensure they don't overfit

  - Unsupervised learning can provide powerful tools to understand data, even when no labels are available

  - Choosing a model for a given problem is difficult, but there may be some guidance in the literature
    - Keep in mind the bias-variance tradeoff when building an ML model

- Deep learning is an exciting frontier and powerful paradigm in ML research
  - We will hear more about it tomorrow!

Advertisements

- Tomorrow's lecture on deep learning and computer vision from Jon Shlens from Google Brain!

- Data Science @ HEP workshop on machine learning in high energy physics
  - May 8-12, 2017 at Fermilab
  - https://indico.fnal.gov/conferenceDisplay.py?ovw=True&confId=13497

Useful Python ML software

- Anaconda / Conda → easy to setup python ML / scientific computing environments
  - https://www.continuum.io/downloads
  - http://conda.pydata.org/docs/get-started.html
- Integrating ROOT / PyROOT into conda
  - https://nlesc.gitbooks.io/cern-root-conda-recipes/content/index.html
  - https://conda.anaconda.org/NLeSC
- Converting ROOT trees to python numpy arrays / panda dataframes
  - https://pypi.python.org/pypi/root_numpy/
  - https://github.com/ibab/root_pandas
- Scikit-learn → general ML library
  - http://scikit-learn.org/stable/
- Deep learning frameworks / auto-differentiation packages
  - https://www.tensorflow.org/
  - http://deeplearning.net/software/theano/
- High level deep learning package build on top of Theano / Tensorflow
  - https://keras.io/

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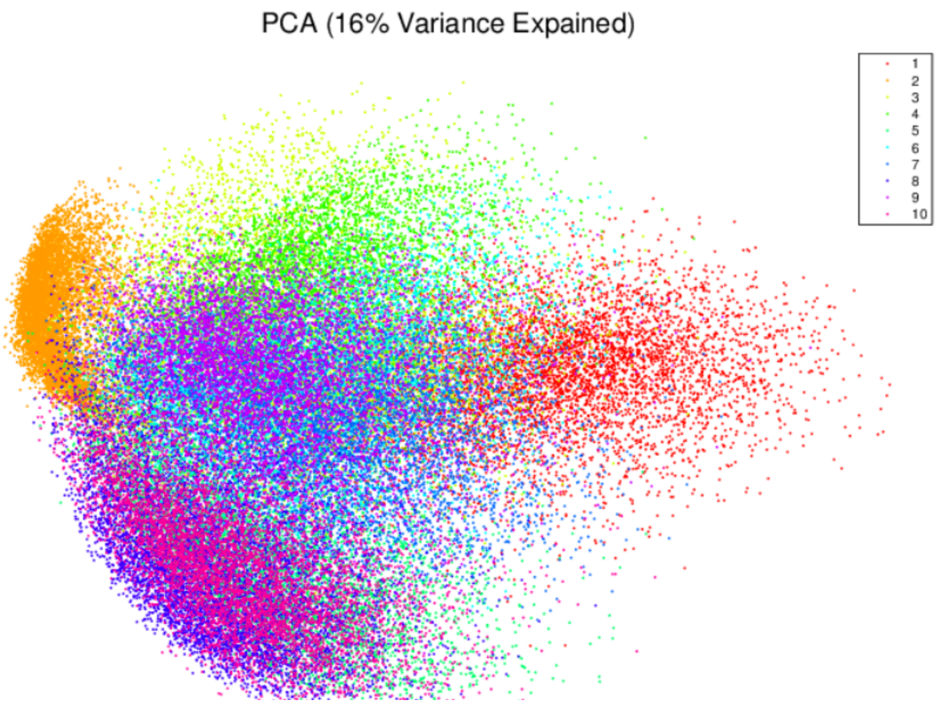
  - http://cs229.stanford.edu/
- [Rogozhnikov] Machine learning in high energy physics, Alex Rogozhnikov
  - https://indico.cern.ch/event/497368/

Example

- Classifying hand written digits
  - 10-class classification
  - Right plot shows projection of 10-class output onto 2 dimensions



Error Analysis

- Anti-spam classifier using logistic regression.
- How much did each component of the system help?
- Remove each component one at a time to see how it breaks

Component	Accuracy
Overall system	99.9%
Spelling correction	99.0
Sender host features	98.9%
Email header features	98.9%
Email text parser features	95%
Javascript parser	94.5%
Features from images	94.0%

Removing text parser caused largest drop in performance (Email text parser features)

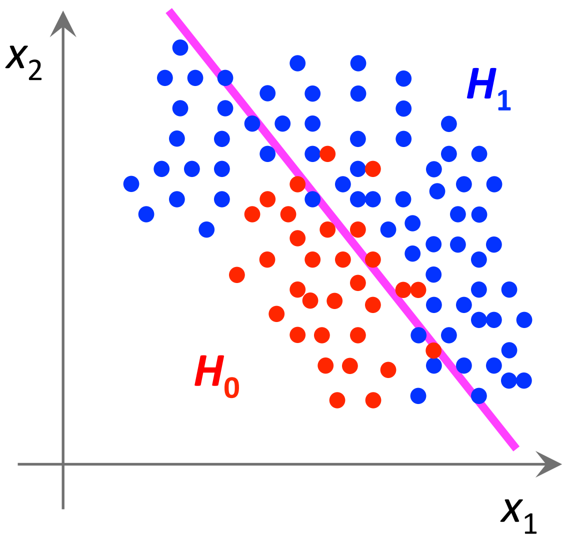
[baseline] (Features from images)

Ensemble Methods

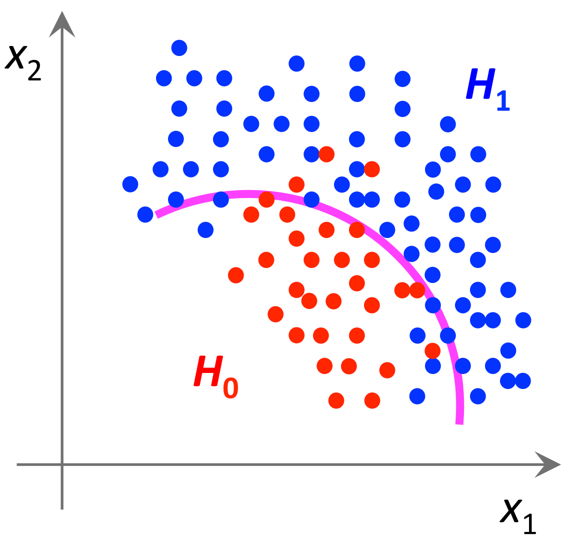
- Combine many decision trees, use the ensemble for prediction
- Averaging: $$D(x) = \frac{1}{N_{tree}} \sum_{i=1}^{N_{tree}} d_i(x)$$
  - **Random Forest**, averaging combined with:
    - **Bagging:** Only use a subset of events for each tree training
    - **Feature subsets**: Only use a subset of features for each tree
- Boosting (weighted voting): $$D(x) = \sum_{i=1}^{N_{tree}} \alpha_i d_i(x)$$
  - Weight computed such that events in current tree have higher weight misclassified in previous trees
  - Several boosting algorithms
    - AdaBoost
    - Gradient Boosting
    - XGBoost

Non-Linear Activations

- The activation function in the NN must be a non-linear function
  - If all the activations were linear, the network would be linear: $f(X) = W_n(W_{n-1} (\ldots W_1 X)) = UX$, where $U = \Pi_i W_i$
- Linear functions can only correctly classify linearly separable data!
- For complex datasets, need nonlinearities to properly learn data structure



Linear Classifier



Non-linear Classifier

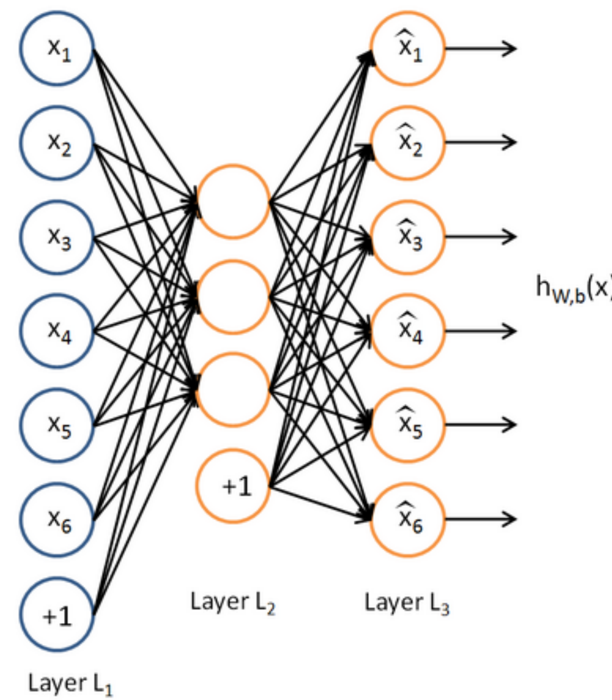
Neural Networks and Local Minima

- Large NN's difficult to train…trapping in local minimum?

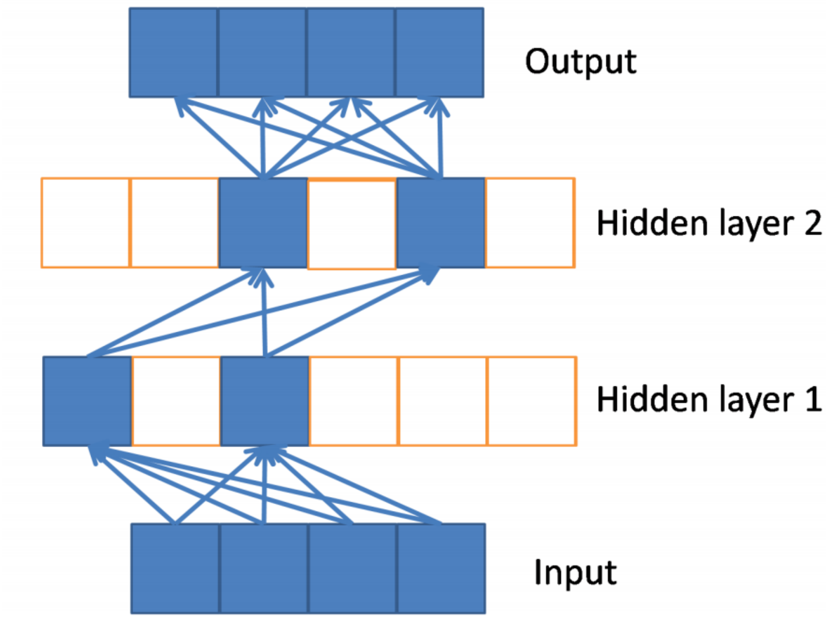
- Not in large neural networks *https://arxiv.org/abs/1412.0233*
  - Most local minima equivalent, and resonable
  - Global minima may represent overtraining
  - Most bad (high error) critical points are saddle points (different than small NN's)

Weight Initializations and Training Procedures

- Used to set weights to some small initial value
  - Creates an almost linear classifier
- Now initialize such that node outputs are normally distributed
- Pre-training with auto-encoder
  - Network reproduces the inputs
  - Hidden layer is a non-linear dimensionality reduction
  - Learn important features of the input
  - Not as common anymore, except in certain circumstances…
- Adversarial training, invented 2014
  - Will potential HEP applications later



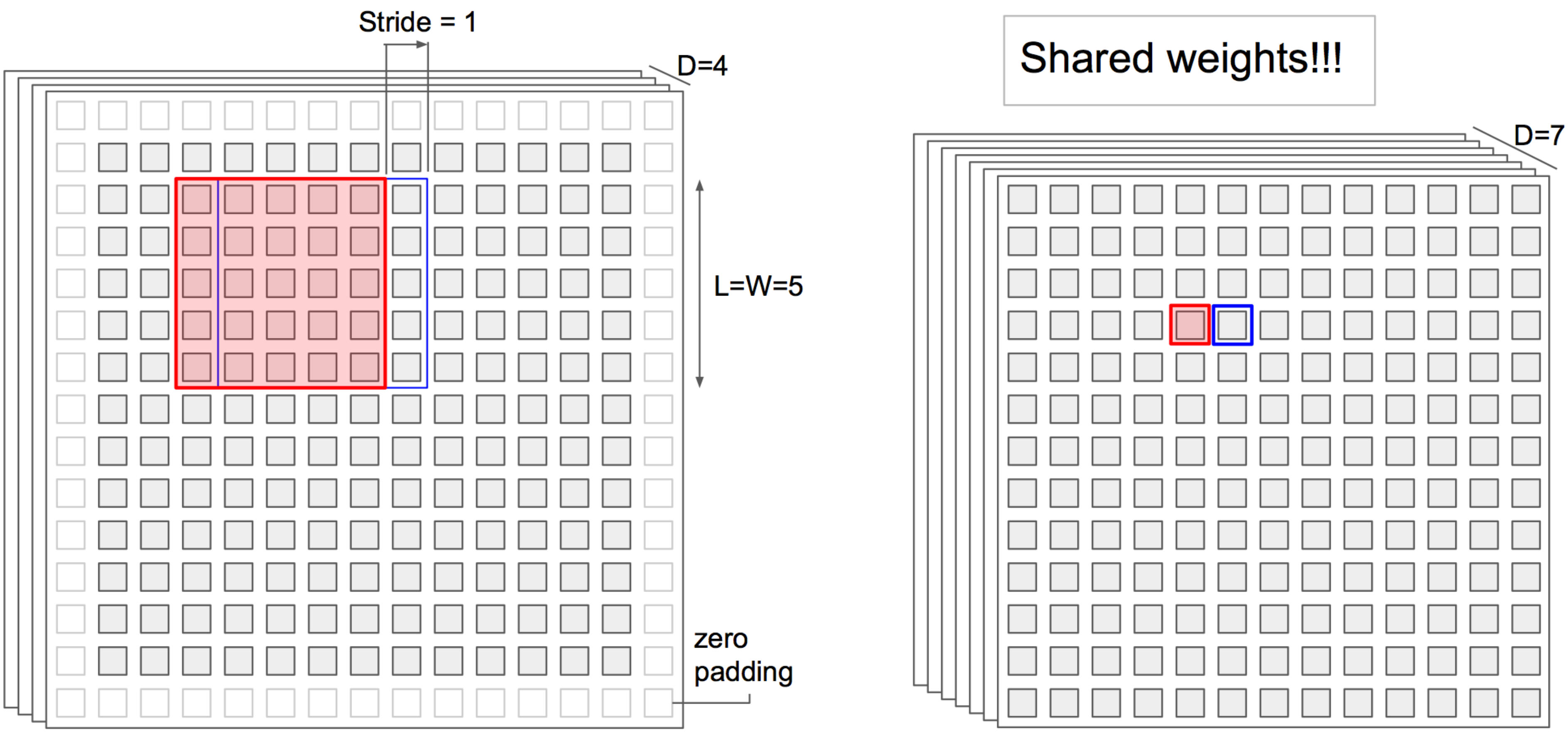
ReLU Networks



http://www.jmlr.org/proceedings/papers/v15/glorot11a/glorot11a.pdf

- Sparse propagation of activations and gradients in a network of rectifier units. The input selects a subset of active neurons and computation is linear in this subset.
- Model is "linear-by-parts", and can thus be seen as an exponential number of linear models that share parameters
- Non-linearity in model comes from path selection

Convolutions in 2D

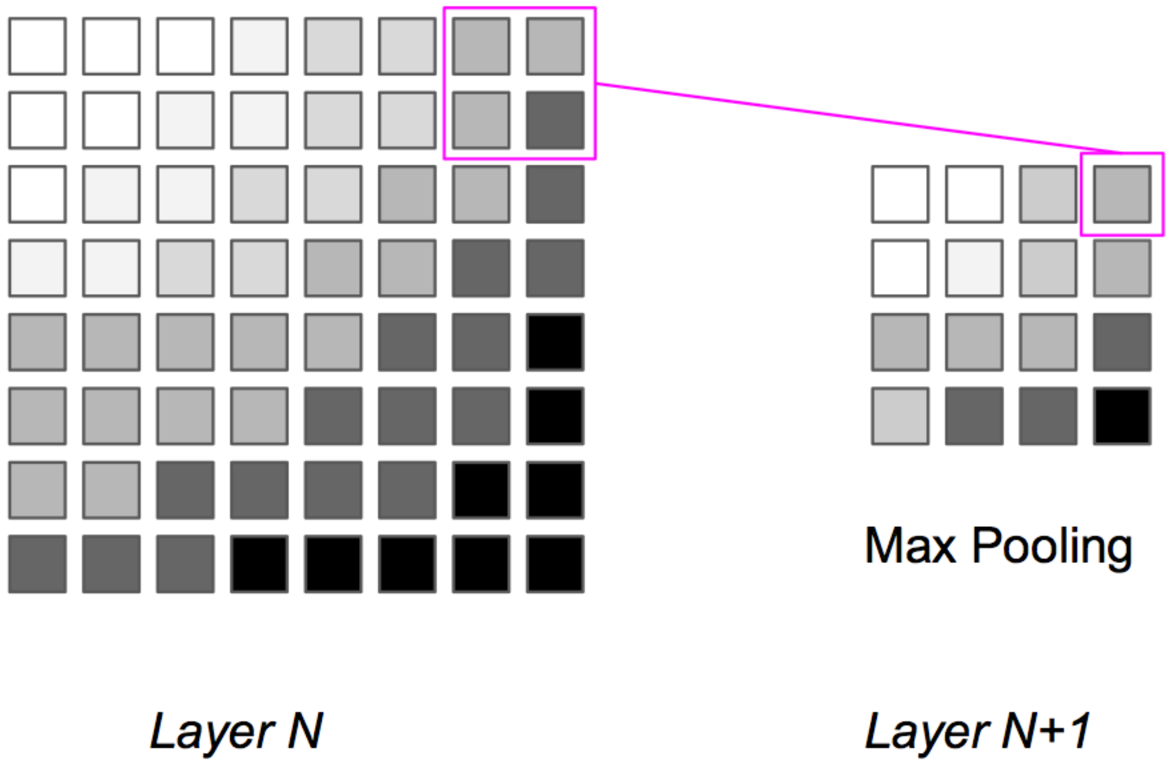


Input image

Convolved image

- Scan the filters over the 2D image, producing the convolved images

Max Pooling

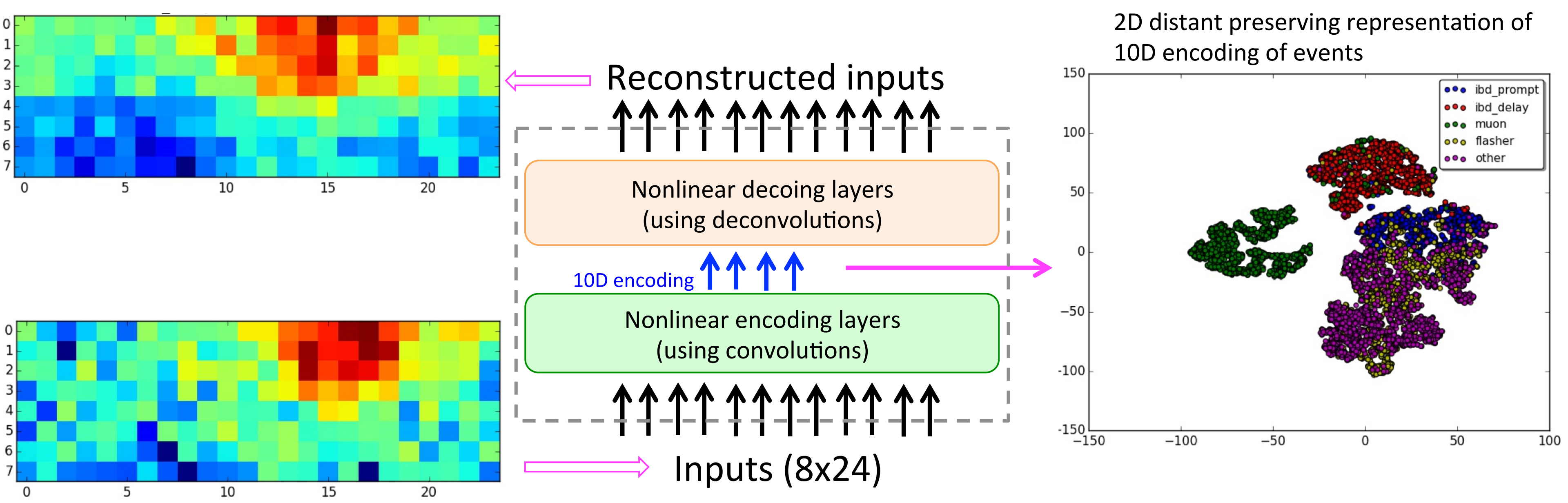


- Down-sample the input by taking MAX or average over a region of inputs
  - Keep only the most useful information

Daya Bay Neutrino Experiment

arXiv:1601.07621

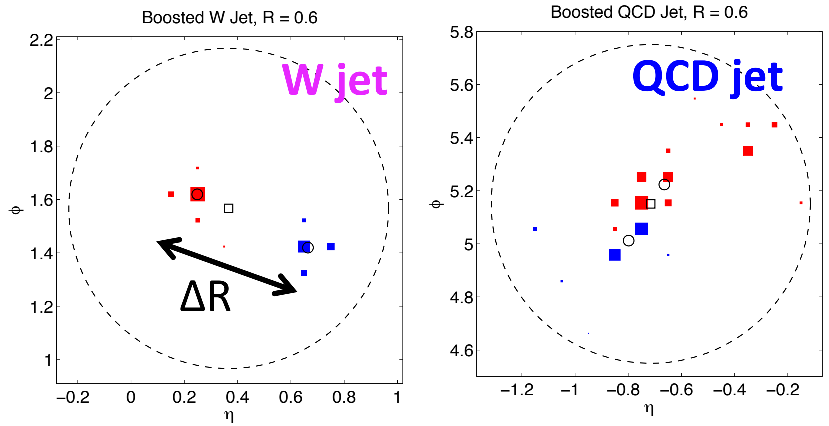
- Aim to reconstruct inverse β-decay interactions from scintillation light recorded in 8x24 PMT's
- Study discrimination power using CNN's
  - Supervised learning → observed excellent performance (97% accuracy)
  - Unsupervised learning: ML learns itself what is interesting!

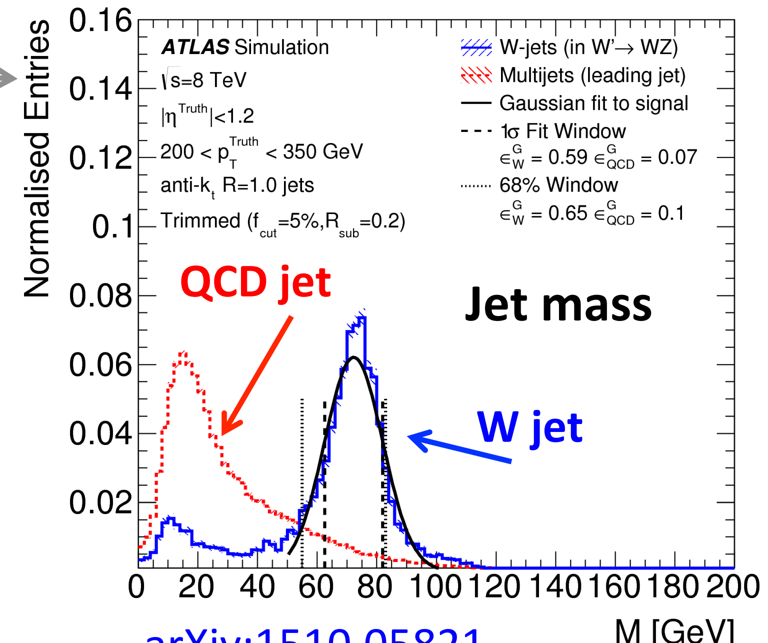


Jet tagging using jet substructure

- **Typical approach:**
  Use physics inspired variables to provide signal / background discrimination

- Typical physics inspired variables exploit differences in:
  - **Jet mass**
  - **N-prong structure**:
    - 1-prong (QCD)
    - 2-prong (W,Z,H)
    - 3-prong (top)
  - **Radiation pattern:**
    - Soft gluon emission
    - Color flow





arXiv:1510.05821

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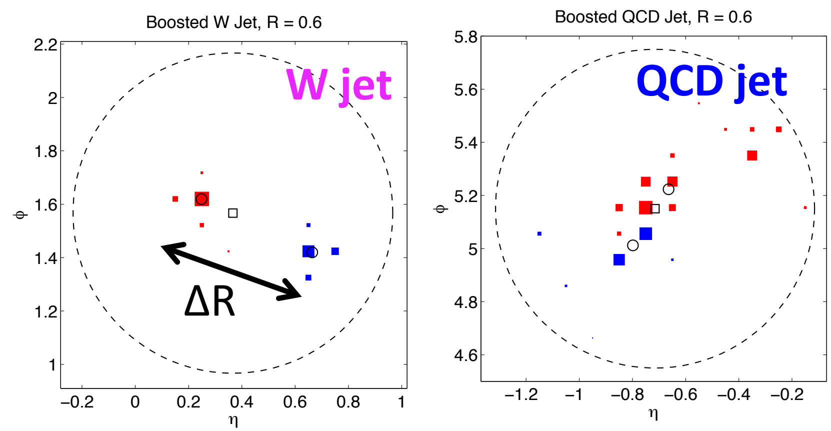
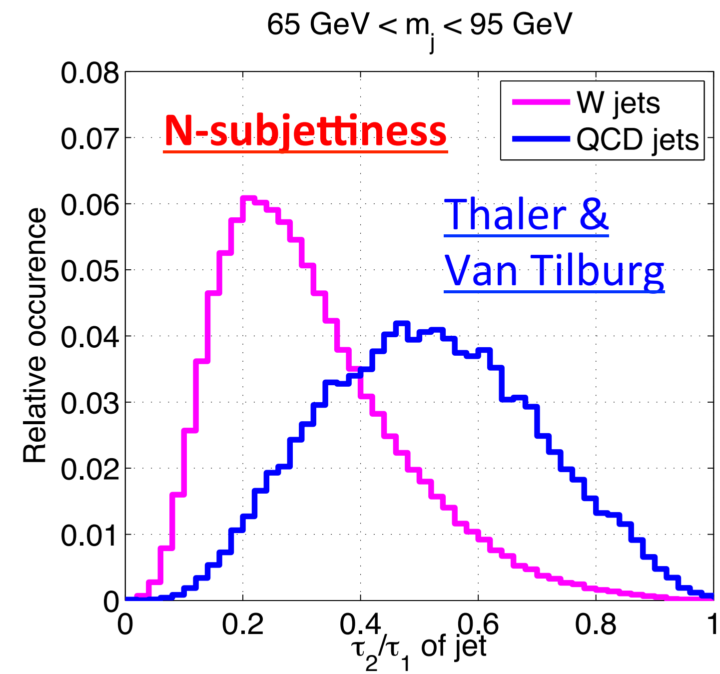


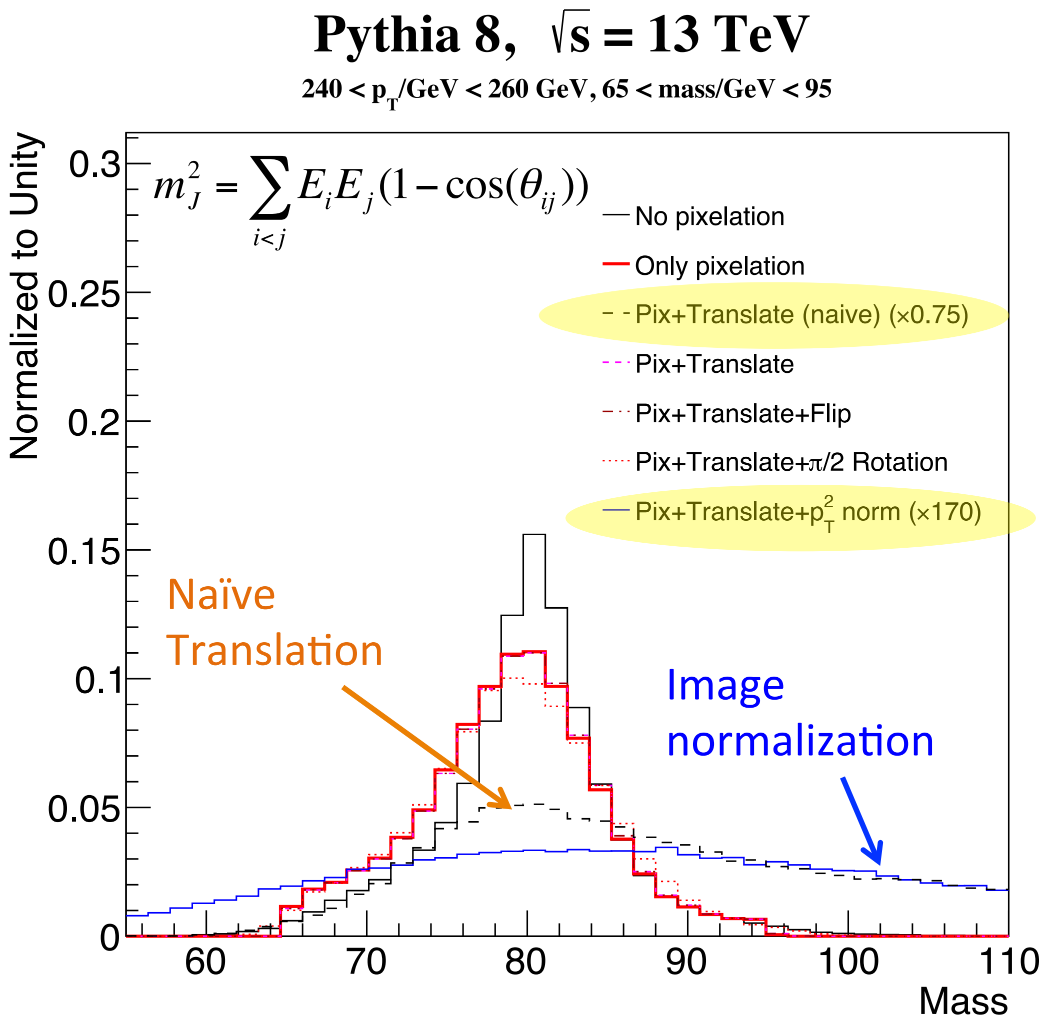


$$\tau_N = \frac{1}{d_0} \sum p_{T,k} \min\{\Delta R_{k,axis-1}, \ldots, \Delta R_{k,axis-n}\}$$

Pre-processing and space-time symmetries

Pre-processing steps may not be Lorentz Invariant

- Translations in η are Lorentz boosts along z-axis
  - Do not preserve the pixel energies
  - Use p_T rather than E as pixel intensity
- Jet mass is not invariant under Image normalization

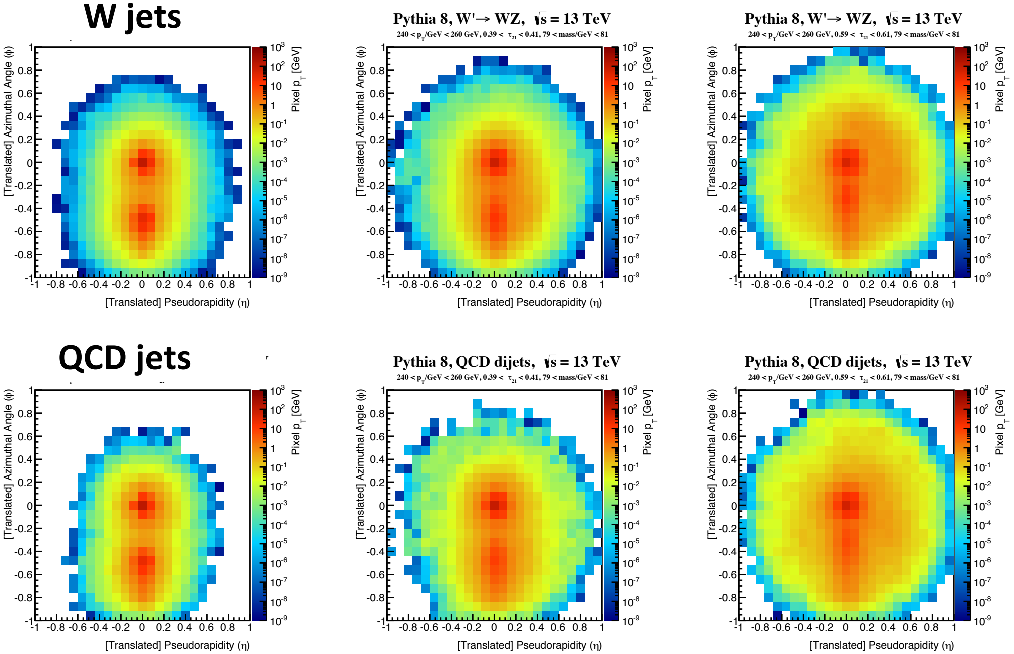


Restricted phase space

2-prong τ_{21} **1-prong**

W jets

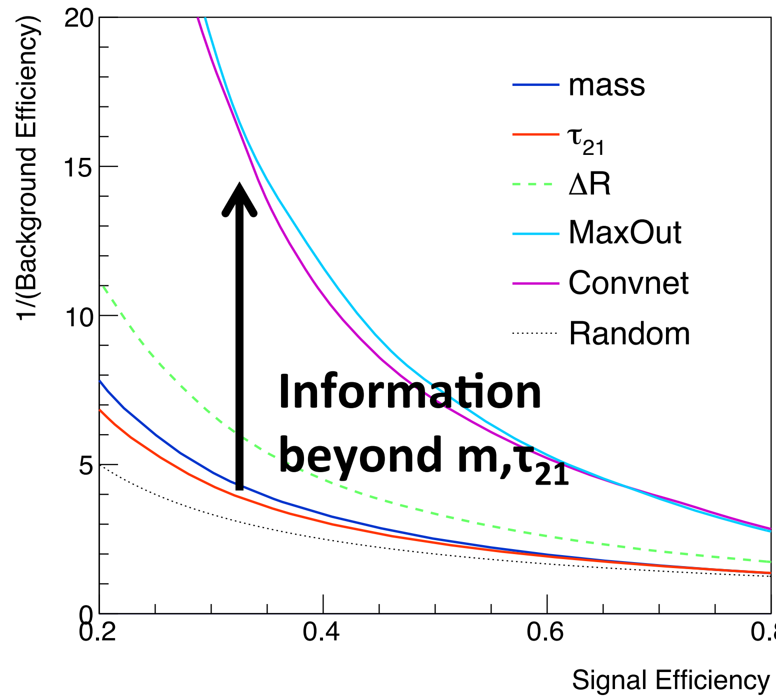
QCD jets



[0.19, 0.21] **[0.39, 0.41]** **[0.59, 0.61]**

79 < m < 81 GeV

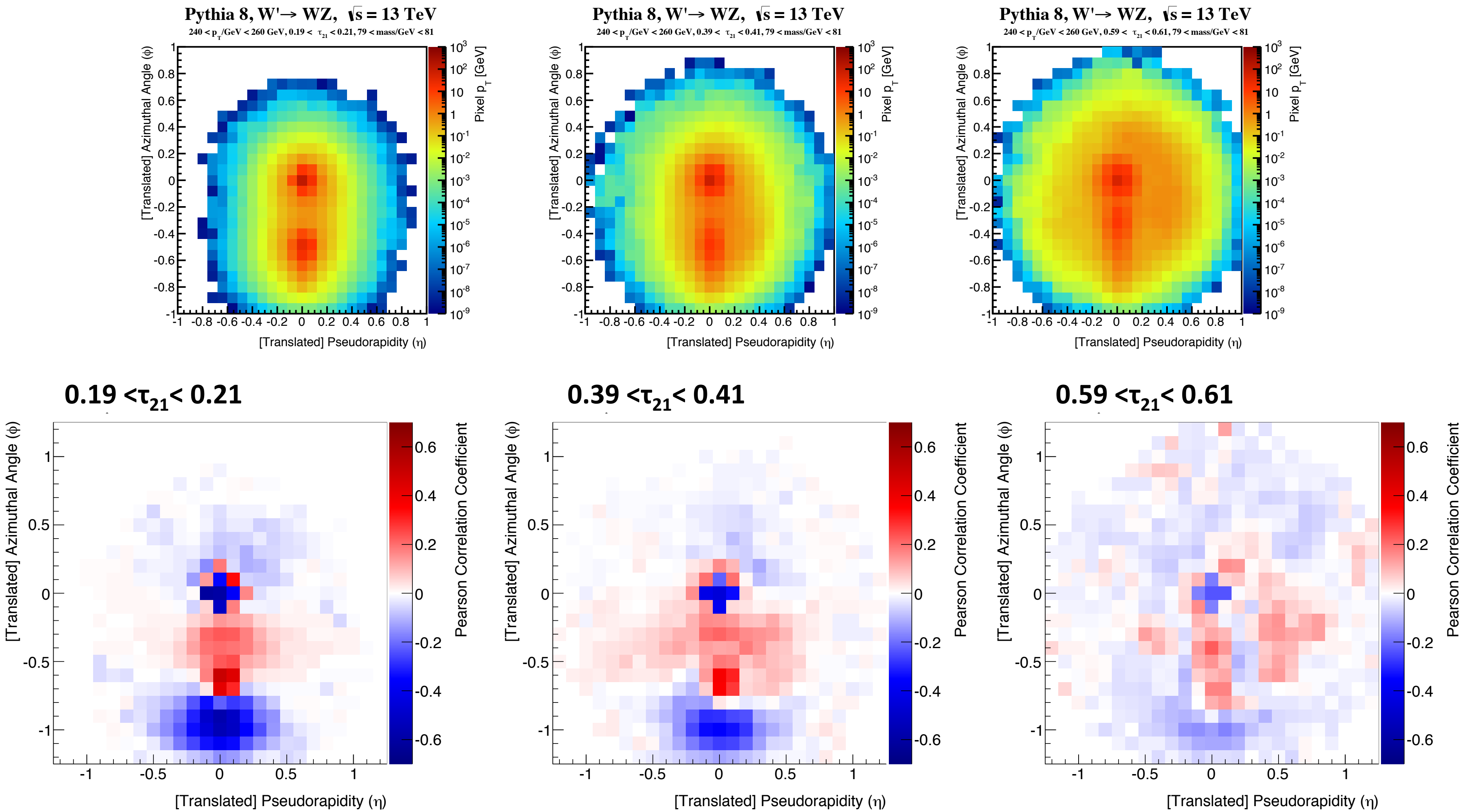
$0.19 < \tau_{21} < 0.21$



Restrict the phase space in very small mass and τ_{21} bins:

Improvement in discrimination from new, unique, information learned by the network

Deep correlation jet images



Spatial information indicative of radiation pattern for W and QCD: where in the image the network is looking for discriminating features