PY410 / 505
Computational Physics 1

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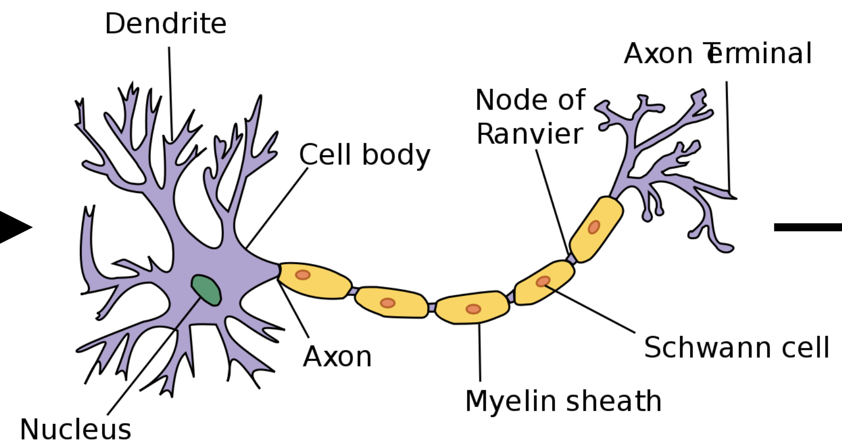
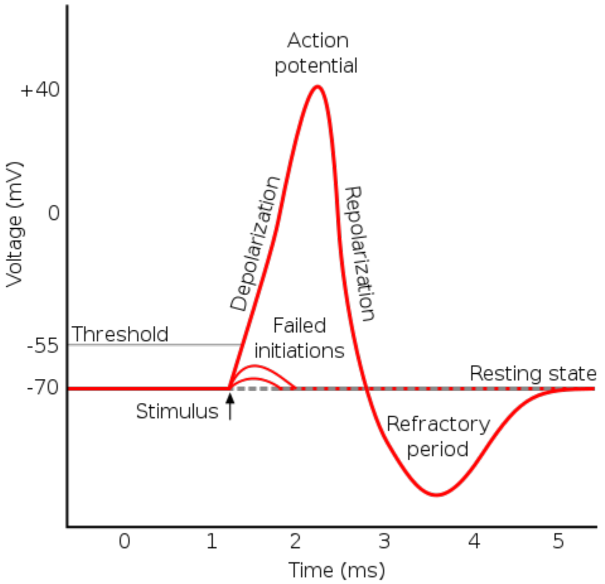
Real Neural Networks

Chemical concentration input

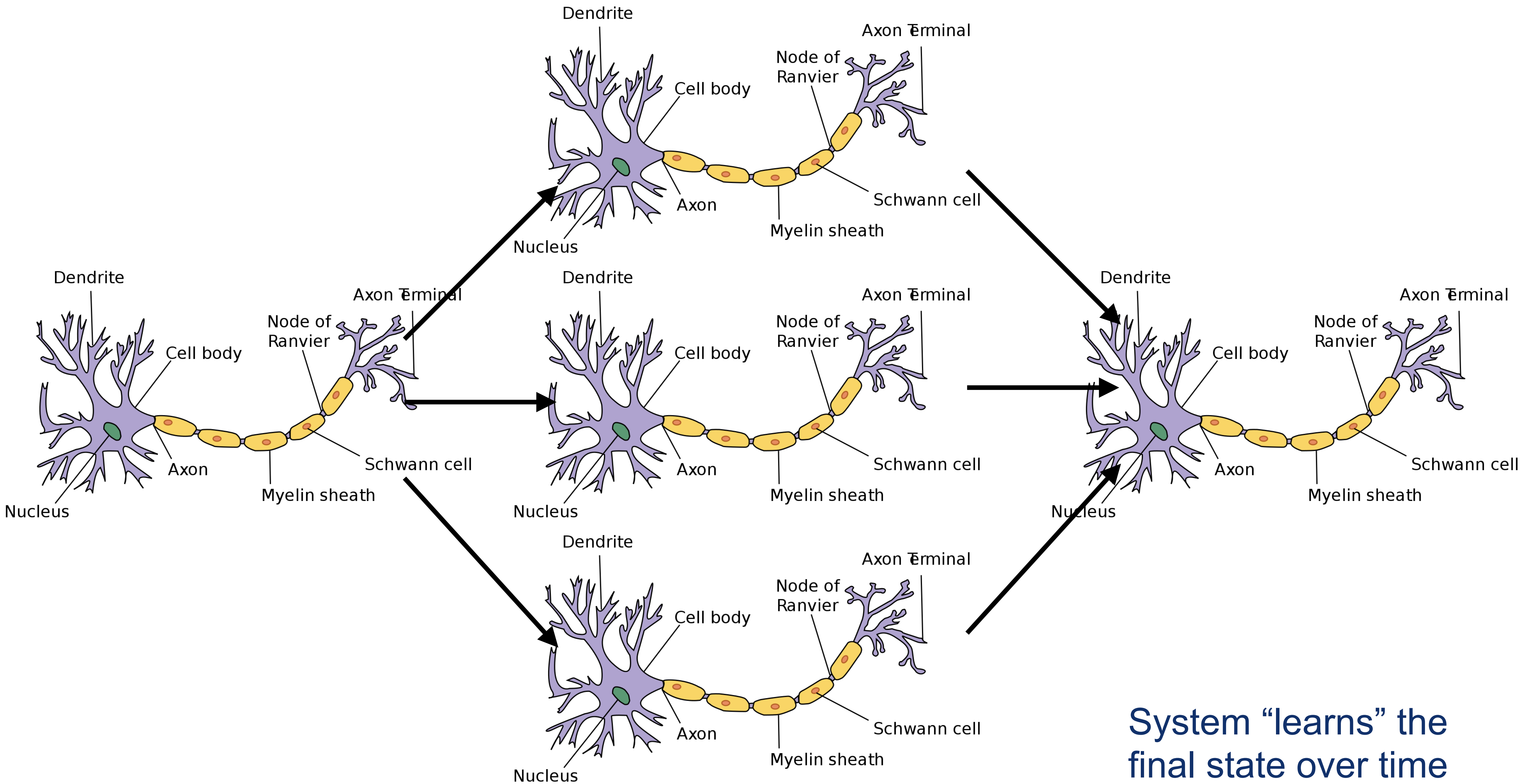


Chemical concentration output

Activation



Real Neural Networks



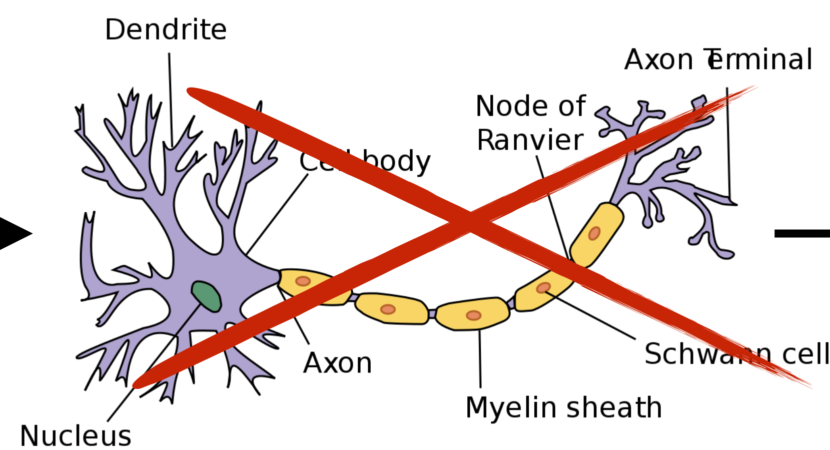
System “learns” the final state over time

Neurons affect other neurons, and the “state” is saved

Artificial Neural Networks

Number

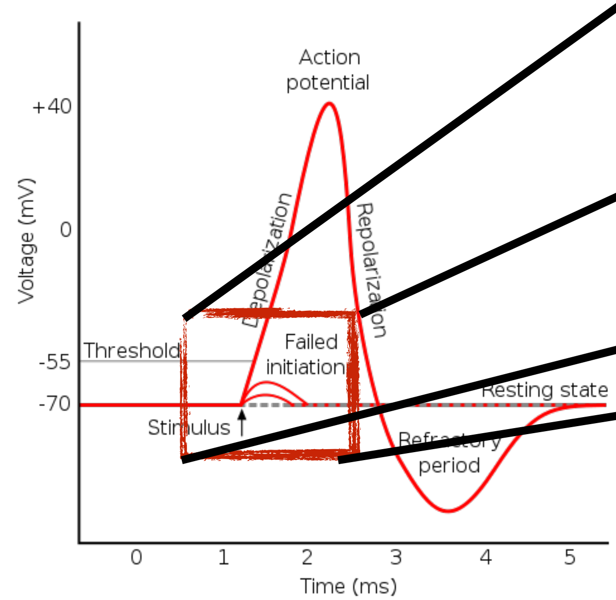
~~Chemical concentration~~ input

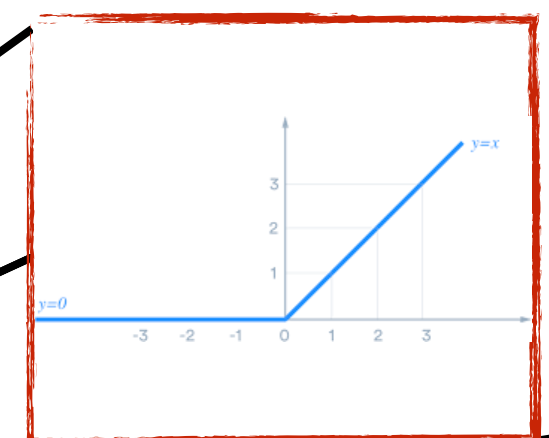


Number

~~Chemical concentration~~ output

Activation

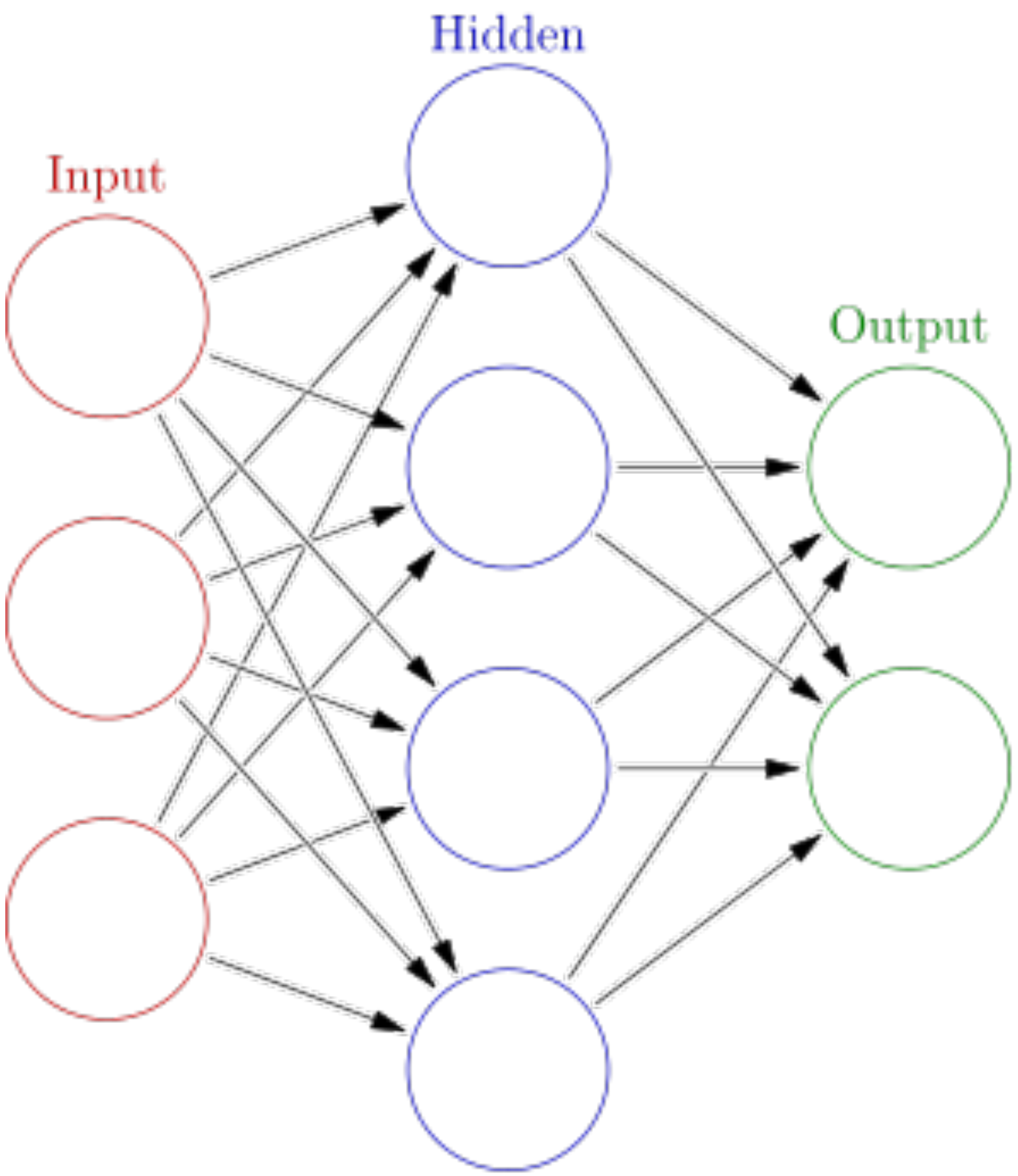




“Rectified linear unit”

Neural Networks

- The neural network is a group of neurons working together in such a persistent state:



https://en.wikipedia.org/wiki/Artificial_neural_network

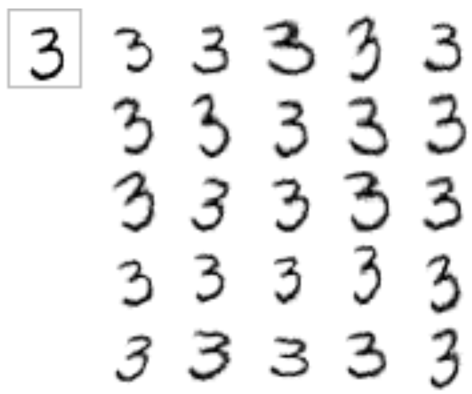
Neural Networks

- Training:
  - Feed a sample where you know the answer to the network
  - Tell the network the answer

- Discrimination:
  - Network takes inputs from UNKNOWN source
  - Outputs weights relative to known outcomes

Example to recognize handwriting:

"These are all the number 3":



"Is this a 3"?

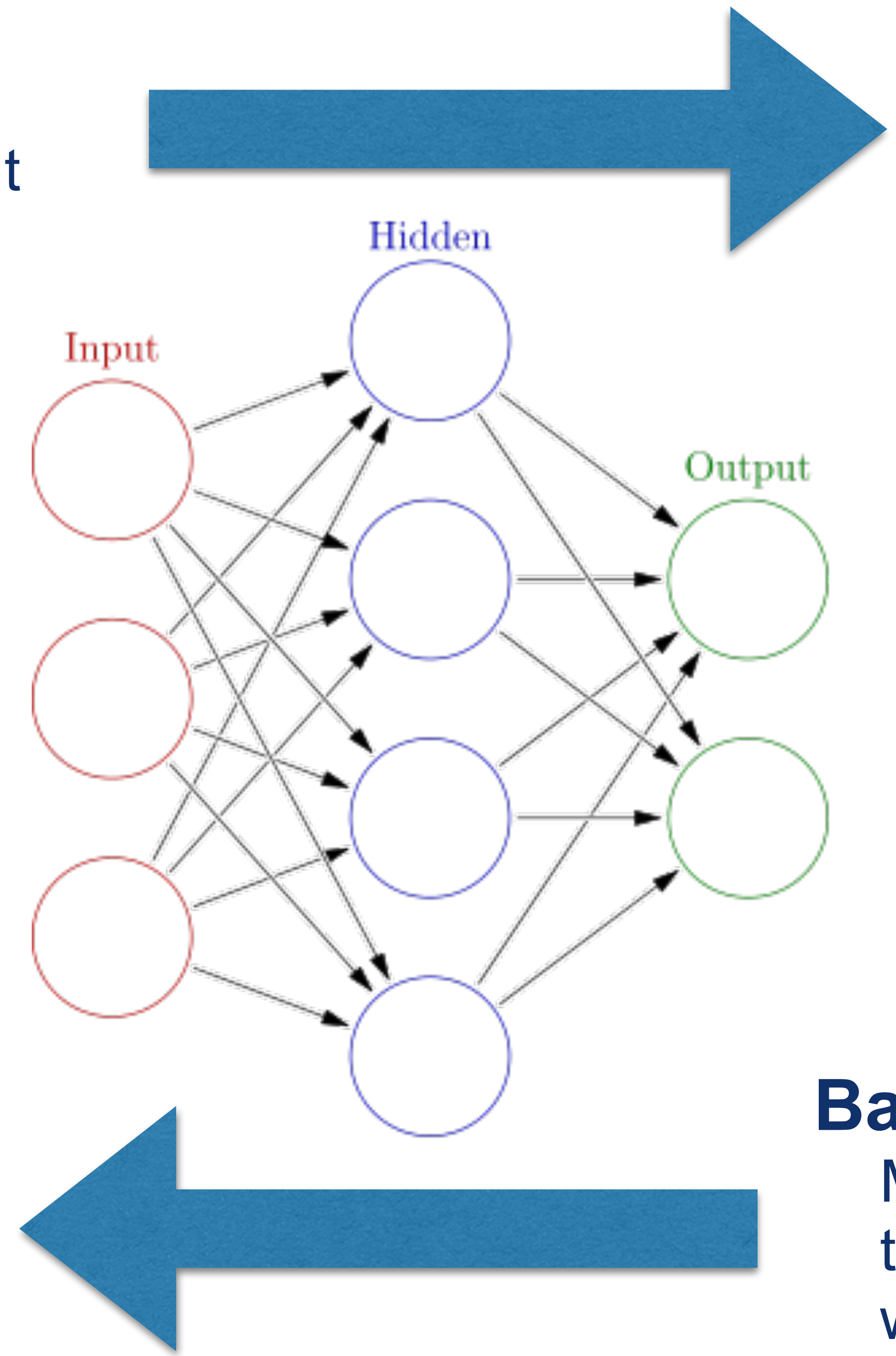
Outputs "yes"

Outputs "no"

https://www.codeproject.com/Articles/16650/Neural-Network-for-Recognition-of-Handwritten-Digi

Neural Networks

Feed forward:
Weight inputs, get output

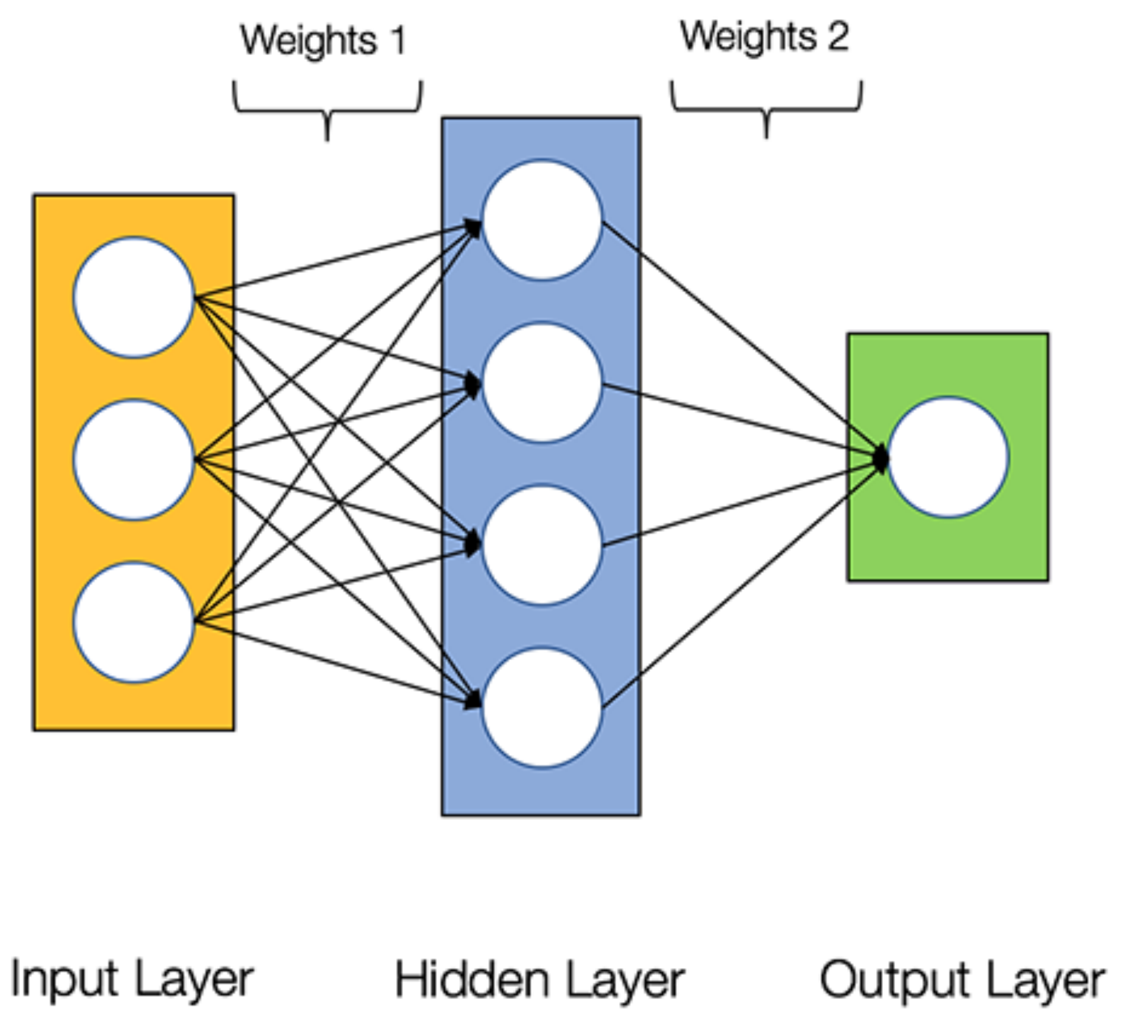


Back-propagate:
Minimize difference between target output and current weights

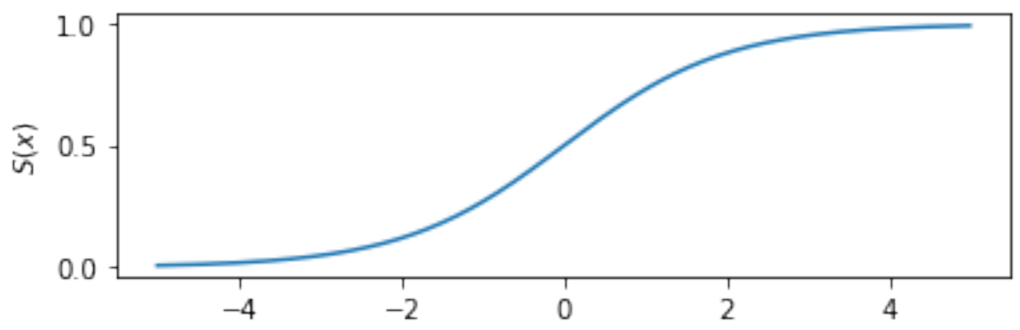
Neural Networks

- Consider a 2-layer network

- A bit more formally:
  - Input vector $\vec{x}$
  - Output vector $\vec{y}$
  - Weights and biases between layers W and b
  - Activation function σ



Usually rectified linear unit (ReLU), but we will use sigmoid because it is differentiable.



Adapted from https://towardsdatascience.com/how-to-build-your-own-neural-network-from-scratch-in-python-68998a08e4f6

Neural Networks

- For each training step:
  - Feed forward $\vec{x} \rightarrow \hat{y}$:
  - $\hat{y} = \sigma(W_2\sigma(W_1\vec{x} + b_1) + b_2)$
  - Compute loss function (least squares):
    $L(y, \hat{y}) = \sum_i (y - \hat{y})^2$
  - Compute gradient of loss function wrt weights
    $\frac{\partial L(y,\hat{y})}{\partial W}$
  - Back propagate :
    - Optimize using gradient descent (like BFGS!)

Caveats about optimization in multiple dimensions hold here!

Adapted from
https://towardsdatascience.com/how-to-build-your-own-neural-network-from-scratch-in-python-68998a08e4f6

Deep Learning and Neural Networks

- Next step: instead of teaching, let the neural network learn on its own
  - Example 1: Convolutional Neural Network
    - Extract features using convolution, pass features to neural network
    - Fixed-size inputs: Suitable for images
  - Example 2: Recurrent Neural Network
    - Instead of “feed forward” like last time, has possible recurrent links
    - Any size inputs: Suitable for text / speech / handwriting recognition
    - Can also be Recursive (don’t get confused!)

https://en.wikipedia.org/wiki/Deep_learning

https://en.wikipedia.org/wiki/Recurrent_neural_network

https://en.wikipedia.org/wiki/Recursive_neural_network

https://en.wikipedia.org/wiki/Convolutional_neural_network

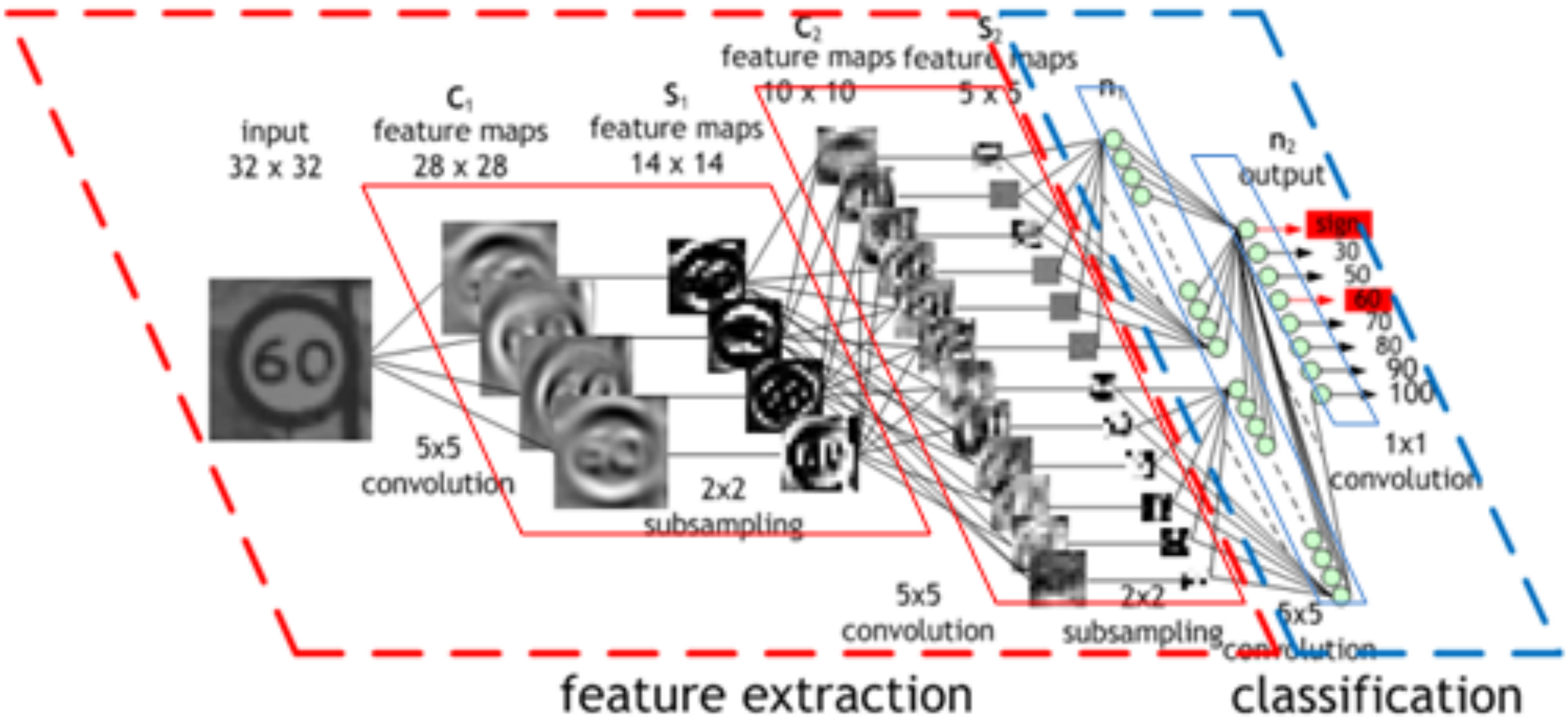
https://devblogs.nvidia.com/parallelforall/deep-learning-nutshell-core-concepts/

Deep Learning and Neural Networks

- Options to train:
- Supervised
  - Give inputs, tell it what the output is
- Unsupervised
  - Give inputs, tell it to optimize a function

Convolutional Neural Networks

- Preprocessing to perform feature extraction
  - Convolution or otherwise
- Classification
  - Standard neural network

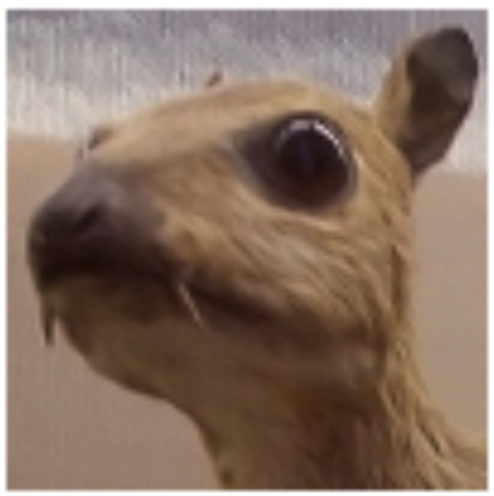


Convolutional Neural Networks

- Does "preprocessing" of the image by convoluting with kernels:

2-d Fourier transform!

Input image



Convolution Kernel

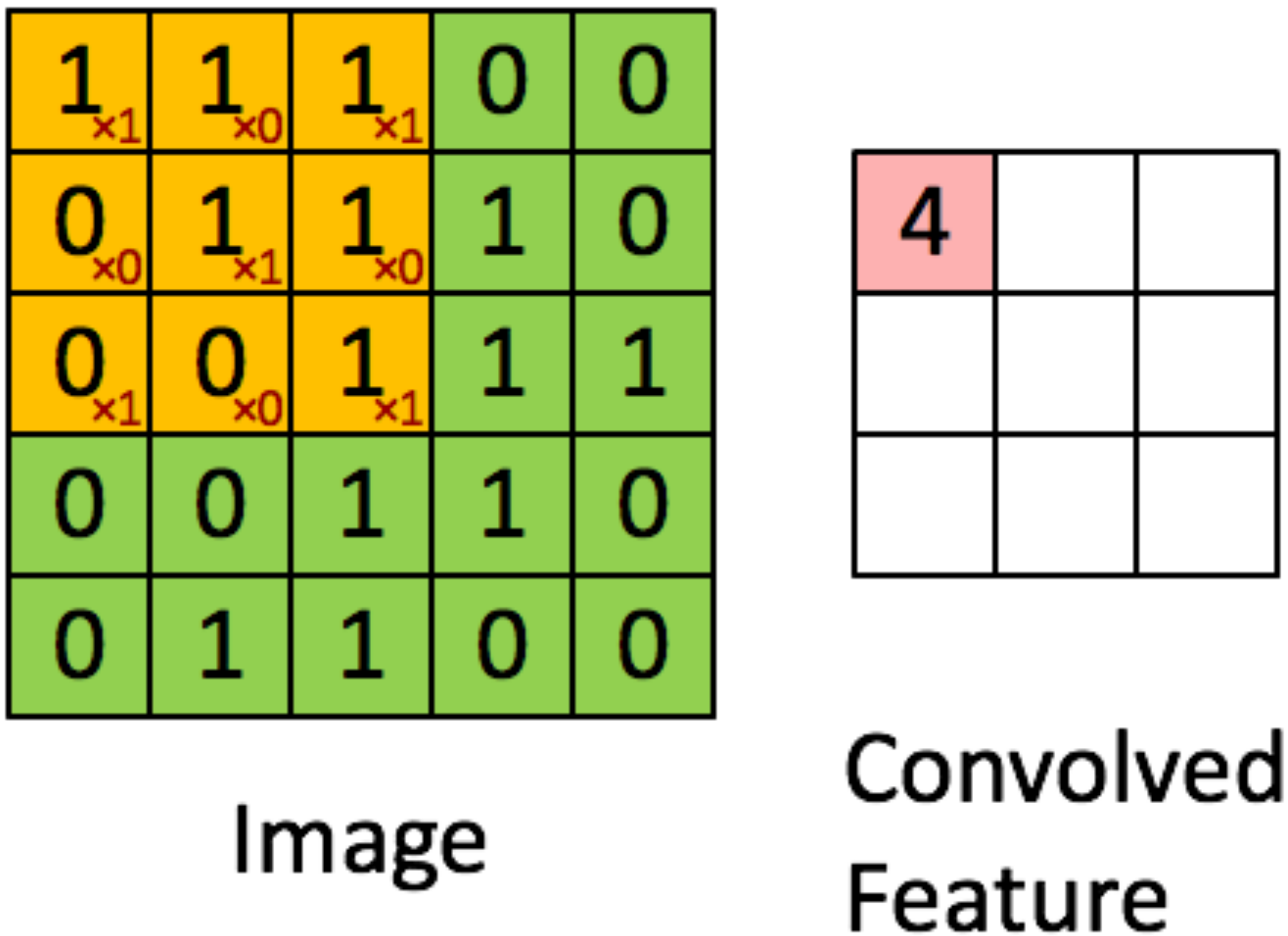
$$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$$

Feature map

Convolutional Neural Networks

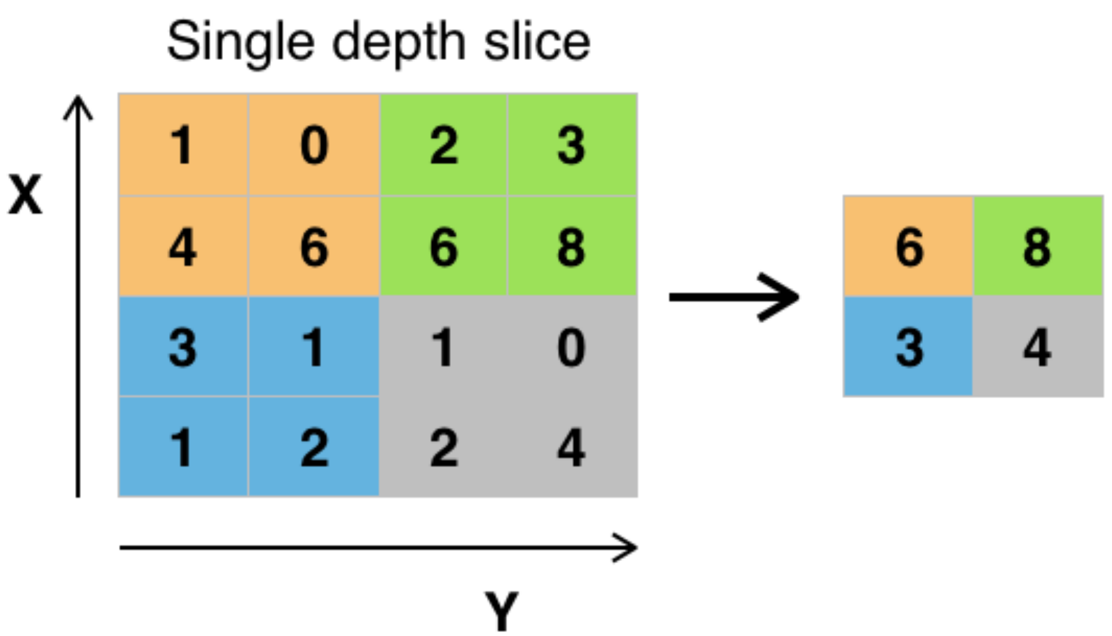
- Animation of convolution:
- Kernel:

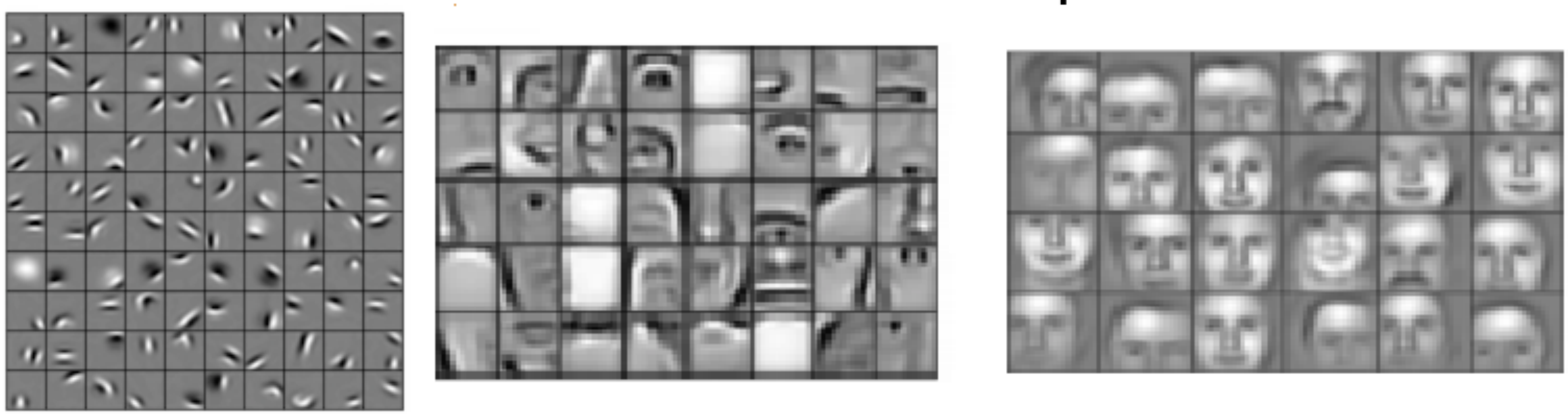
1	0	1
0	1	0
1	0	1



Convolutional Neural Networks

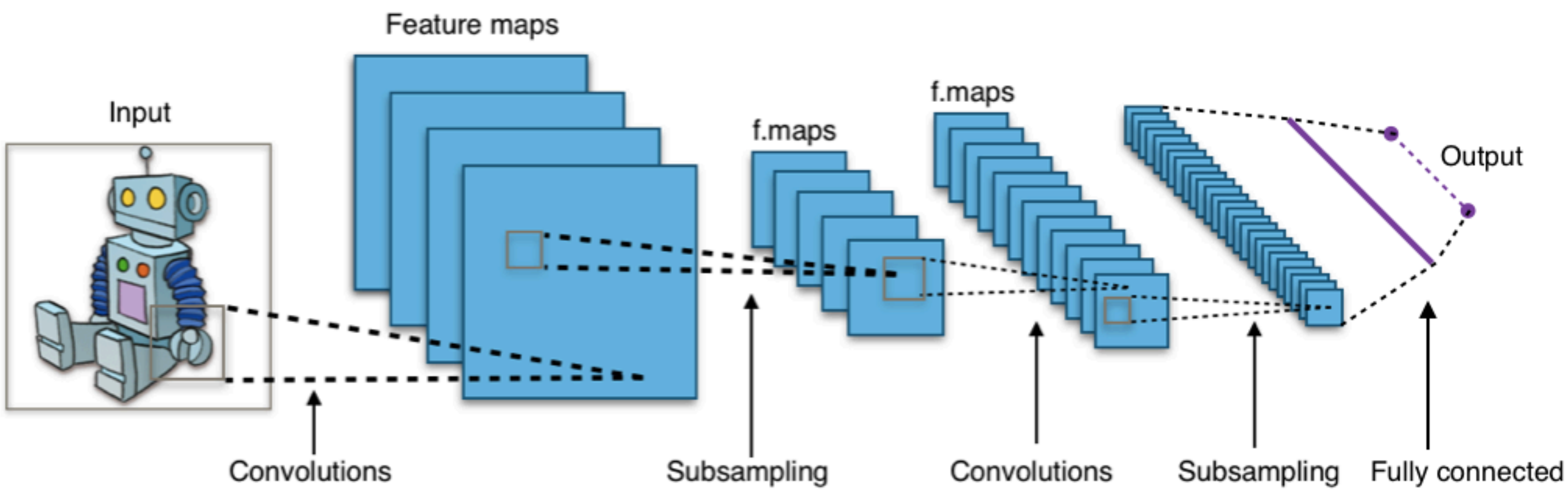
- Pooling layer : used to obtain very big features
  - Downsampled to extract gross features
  - Is it “pointy”?
  - Is it “round”?
  - Does it have a face?





Convolutional Neural Networks

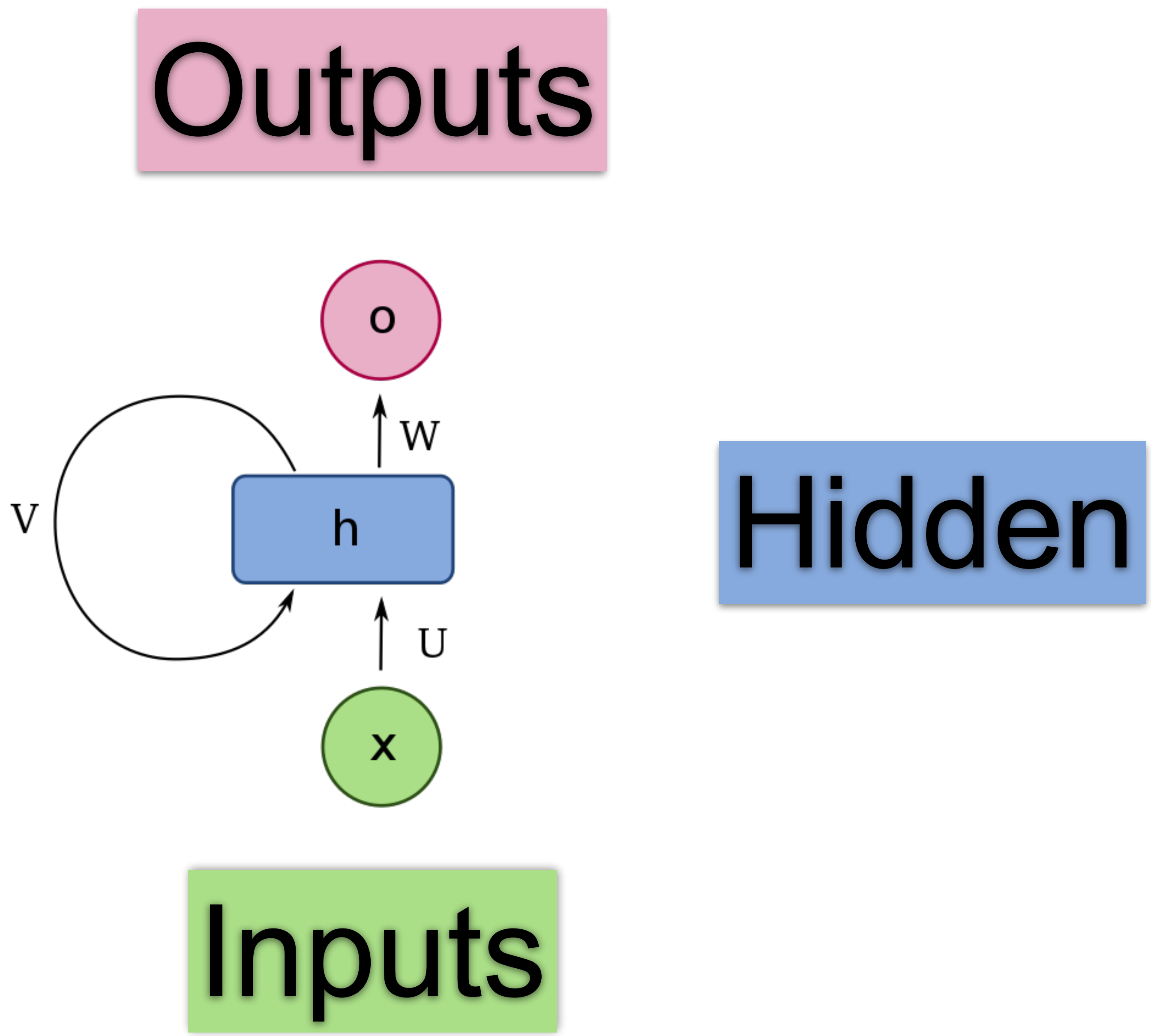
- Putting it together:
  - Convolutional layer
    - Discern features
  - Pooling layer
    - Extract global features
  - Activation function (“Rectified Linear Units”)
    - Standard NN
  - Fully connected layer
    - Standard NN
  - Loss layer
    - How well did it do?



https://en.wikipedia.org/wiki/Convolutional_neural_network

Recurrent Neural Networks

Dynamic directed graph to process **sequences** of inputs

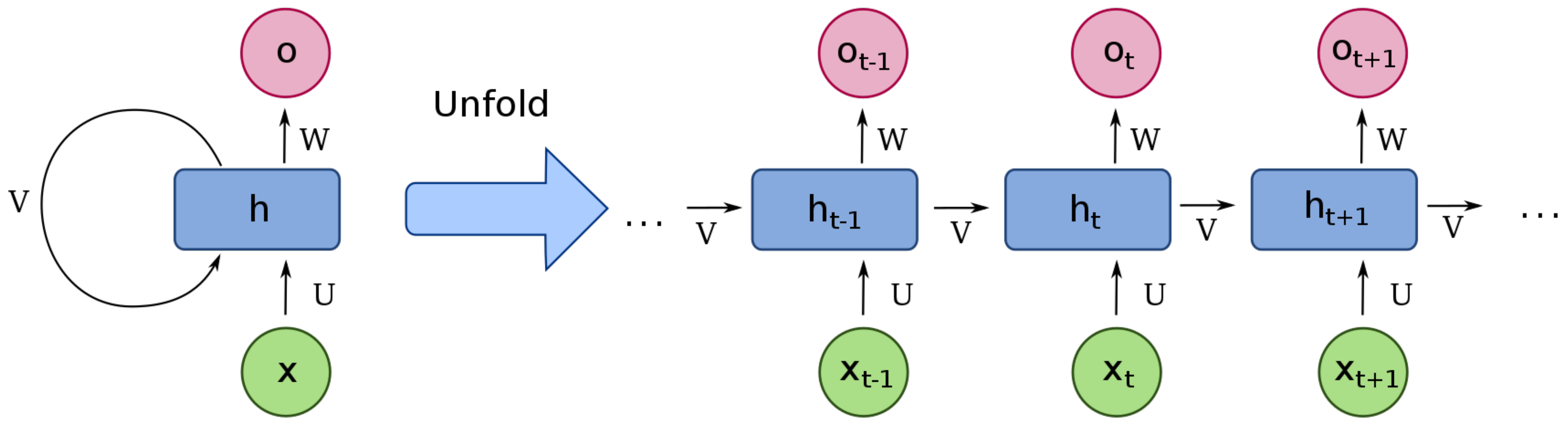


https://en.wikipedia.org/wiki/Recurrent_neural_network

Recurrent Neural Networks

Dynamic directed graph to process **sequences** of inputs

“Dynamic” in the sense that it changes over time



https://en.wikipedia.org/wiki/Recurrent_neural_network

Recurrent Neural Networks

- “Recurrent” : Can “save state” of the inputs
  - (CNNs do not)

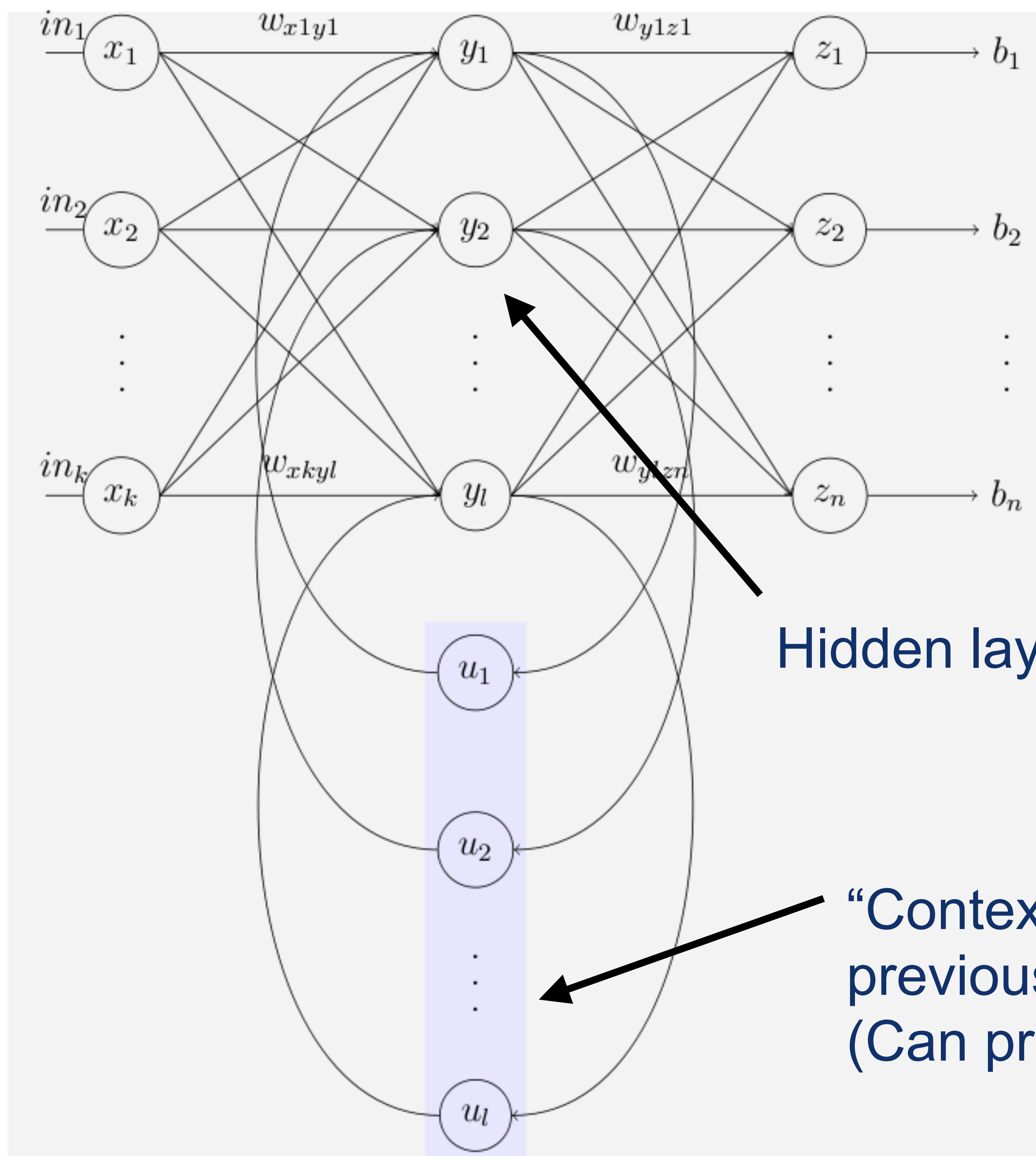
- Has use in predicting the next value in a sequence (speech, text recognition)

- Can also see how similar two sequences are

Recurrent Neural Networks

- Example: Elman network

Inputs



Outputs

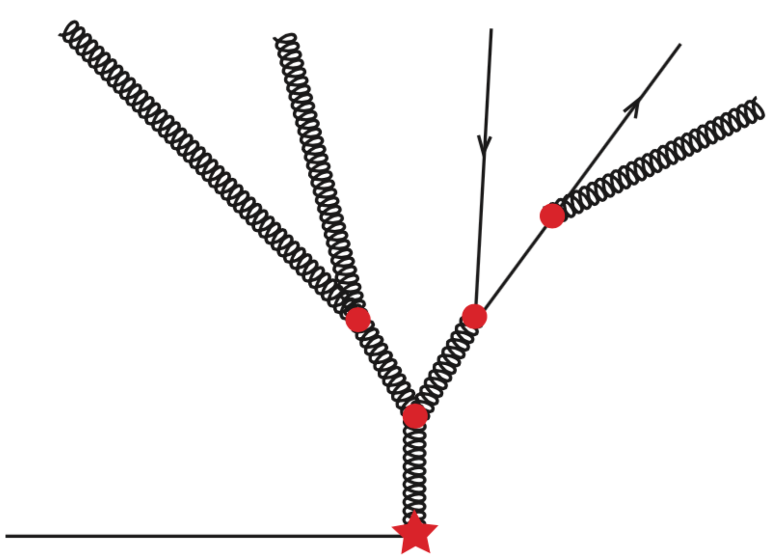
Hidden layer

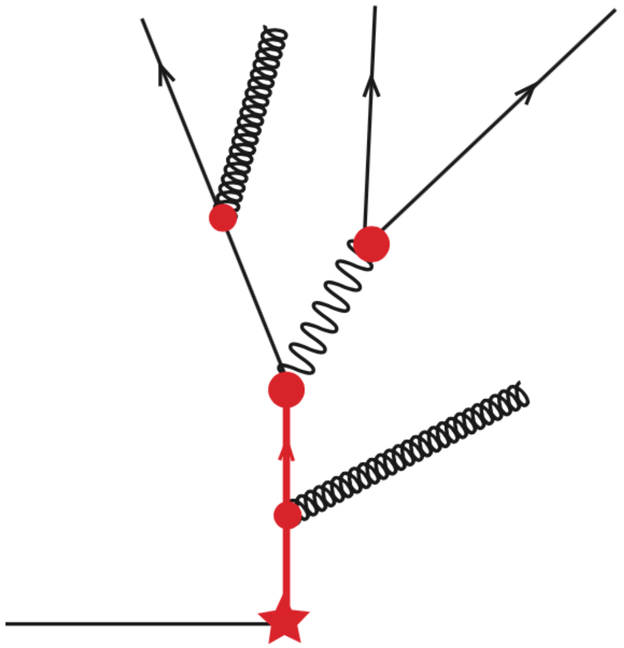
“Context” layer : Stores previous hidden layer. (Can predict!)

Highly Lorentz-Boosted Jets

- Example from physics:
  - "Learning" the origin of a jet at the LHC

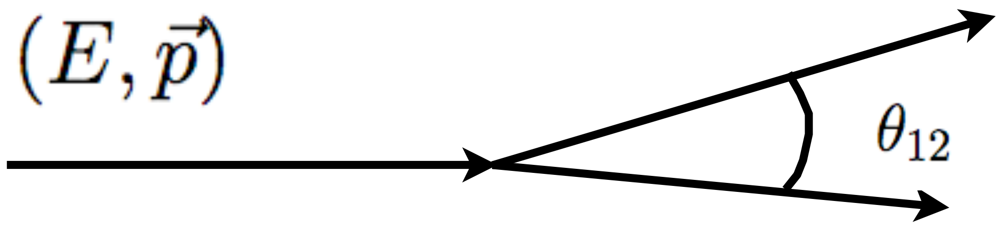
- W bosons can decay to quarks
  - If they obtain a high energy, their decay products merge together
  - How to distinguish between this and standard QCD jets?





Highly Lorentz-Boosted Jets

$$p^\mu = (E, \vec{p})$$



$$p_1^\mu = (E_1, \vec{p_1})$$

$$p_2^\mu = (E_2, \vec{p_2})$$

$$\begin{aligned} p^\mu p_\mu &= (p_1 + p_2)^\mu (p_1 + p_2)_\mu \\ m^2 &= (E_1 + E_2)^2 - (\vec{p_1} + \vec{p_2}) \cdot (\vec{p_1} + \vec{p_2}) \\ m^2 &\approx 2E_1 E_2 (1 - \cos(\theta_{12})) \end{aligned}$$

Assume E1=E2 = E/2

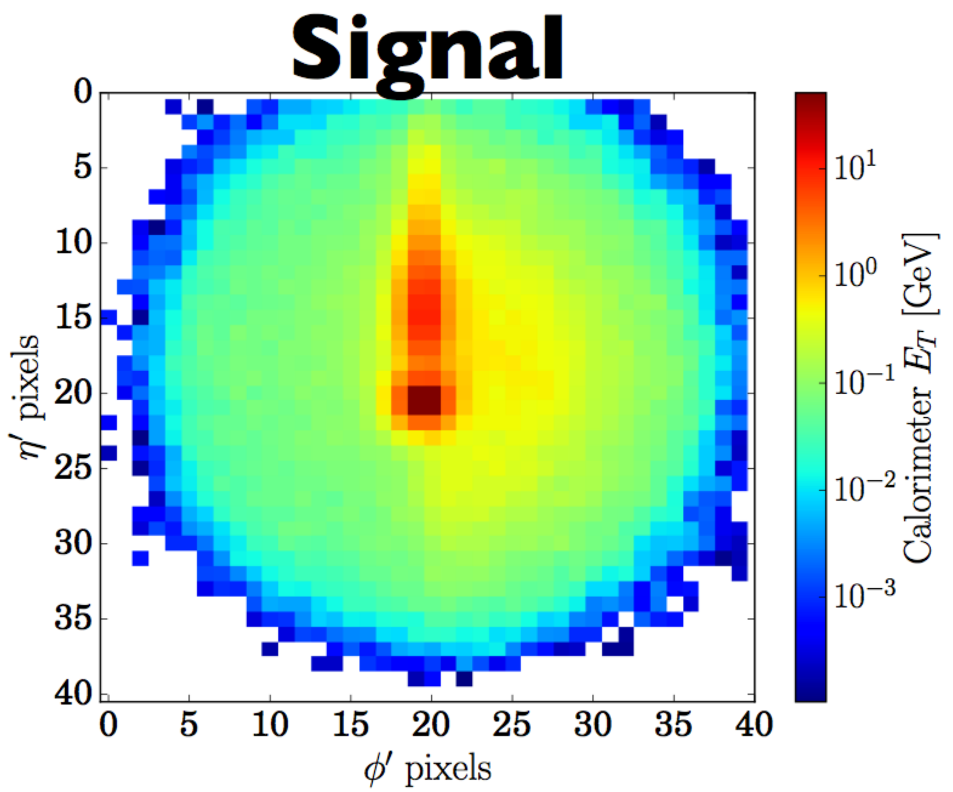
$$\begin{aligned} m^2 &\approx E^2 (1 - \cos(\theta_{12})) \\ \cos(\theta_{12}) &\approx 1 - \frac{m^2}{E^2} \approx 1 - \frac{1}{\gamma^2} \end{aligned}$$

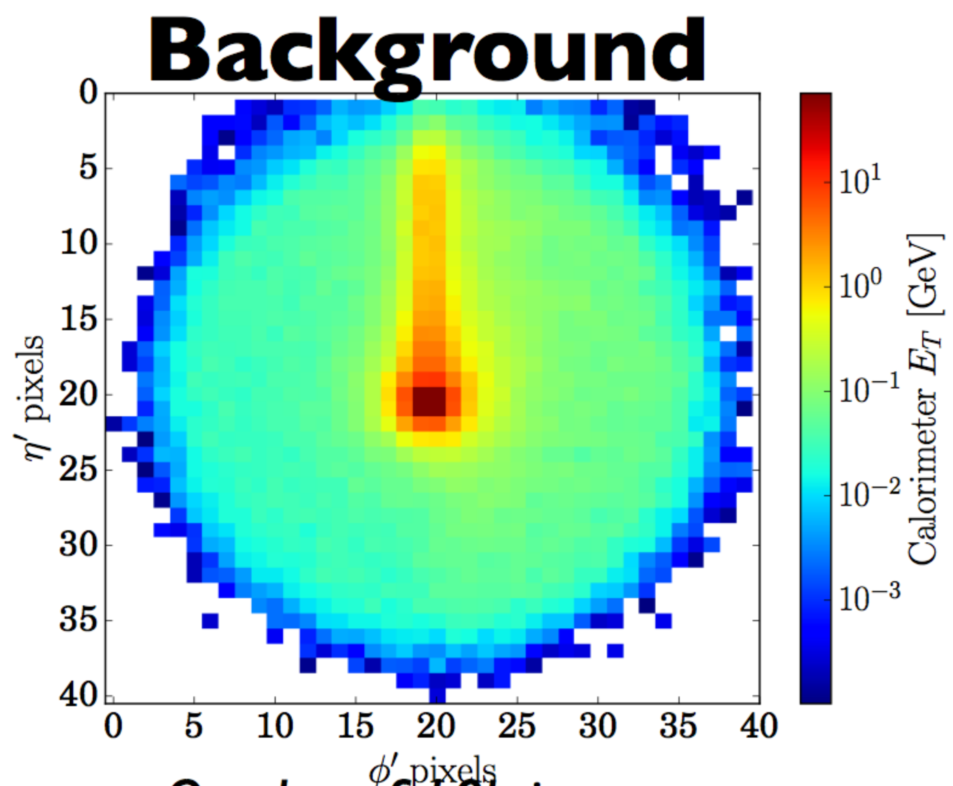
$$\boxed{\theta_{12} \approx \frac{2m}{E} = \frac{2}{\gamma}}$$

Highly Lorentz-Boosted Jets

- Plot energy of particles as a 2d projection
- Take average, put at center
- Take “next blob”, put at top center
- Look at sum of many images

- Use image processing techniques!





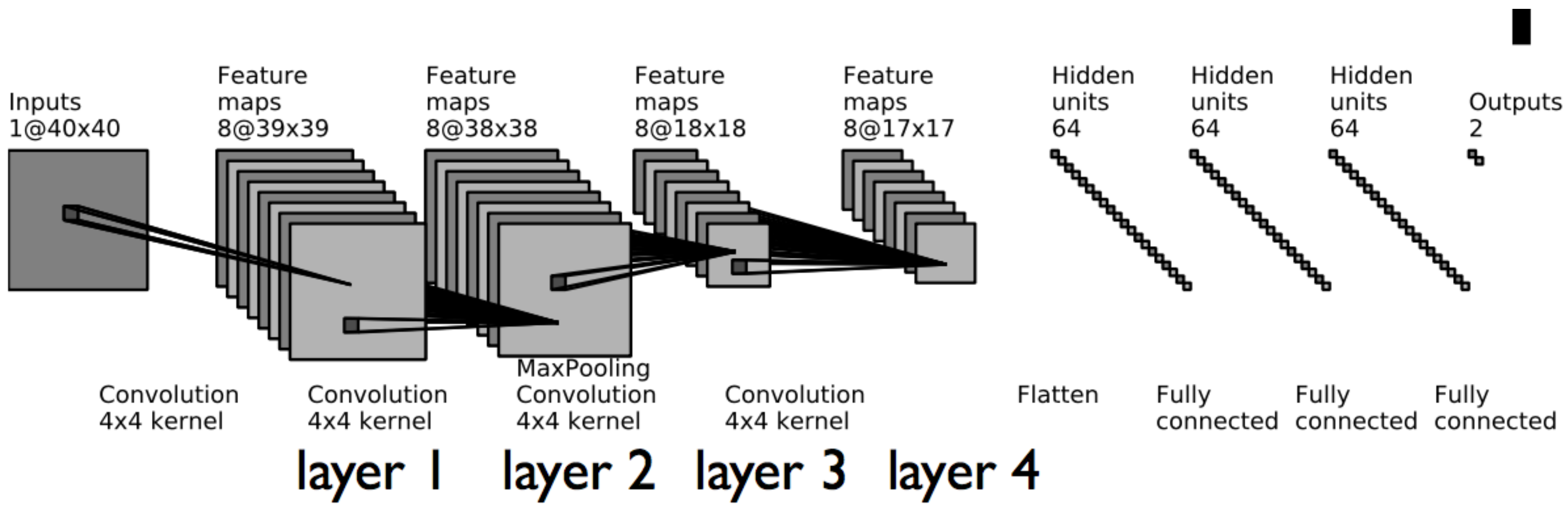
Overlay of 10k images

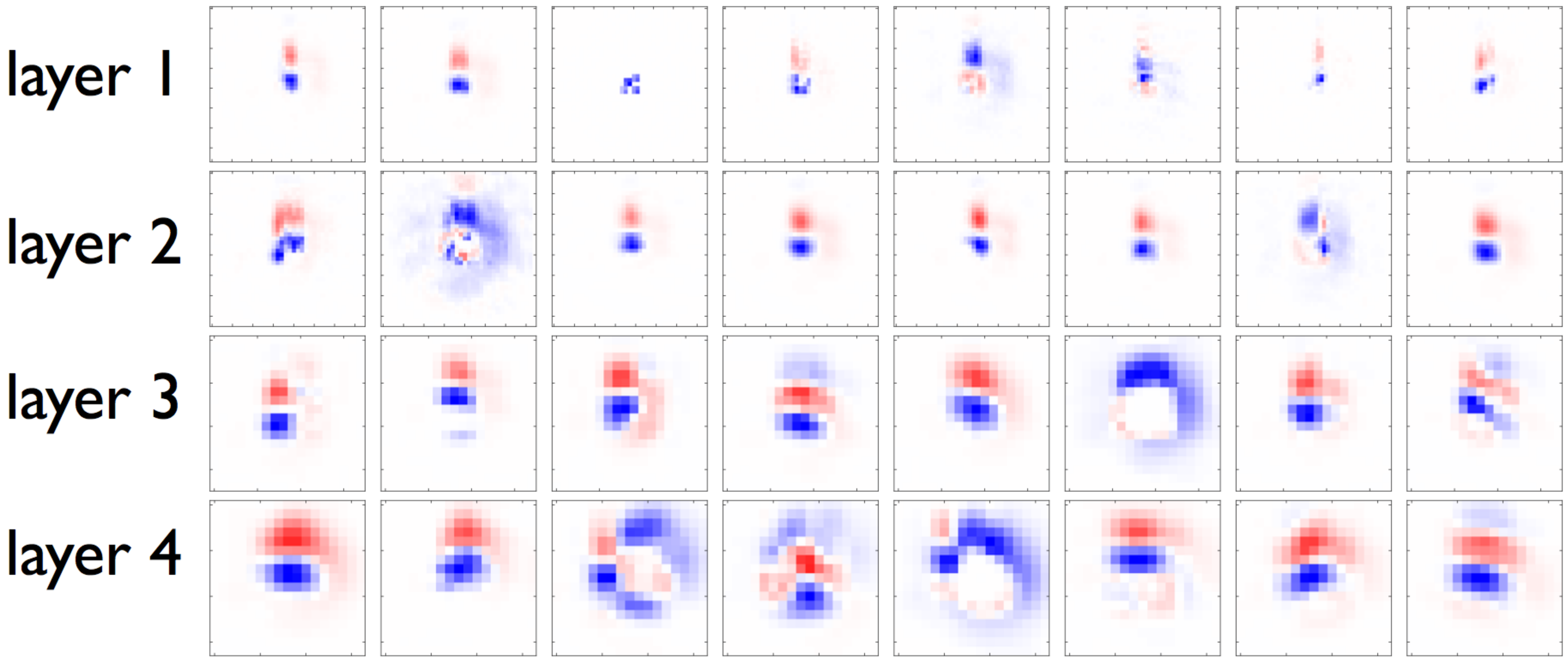
arXiv:1407.5675

JHEP 1607 069

JHEP 05 (2017) 006

Highly Lorentz-Boosted Jets





Software

- Lots of Deep Network software out there
- Popular ones:
  - Theano
  - TensorFlow
  - Scikit-learn
  - etc

- Theano and tensorflow are both installed in vidia, so we can work through an example there:
  - https://www.tensorflow.org/tutorials/

The Inverse Problem

- The inverse problem is, to first order, "simply" inverting functions

- Linear functions: trivial:

$$f(x) = mx + b$$

  - But! If m = 0, ????

$$f^{-1}(x) = \frac{1}{m}x - \frac{b}{m}$$

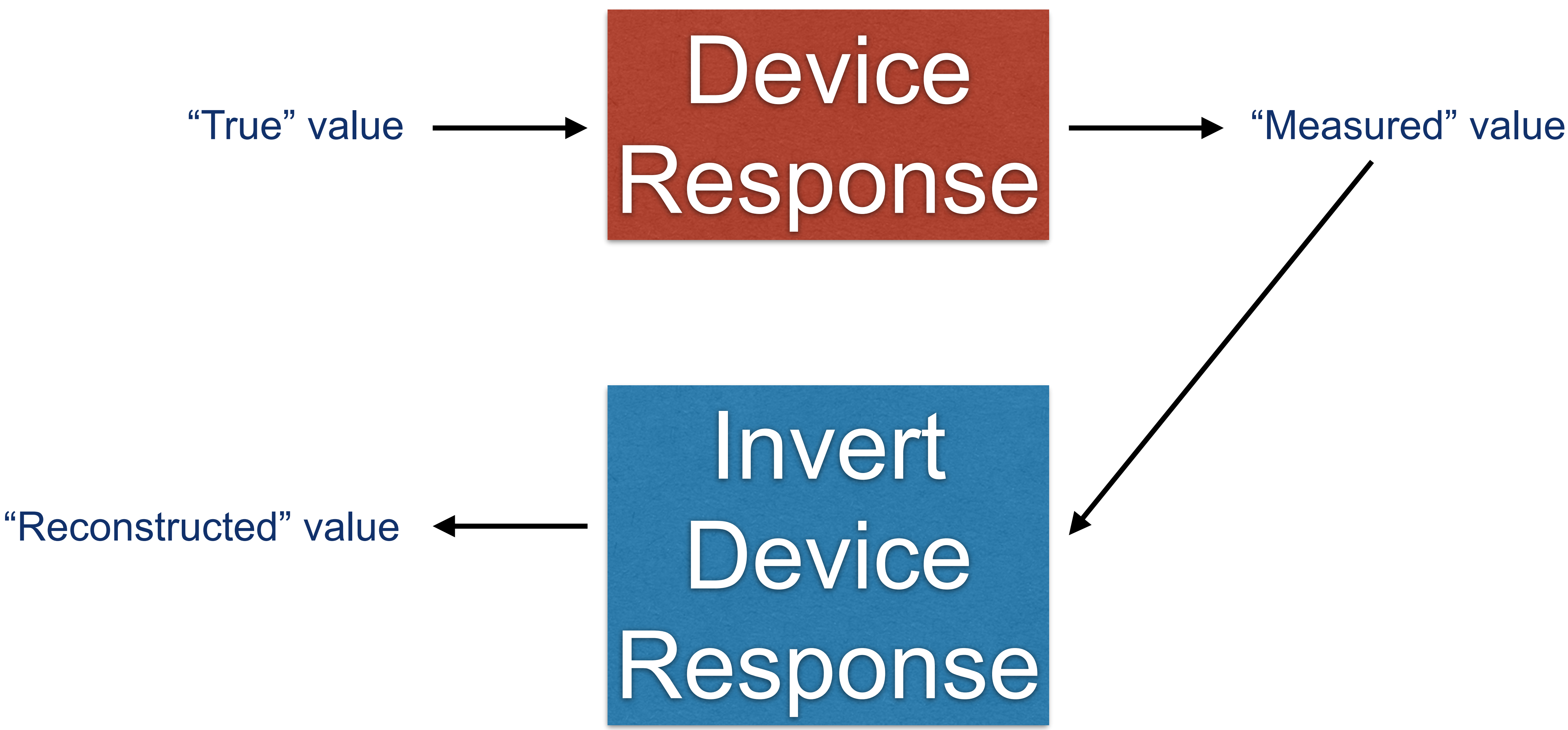
- Everything else: not even guaranteed to exist!
  - Can be many-to-one mapping
  - Can be non-invertible

- Becomes even trickier in multiple dimensions!

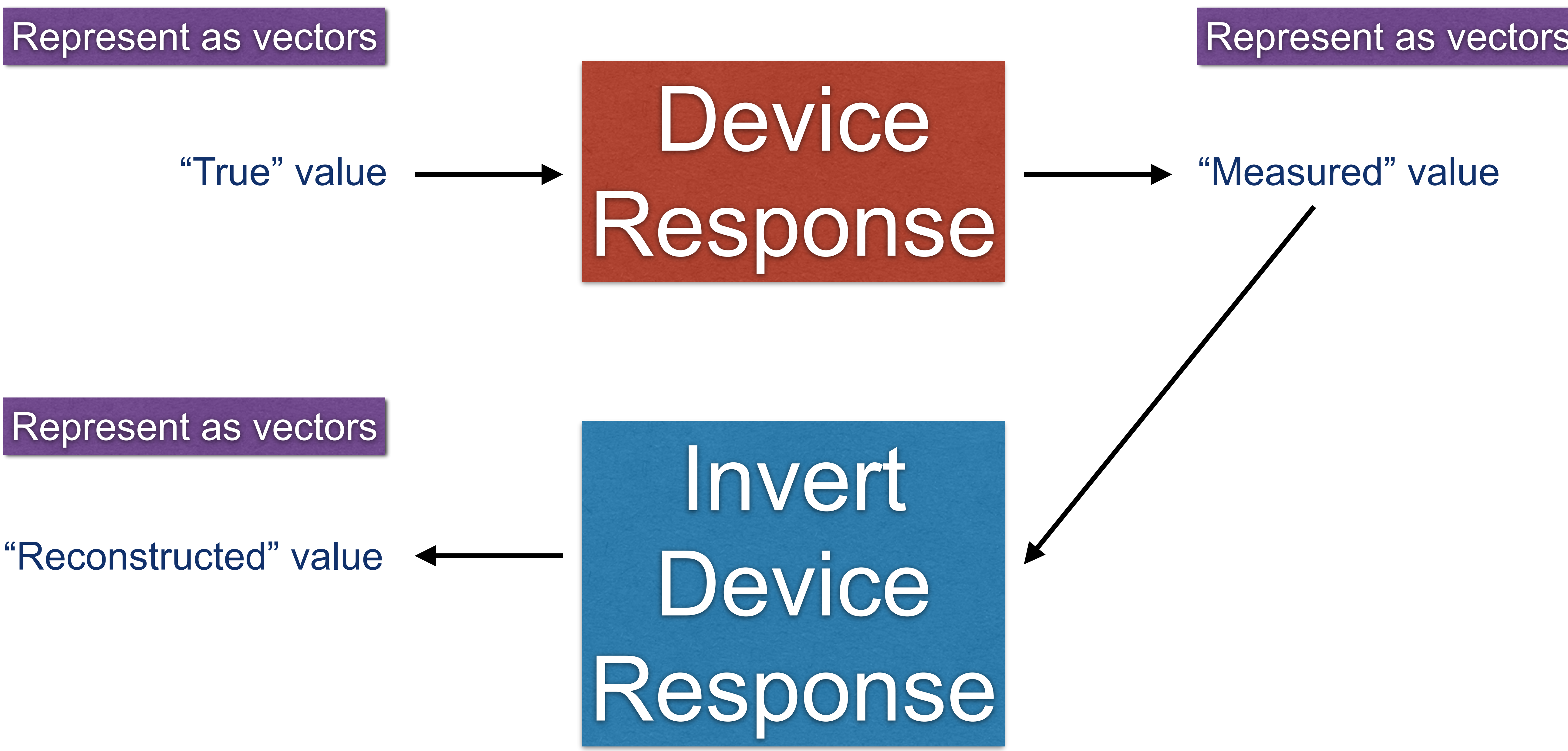
The Inverse Problem

“True” value → Device Response → “Measured” value

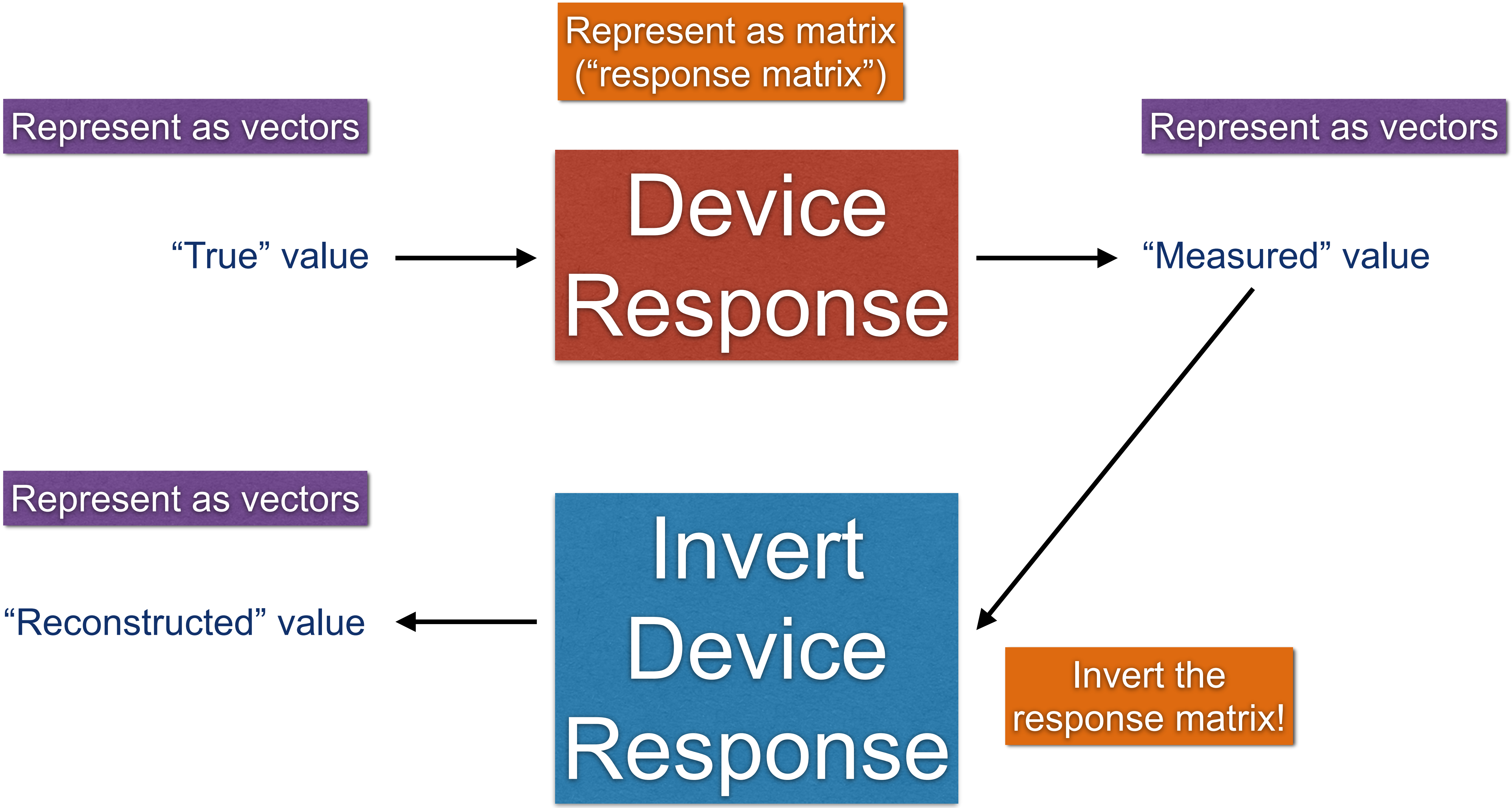
The Inverse Problem



The Inverse Problem

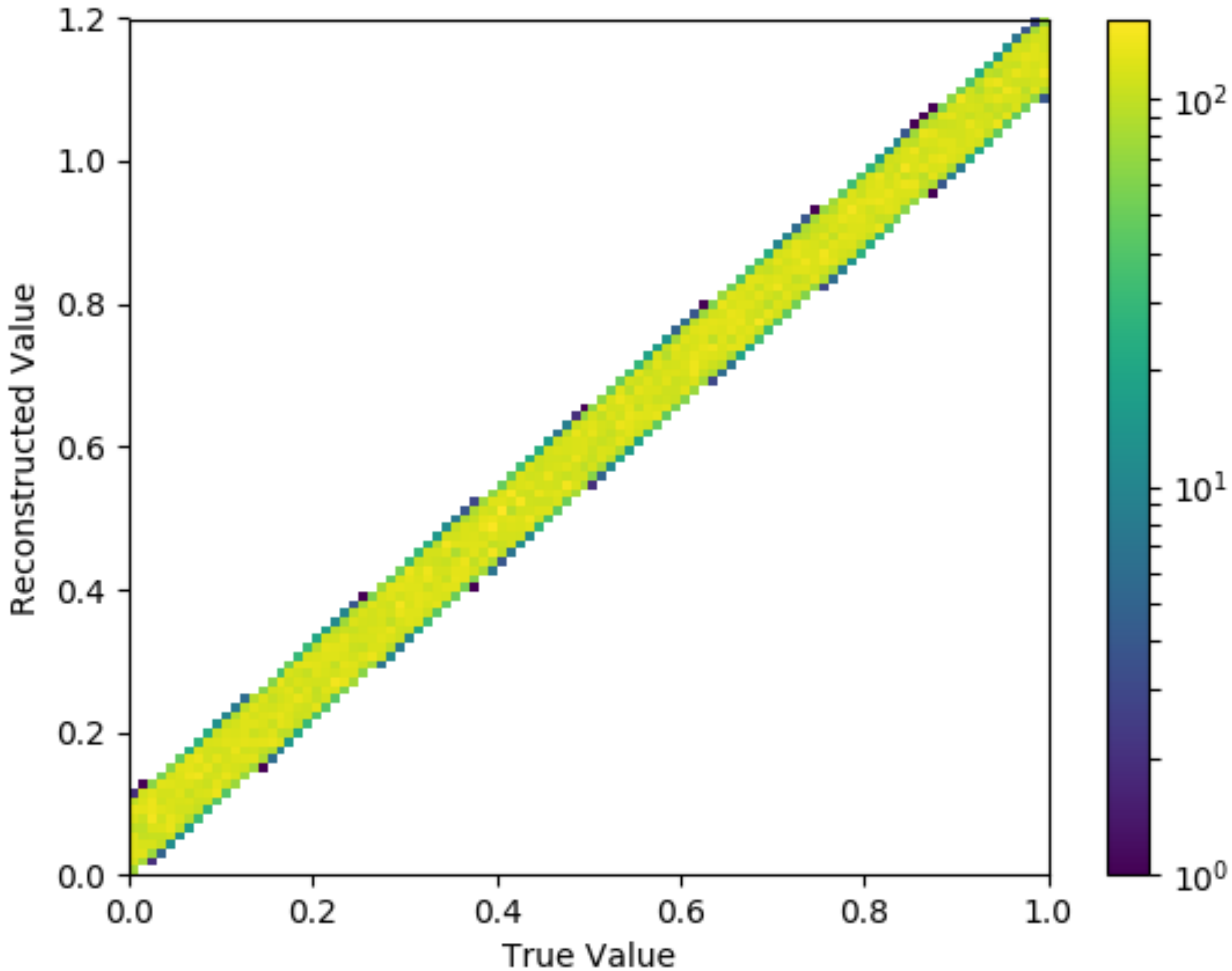


The Inverse Problem



The Inverse Problem

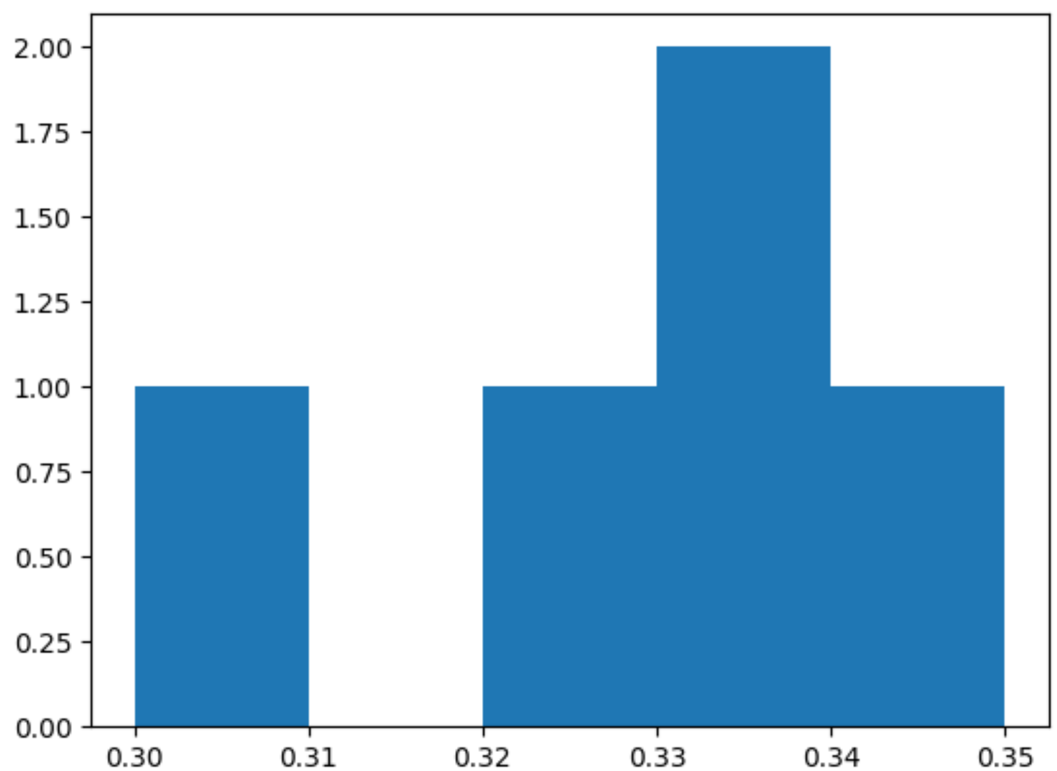
- But! Need one of these for EVERY possible input (0, 0.1, 0.1… 1.0)
- Represent as a matrix:



$$\sim \begin{pmatrix} 0.9 & 0.1 & 0 \\ 0.1 & 0.80 & 0.1 \\ 0 & 0.1 & 0.9 \end{pmatrix}$$

The Inverse Problem

- Represent our histogram as a vector

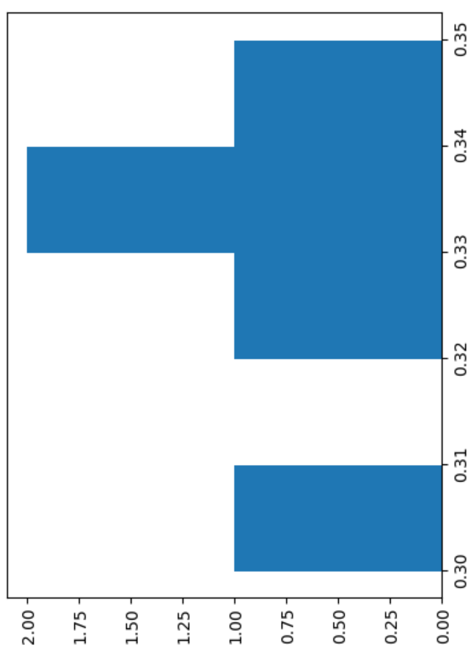


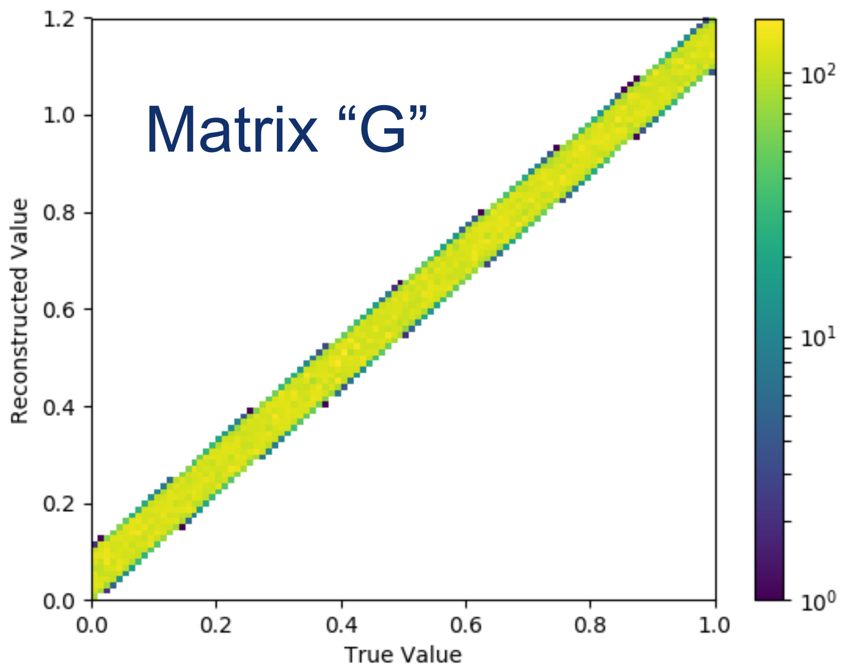
$$\sim \quad \begin{array}{cl} \begin{pmatrix} 0 \\ 0 \\ \dots \\ 1 \\ 0 \\ 1 \\ 2 \\ 1 \\ \dots \\ 0 \end{pmatrix} & \begin{array}{l} \text{Index=0: 0.0} \\ \\ \\ \text{Index=30: 0.3} \\ \\ \\ \\ \\ \\ \\ \end{array} \end{array}$$

The Inverse Problem

$$d = Gm$$

Vector “d”





Invert G to get vector “m”

The Inverse Problem

- You’re aware of the first case: Linear inverses (i.e. inverting matrices)
- There are generalizations

- Reminder:
  - To solve $\vec{y} = A\vec{x} + \vec{b}$:
  - Invert the matrix:

$$\vec{x} = A^{-1}\left(\vec{y} - \vec{b}\right)$$

  - Gauss-Jordan elimination, other techniques we did last semester

The Inverse Problem

- What if the matrix is not invertible?
  - Can still get information, but not perfectly determined
  - Often sufficient to have partial information
- Examine the over-constrained case:
- Suppose we have a matrix G (the "observation matrix") with data "d" and true value "m".
- Want to minimize the difference between the prediction (Gm) and the data: $$\phi = |d - Gm|^2$$
- Where $$|a|^2 = \left(a^T a\right)$$
- Want to find the place where the difference is minimized!

https://en.wikipedia.org/wiki/Inverse_problem

The Inverse Problem

- Difference minimized when

$$\nabla_m \phi = 0$$

- That is, the gradient wrt the “m” components is zero
- Using chain rules for matrix functions:

$$\nabla_m \phi = 2\left(G^T G m - G^T d\right) = 0$$

- Needs to be satisfied for all of the components, so require each to vanish:

$$G^T G m = G^T d$$

- So we solve for m:

$$m = \left(G^T G\right)^{-1} G^T d$$

Least squares distance from last semester!

https://en.wikipedia.org/wiki/Inverse_problem
https://atmos.washington.edu/~dennis/MatrixCalculus.pdf

The Inverse Problem

- So the inverse problem is similar to least squares
- Don't get the "full inverse" but do get the closest to it

- For intuition, remember our "design matrix" from last semester:

$$A_{ij} = \frac{Y_j(x_i)}{\sigma_i}$$

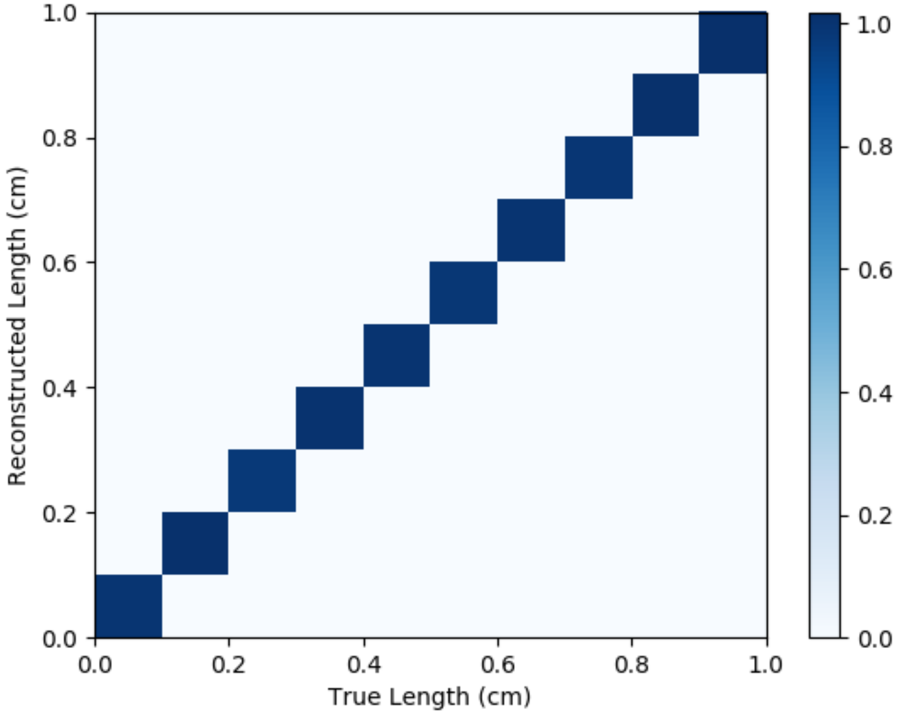
$$\mathbf{A} = \begin{bmatrix} Y_1(x_1)/\sigma_1 & Y_2(x_1)/\sigma_1 & \dots \\ Y_1(x_2)/\sigma_2 & Y_2(x_2)/\sigma_2 & \dots \\ \dots & \dots & \dots \end{bmatrix}$$

$$\vec{a} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\vec{b}$$

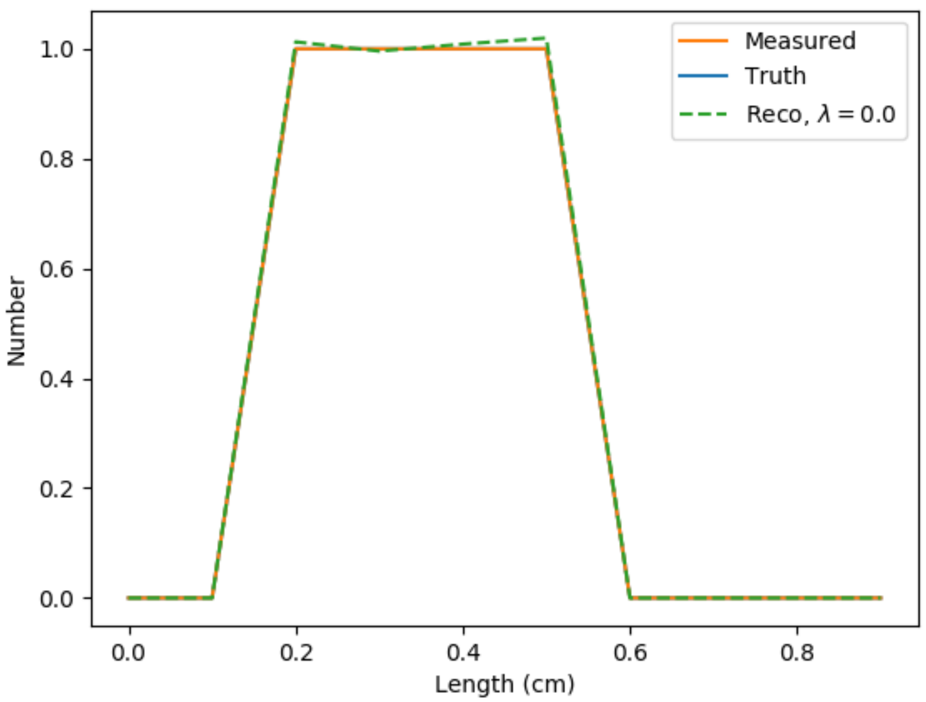
- Then for polynomial fits $A_{ij} = a_j x_i^j / \sigma_i$

The Inverse Problem

- Try to invert the response of some experimental device or detector to get “true” values
  - Example 1:
    - Device to measure length is perfect.
      - Response created from 100000 “pseudo-experiments”:

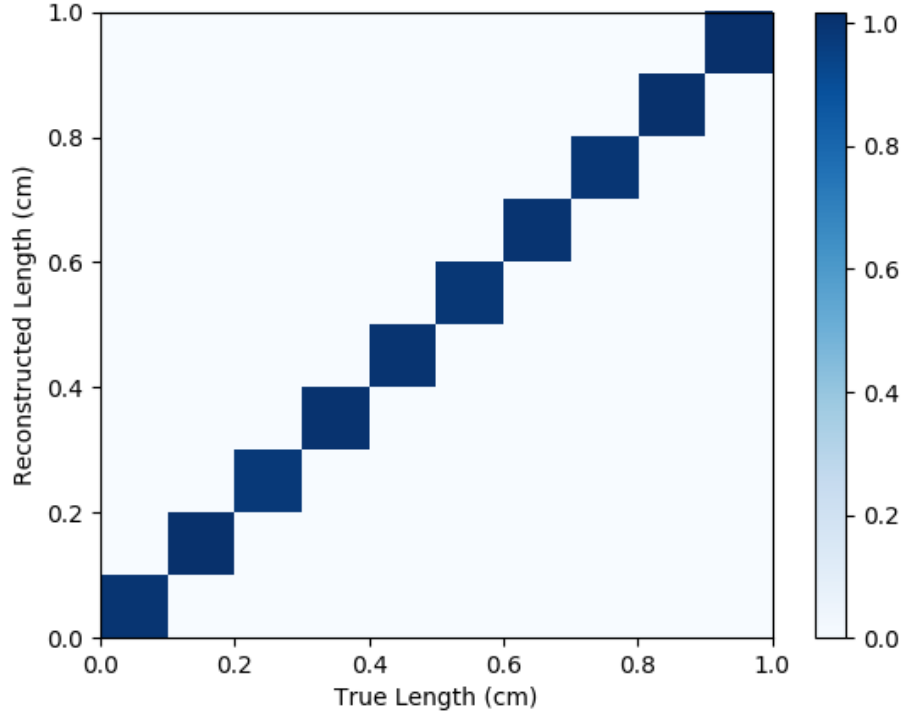


    - You measure 4 objects, and obtain:
      - 0.2 cm, 0.3 cm, 0.4 cm, 0.5 cm
      - Measured vs true histogram:

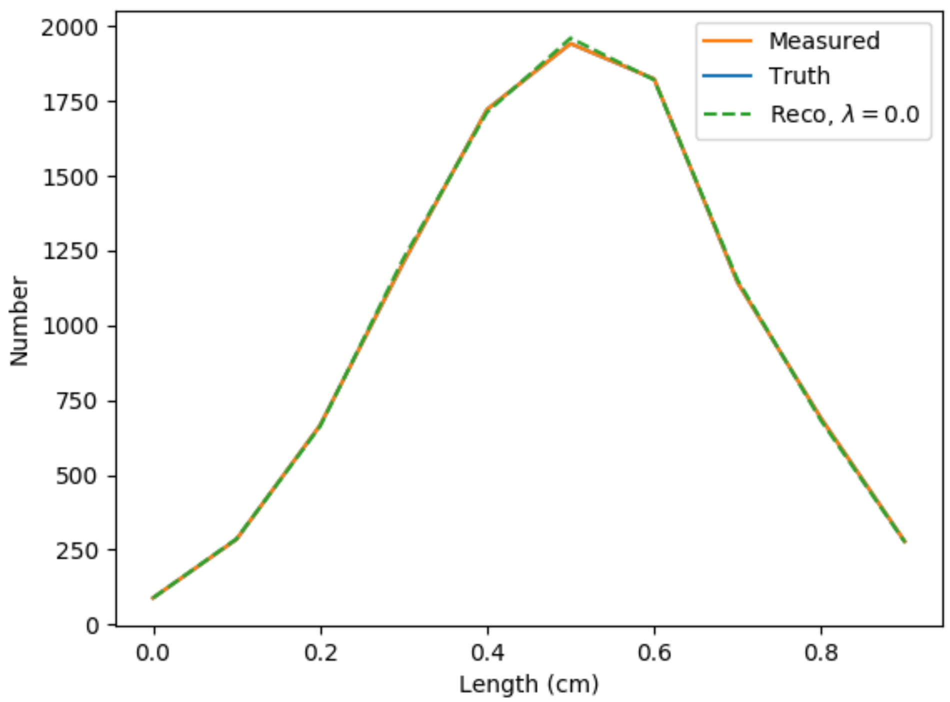


The Inverse Problem

- Try to invert the response of some experimental device or detector to get “true” values
  - Example 2:
    - Device to measure length is perfect.
      - Response created from 100000 “pseudo-experiments”:

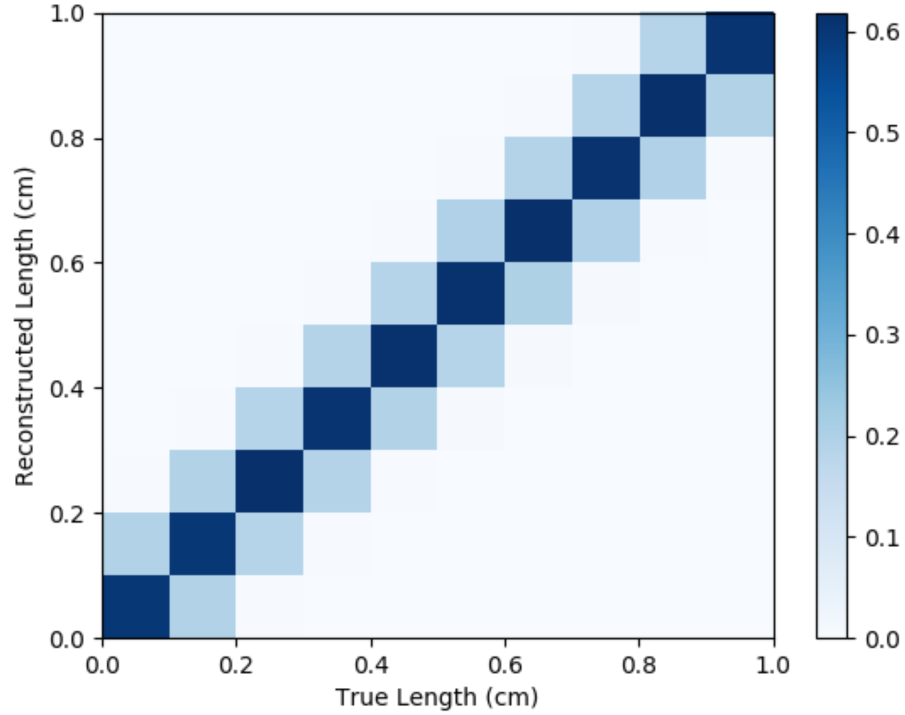


    - You measure 10000 objects, and obtain:
      - Gaussian with width = 0.2, mean = 0.5
      - Measured histogram:

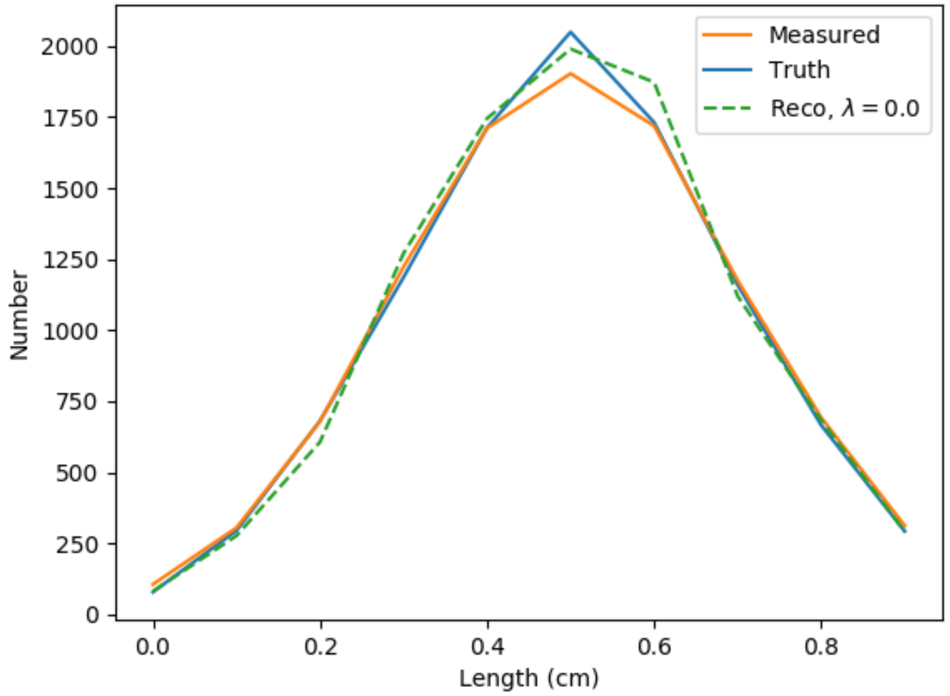


The Inverse Problem

- Try to invert the response of some experimental device or detector to get "true" values
  - Example 3:
    - Device to measure length has resolution of 0.05 cm
      - Response created from 100000 "pseudo-experiments":

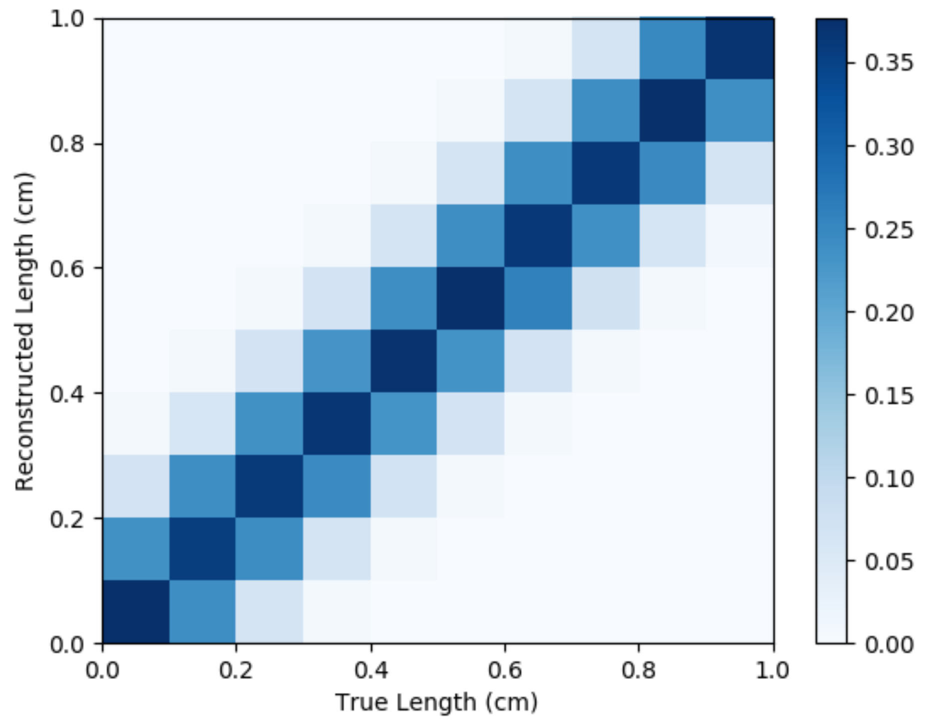


- You measure 10000 objects, and obtain:
  - Gaussian with width = 0.2, mean = 0.5
  - Measured histogram:

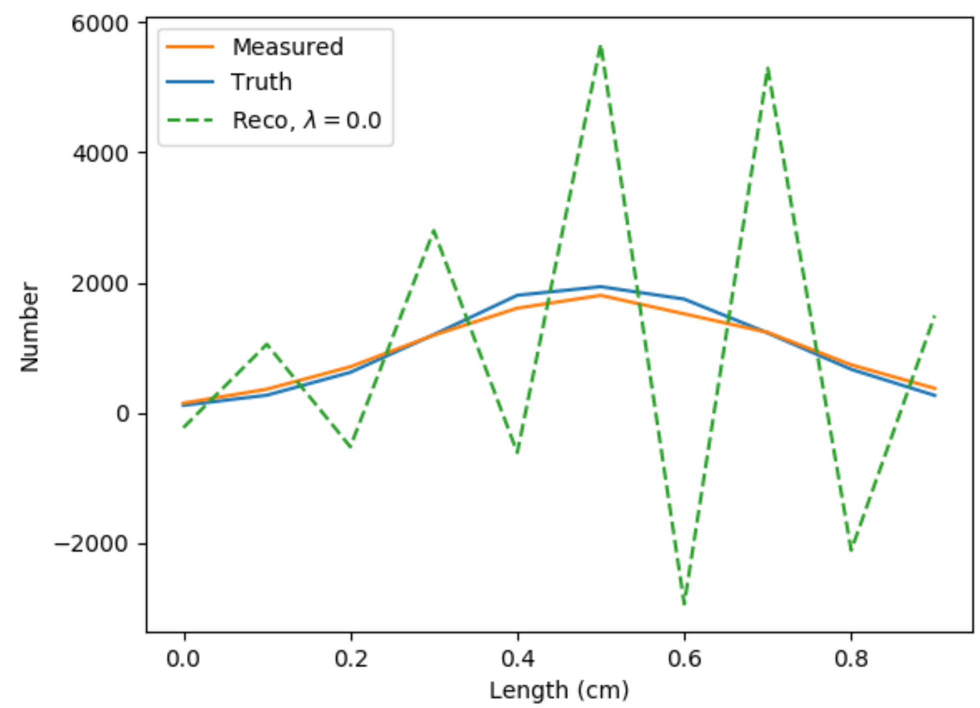


The Inverse Problem

- Try to invert the response of some experimental device or detector to get "true" values
  - Example 4:
    - Device to measure length has resolution of 0.1 cm
      - Response created from 100000 "pseudo-experiments":



    - You measure 10000 objects, and obtain:
      - Gaussian with width = 0.2, mean = 0.5
      - Measured histogram:



The Inverse Problem

- What is going on???
- Statistical uncertainties bin-to-bin are greatly amplified by inversion
  - Need to damp those out… "regularization" (from Tikhonov)

https://en.wikipedia.org/wiki/Tikhonov_regularization

The Inverse Problem

- How to formally do this?
- Ordinary formula for the inversion is:

$$m = \left(G^T G\right)^{-1} G^T d$$

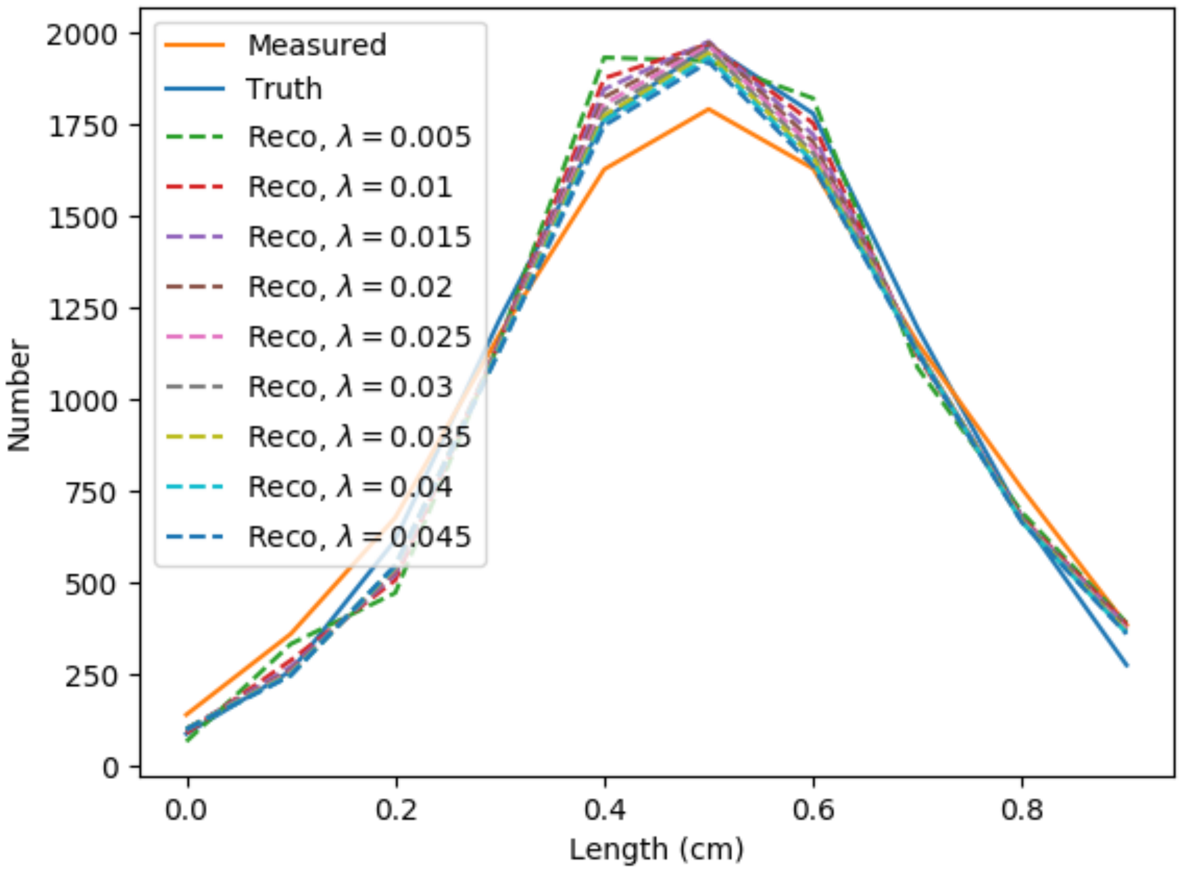
- Introduce a penalty term (here, a Lagrange multiplier) to solve:

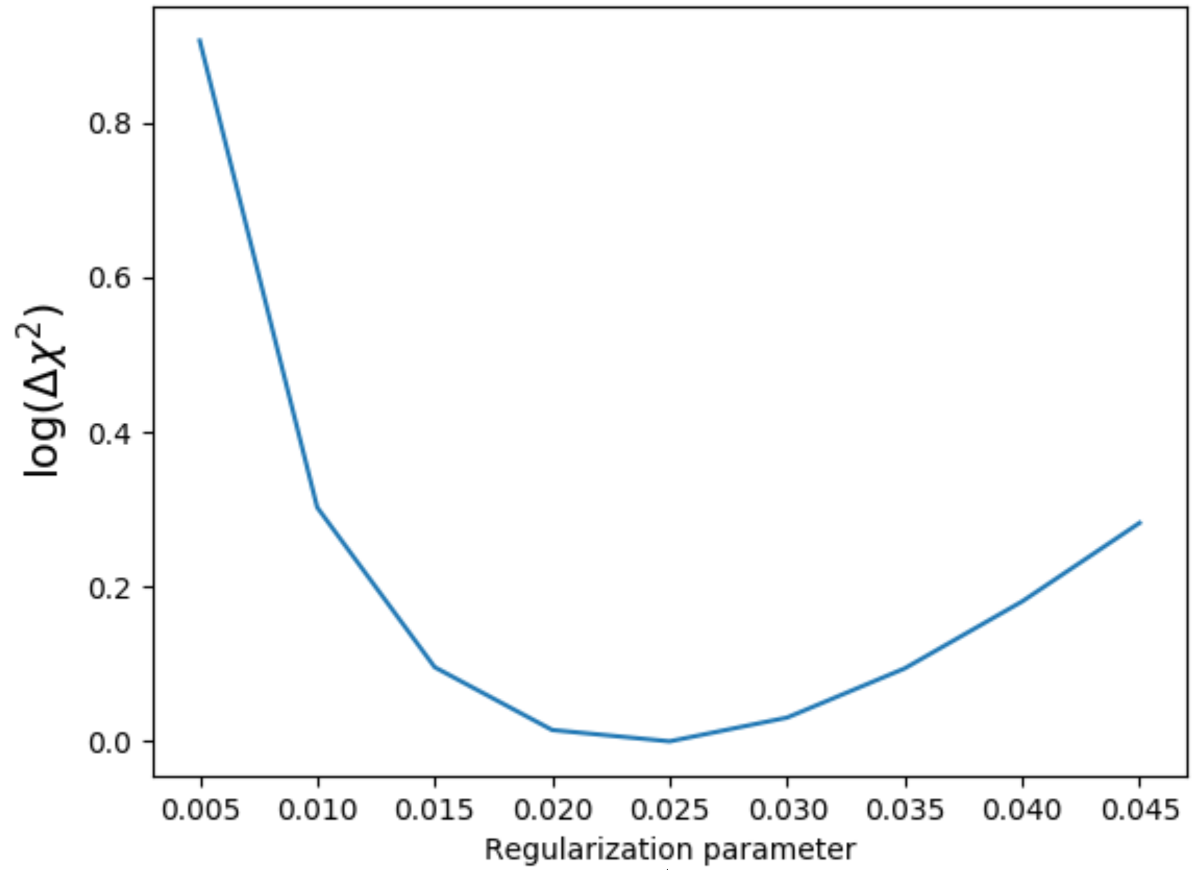
$$m = \left(G^T G + \lambda I\right)^{-1} G^T d$$

- Can then vary as a function of lambda to pick when the regularization is complete

https://www.researchgate.net/publication/274138835_NumPy_SciPy_Recipes_for_Data_Science_Regularized_Least_Squares_Optimization

- Example 4: vary regularization parameter for our example:

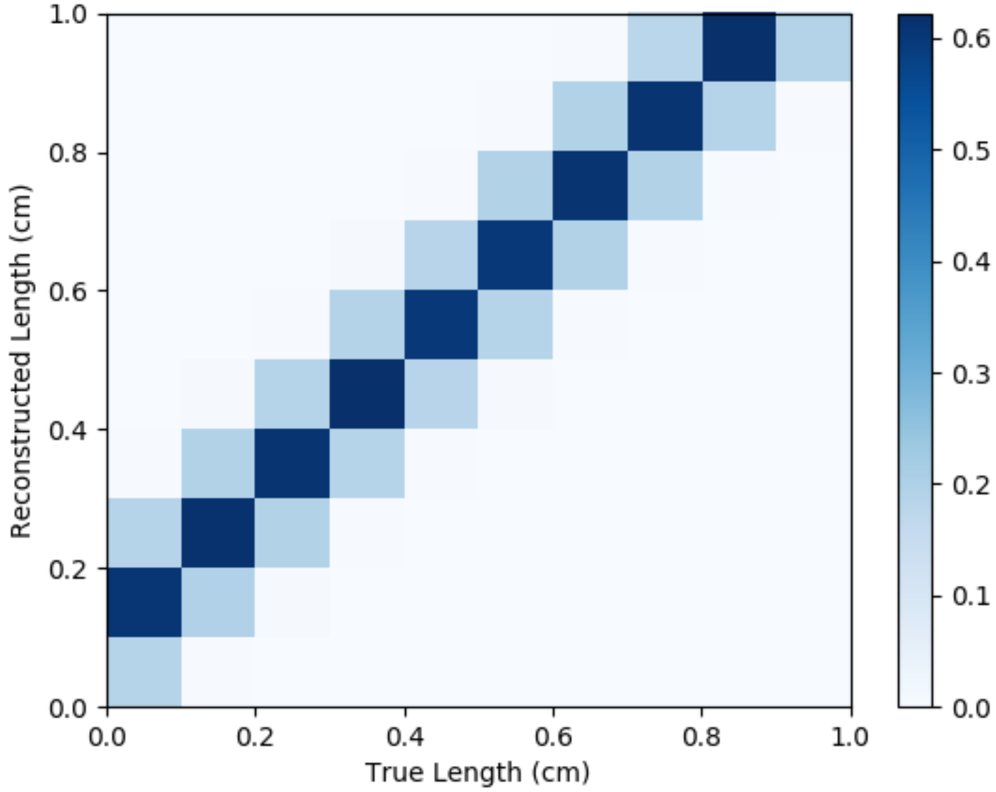


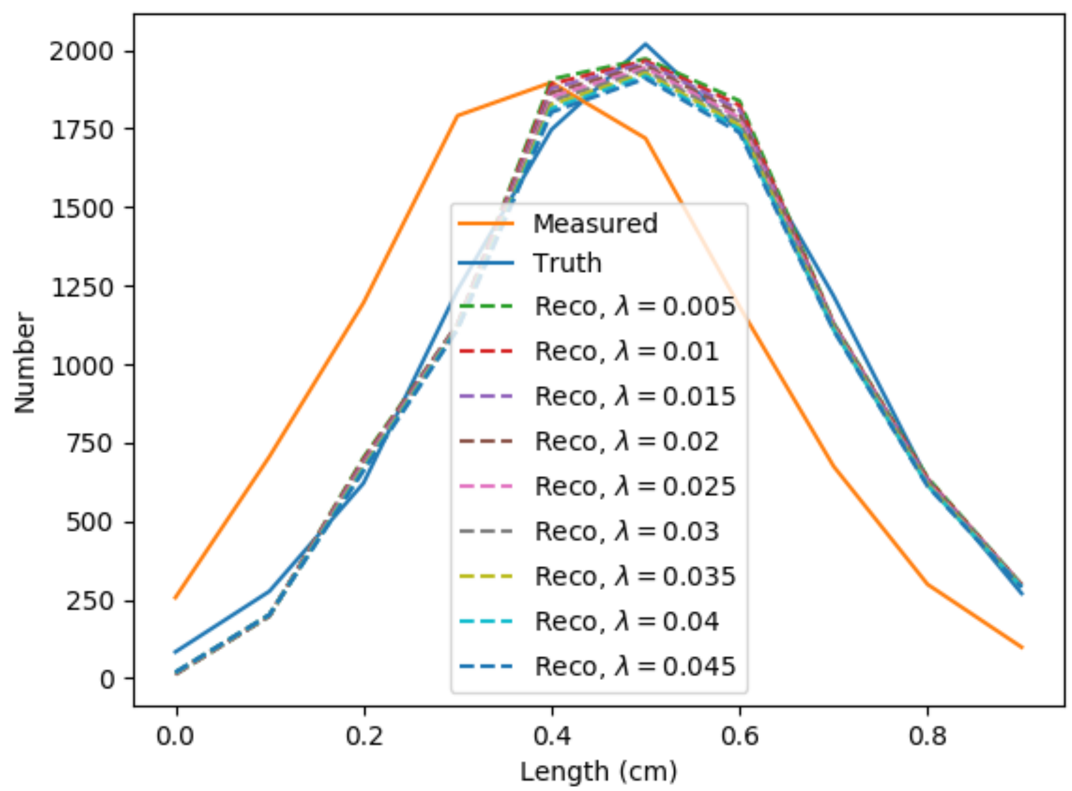


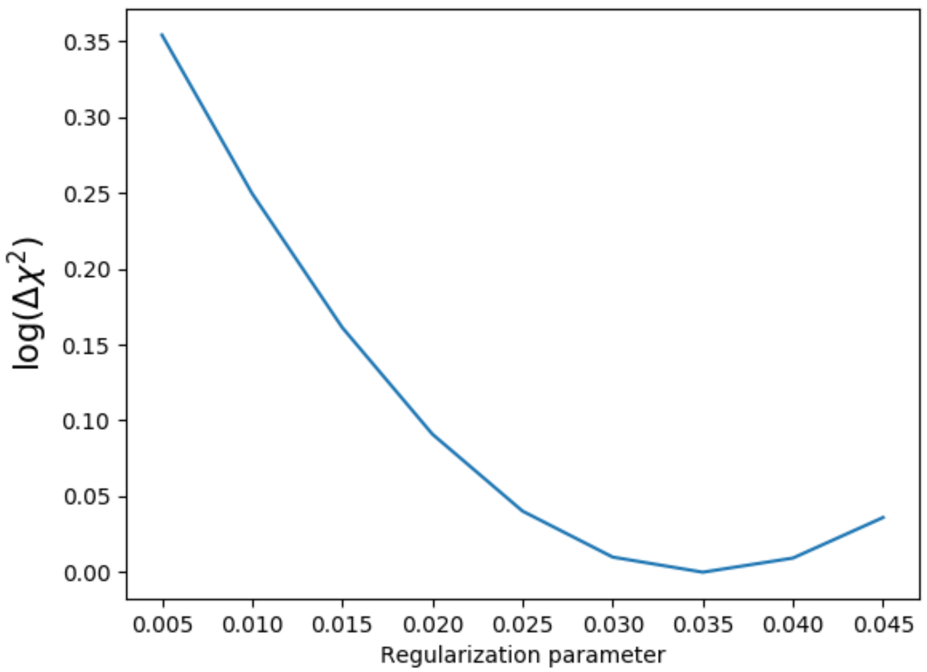
Pick ~0.025

The Inverse Problem

- Example 5: Can also have biases







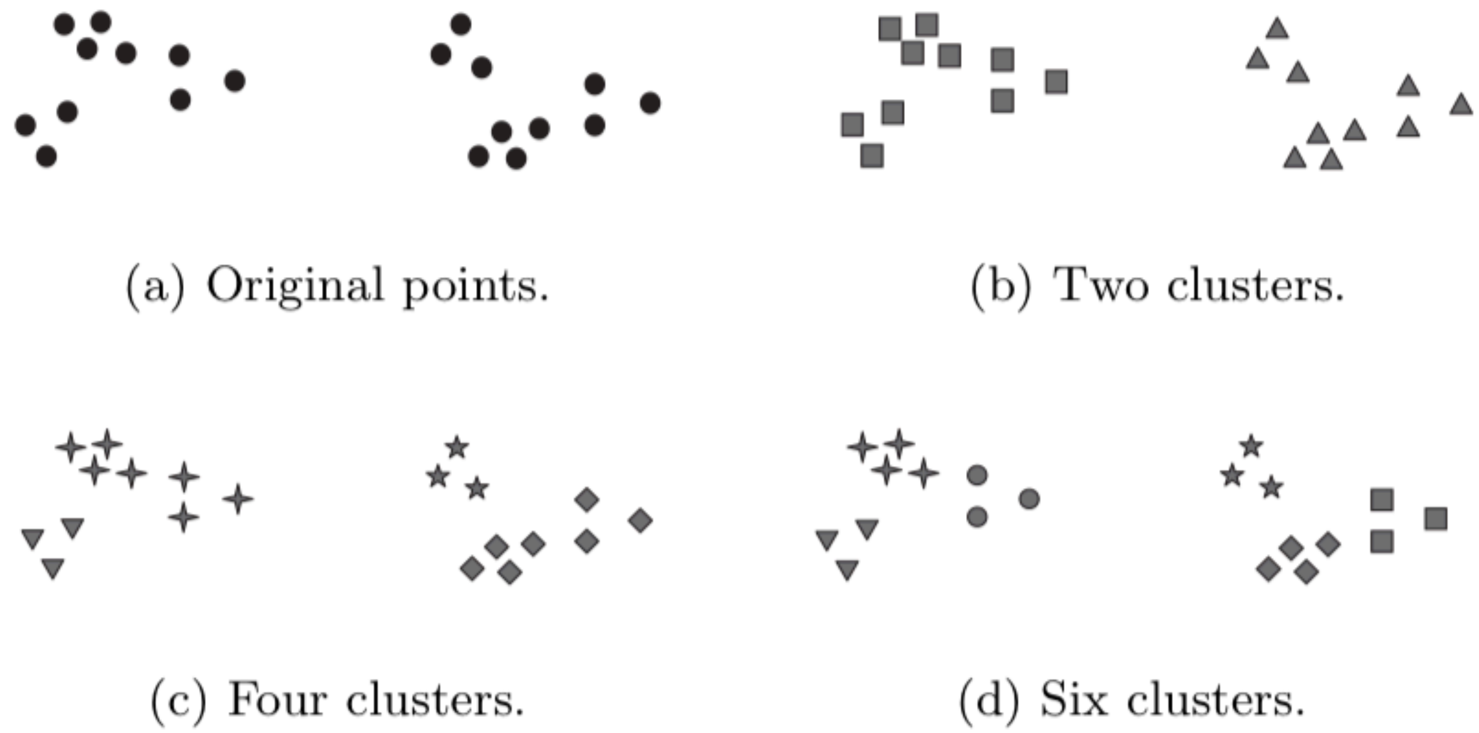
The Inverse Problem

- Sometimes people decide to put the biases in a separate matrix so it is a “diagonal matrix”
- In practice it doesn’t matter.

Clustering

- Goal: Given N points in space, associate to k partitions

- Many applications:
  - Data classification
  - Galaxy clustering
  - Jet clustering
  - Sociology
  - Social networks



https://www-users.cs.umn.edu/~kumar001/dmbook/ch8.pdf

https://en.wikipedia.org/wiki/Cluster_analysis

Clustering

- Goal: Given N points in space, associate to k partitions

- Many applications:
  - Data classification
  - Galaxy clustering
  - Jet clustering
  - Sociology
  - Social networks

Criminal Athlete Princess Nerd

Basket case

https://en.wikipedia.org/wiki/The_Breakfast_Club

Clustering

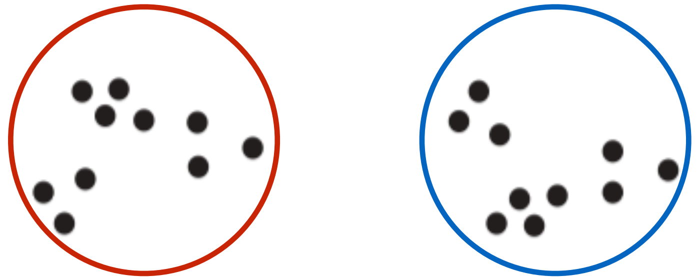
- Goal: Given N points in space, associate to k partitions

- Many applications:
  - Data classification
  - Galaxy clustering
  - Jet clustering
  - Sociology
  - Social networks

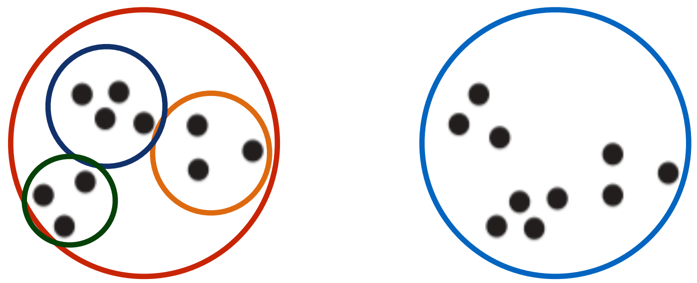
Clustering

- Uses:
  - Summarize / compress "spatial" information
  - Find nearest neighbors
- Types of clustering algorithms:
  - Exclusive:
    - Partitional: divide into k exclusive categories
    - Hierarchical: can have sub-clusters
  - Non-exclusive:
    - Add same element to more than one cluster
  - Fuzzy:
    - Weight elements according to cluster
- Each can be either complete or partial

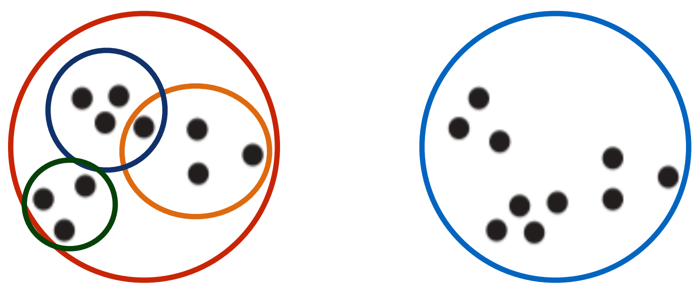
Partitional



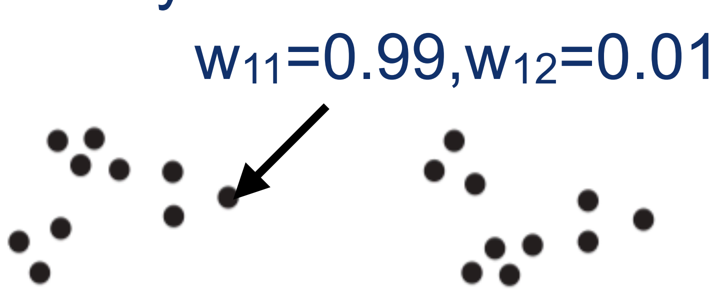
Hierarchical



Non-exclusive



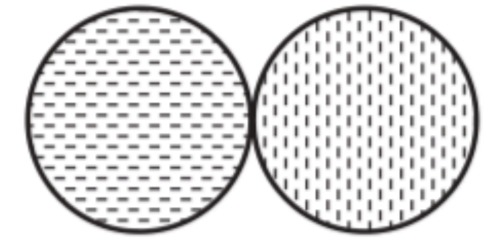
Fuzzy



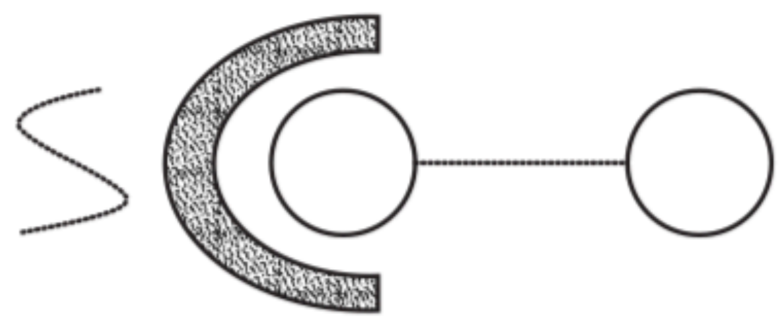
Clustering

- Types of clusters:

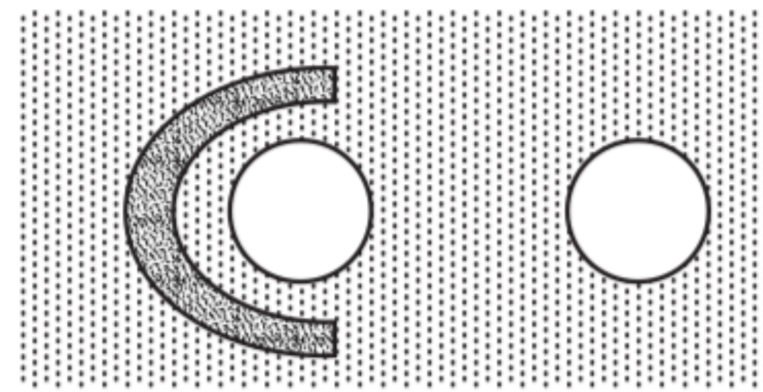
(a) Well-separated clusters. Each point is closer to all of the points in its cluster than to any point in another cluster.



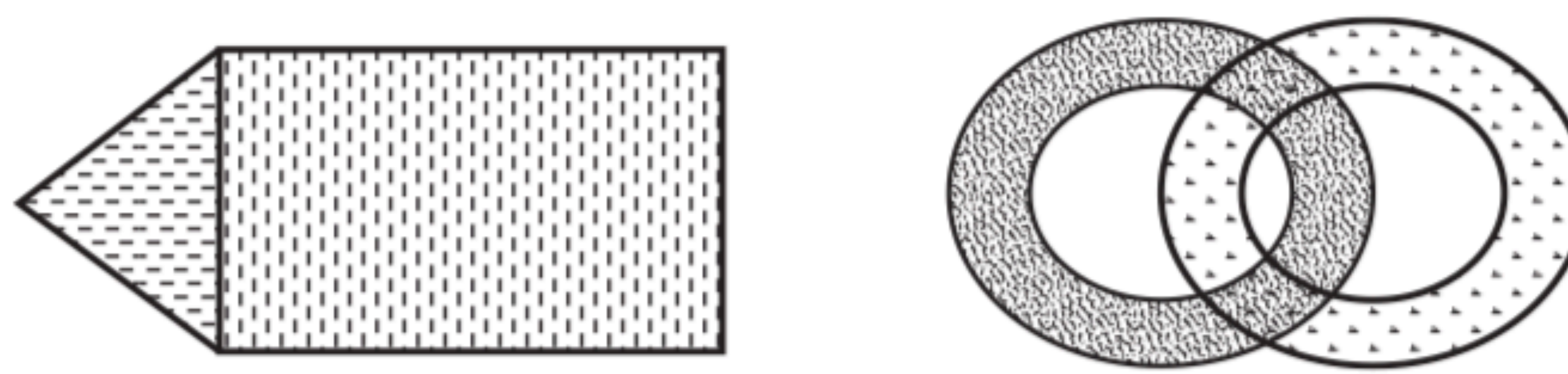
(b) Center-based clusters. Each point is closer to the center of its cluster than to the center of any other cluster.



(c) Contiguity-based clusters. Each point is closer to at least one point in its cluster than to any point in another cluster.



(d) Density-based clusters. Clusters are regions of high density separated by regions of low density.



(e) Conceptual clusters. Points in a cluster share some general property that derives from the entire set of points. (Points in the intersection of the circles belong to both.)

Clustering

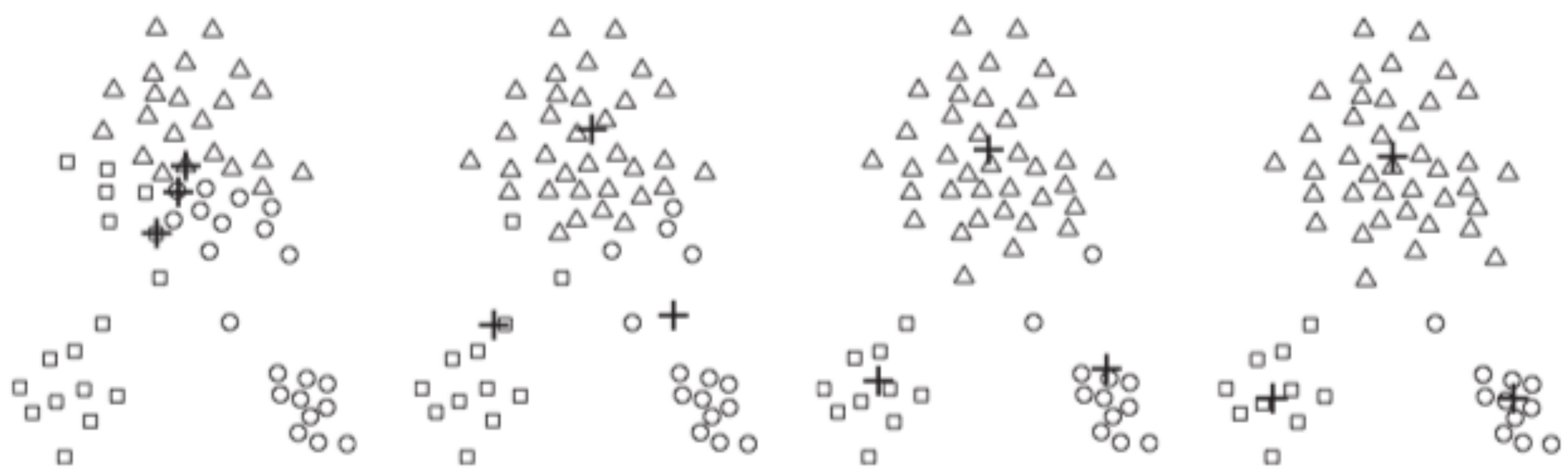
- Popular categories :
  - K-means
    - Partition into k clusters using mean central values (usually exclusively)
  - Agglomerative hierarchical clustering
    - Pair individual elements into clusters given some distance metric
  - Density based scan
    - Considers low-density regions to be noise, not exclusive clustering

Clustering

- K-means algorithm:

Algorithm 8.1 Basic K-means algorithm.

1: Select K points as initial centroids.
2: **repeat**
3: Form K clusters by assigning each point to its closest centroid.
4: Recompute the centroid of each cluster.
5: **until** Centroids do not change.



(a) Iteration 1. (b) Iteration 2. (c) Iteration 3. (d) Iteration 4.

Clustering

- K-means algorithm:
  - Formally, computes RMS:

Number of Centroids

Number of Data points

$$RMS^2 = \sum_{i=1}^{k} \sum_{j=1}^{n} |\vec{c}_i - \vec{x}_j|^2$$

Data positions

Centroid positions

  - Minimize the RMS by adjusting the centroids
  - Note: Other distance metrics can be used, but the principle is the same (minimize the metric)

Clustering

- Computational complexity is ~linear in product of:
  - Number of points
  - Number of “dimensions” (or attributes)
  - Number of clusters
  - Number of iterations to converge

- Shortcomings of k-means:
  - As in all minimization routines, danger of local minima
    - Need heuristic methods to avoid them
  - Can result in empty clusters if initialized poorly
  - Outliers have disproportionate impact
- Can try to split and merge centroids to mitigate these!

Clustering

- Alternative to k-means: Bisecting k-means:

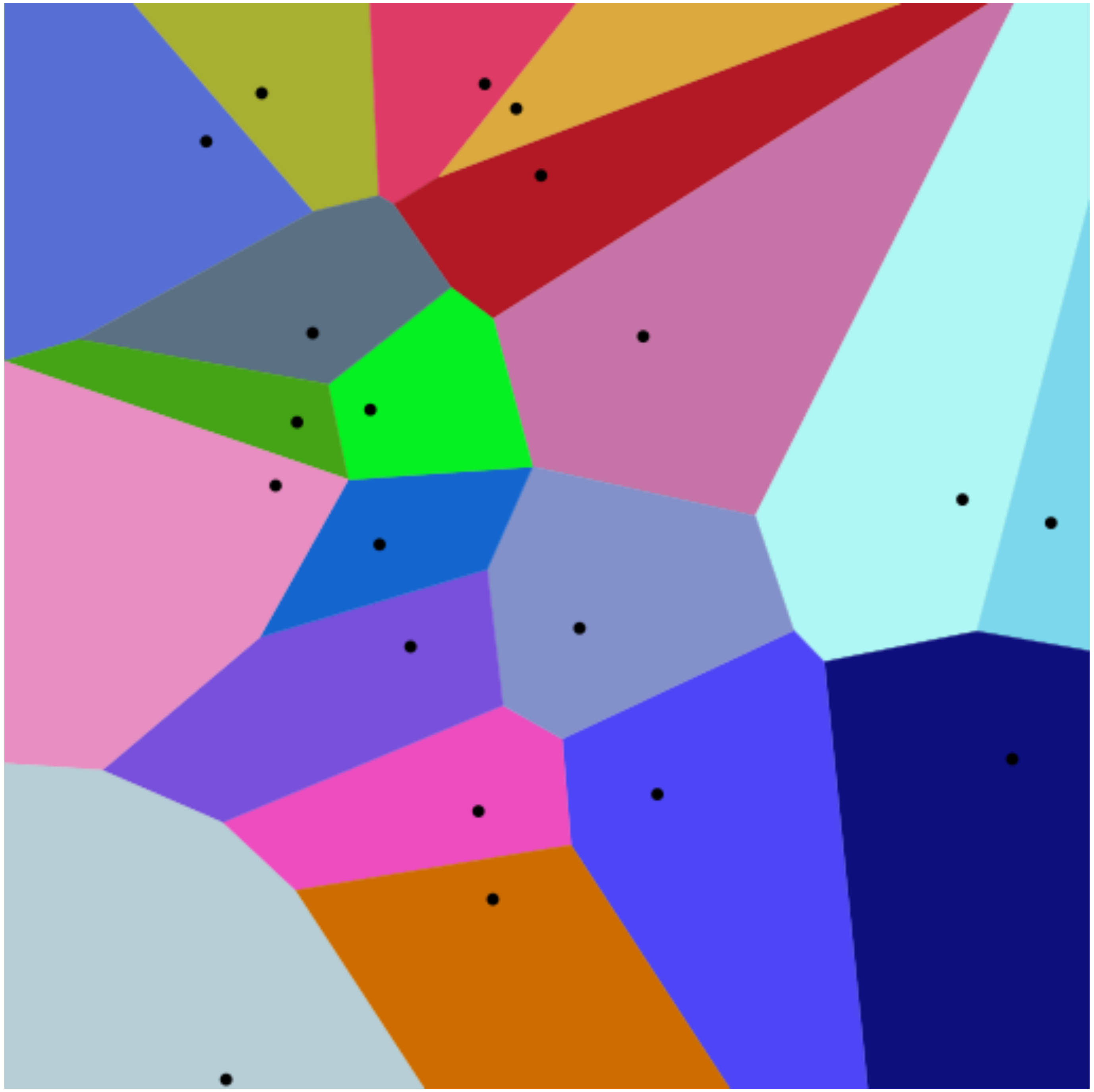
Algorithm 8.2 Bisecting K-means algorithm.

Initialize the list of clusters to contain the cluster consisting of all points.
repeat
    Remove a cluster from the list of clusters.
    {Perform several "trial" bisections of the chosen cluster.}
    for $i = 1$ to $number\ of\ trials$ **do**
        Bisect the selected cluster using basic K-means.
    end for
    Select the two clusters from the bisection with the lowest total SSE.
    Add these two clusters to the list of clusters.
until Until the list of clusters contains K clusters.

Clustering

- Result is a Voronoi diagram
- Each point is closer to all points in its cell than other cells

- Also referred to as “cachement areas”
  - From river basins, water tables, etc… where does the water pool when it rains?

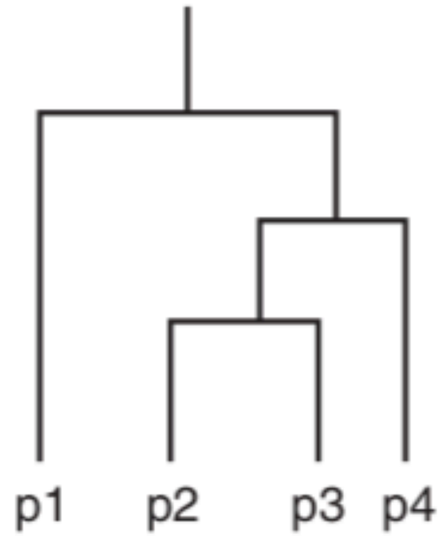


https://en.wikipedia.org/wiki/Voronoi_diagram

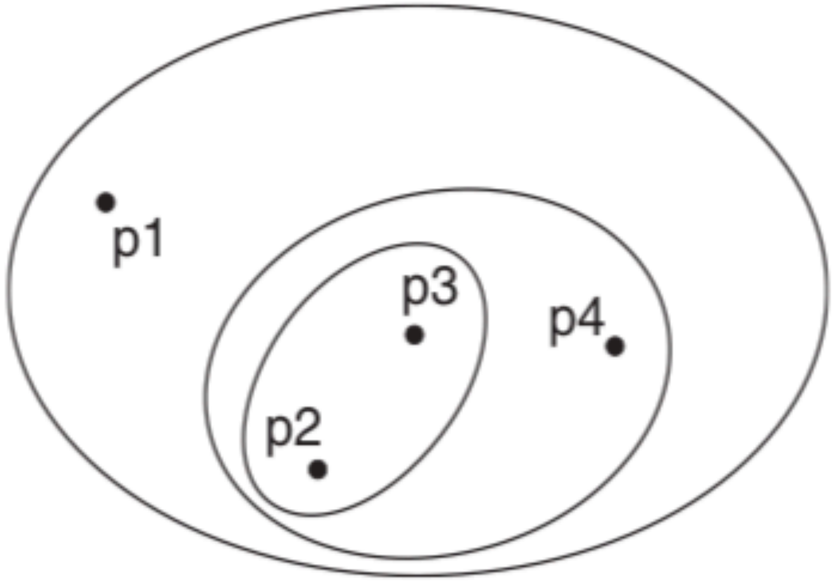
Clustering

- Hierarchical clustering:
  - Agglomerative (“bottom up”):
    - Start with individual constituents, merge until criteria met
  - Divisive (“top down”):
    - Start with conglomerate, split until criteria met (or you get to individual constituents)
  - Represent by a tree (“dendrogram”) or Venn diagram (“nested cluster diagram”):

Basically the same, but in reverse



(a) Dendrogram.



(b) Nested cluster diagram.

Clustering

Algorithm 8.3 Basic agglomerative hierarchical clustering algorithm.

Compute the proximity matrix, if necessary. O(n^2), done once
repeat
  Merge the closest two clusters. O(1), done n times
  Update the proximity matrix to reflect the proximity between the new cluster and the original clusters. O(n^2), done n times
until Only one cluster remains.

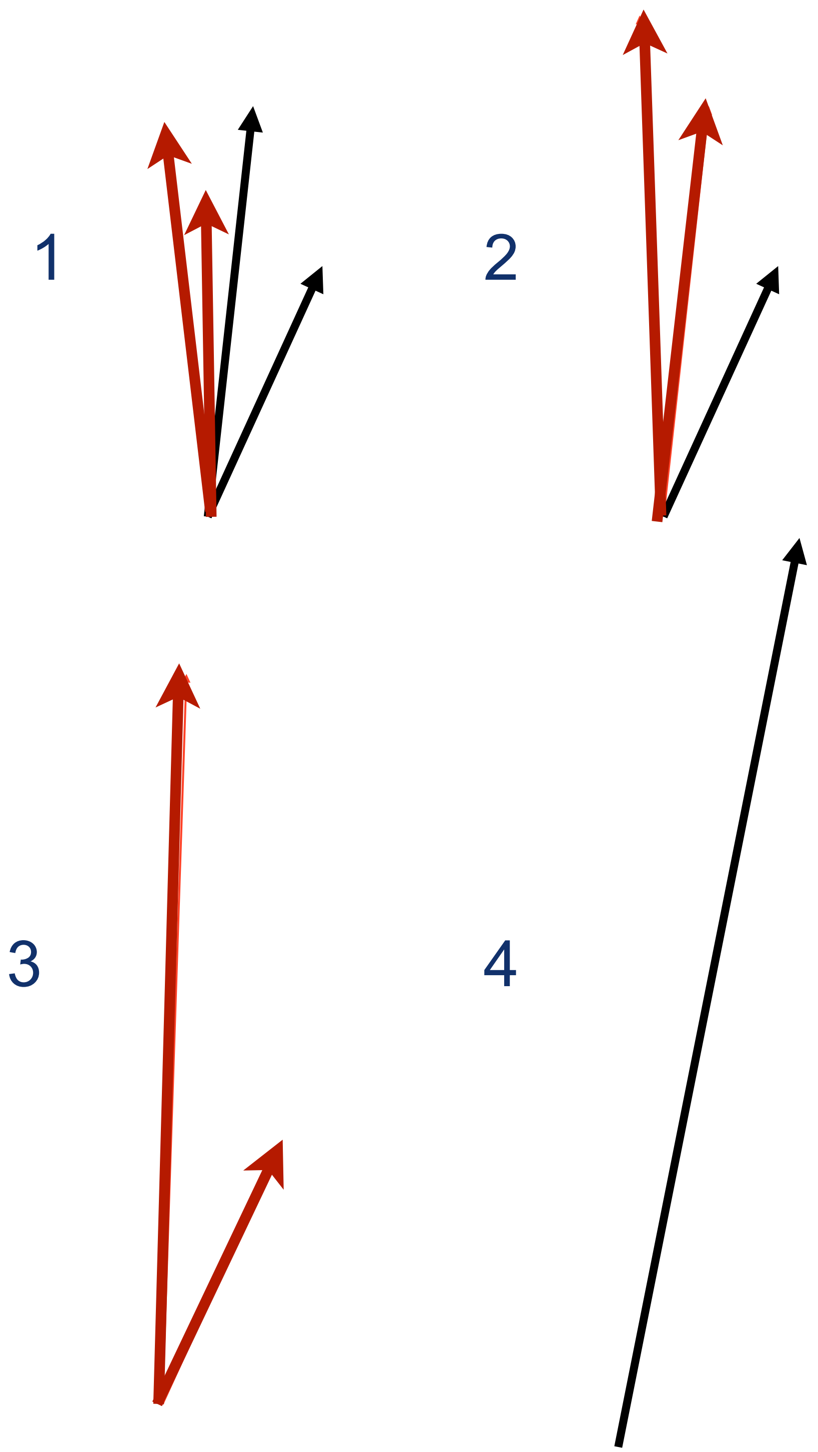
n^3 algorithm?

https://arxiv.org/pdf/hep-ph/0512210.pdf

Clustering

- Faster clustering algorithms (i.e. fastjet):
  - Can precompute nearest neighbors in the metric, and then only look at those instead of all (nearest is nearest is nearest!)

    Calculate nearest neighbors
    while inputs are left:
      Compute distances to neighbors, and self
      If distance to neighbor is smallest, merge + iterate
      Else if distance to self is smallest, stop



https://arxiv.org/pdf/hep-ph/0512210.pdf

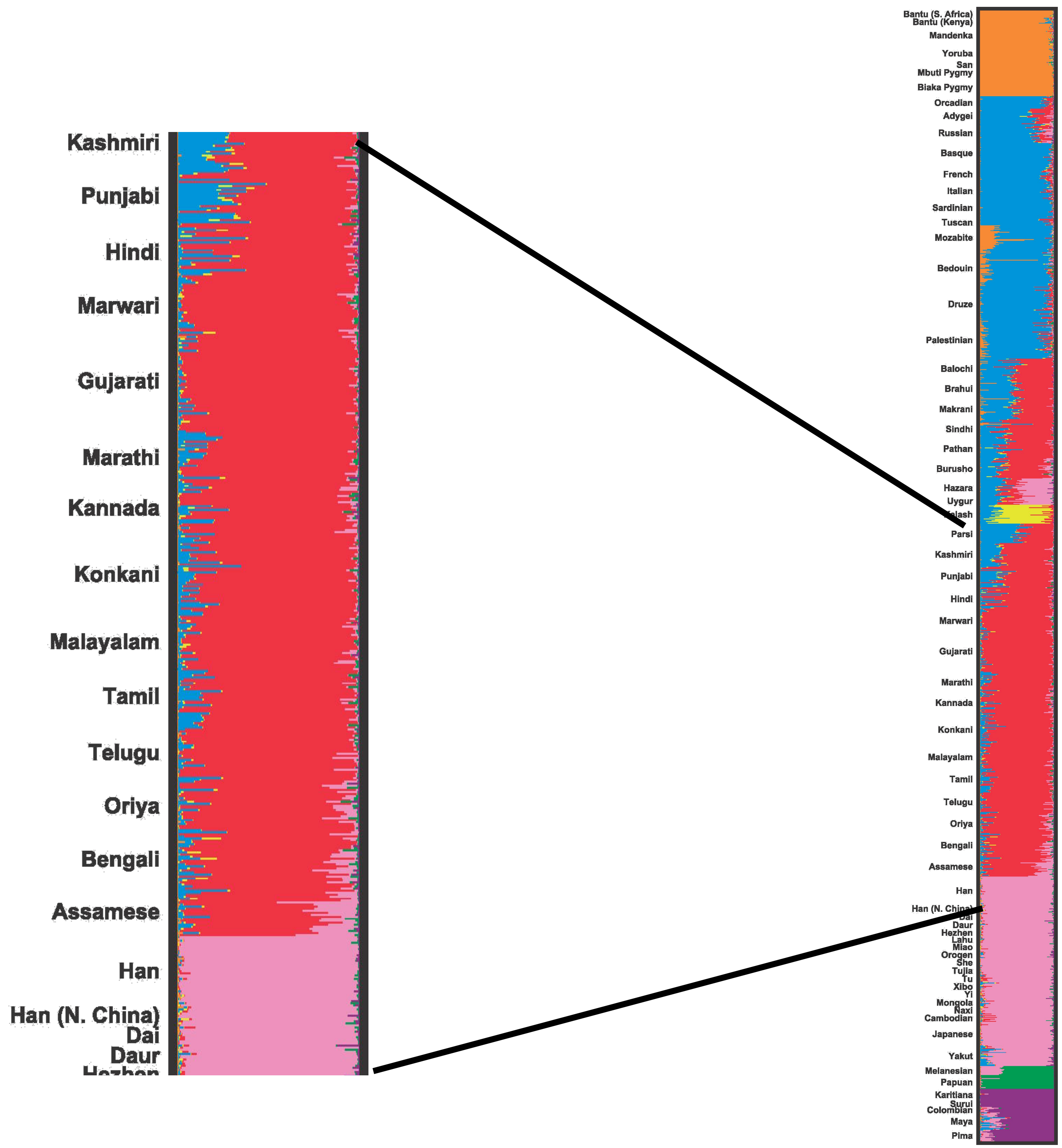
Clustering

- This reduces to $O(n^2)$ complexity

- Can reduce further!
  - To find nearest neighbors, can use Voronoi diagrams (like we had before)
  - This reduces complexity to $O(n \ln(n))$!

Clustering

- Example: Genetic clustering
  - Including those "who are your ancestors" DNA kits!



Clustering

- Example: Finding galaxy clusters using Voronoi tessellations
  - https://www.aanda.org/articles/aa/pdf/2001/12/aa10522.pdf

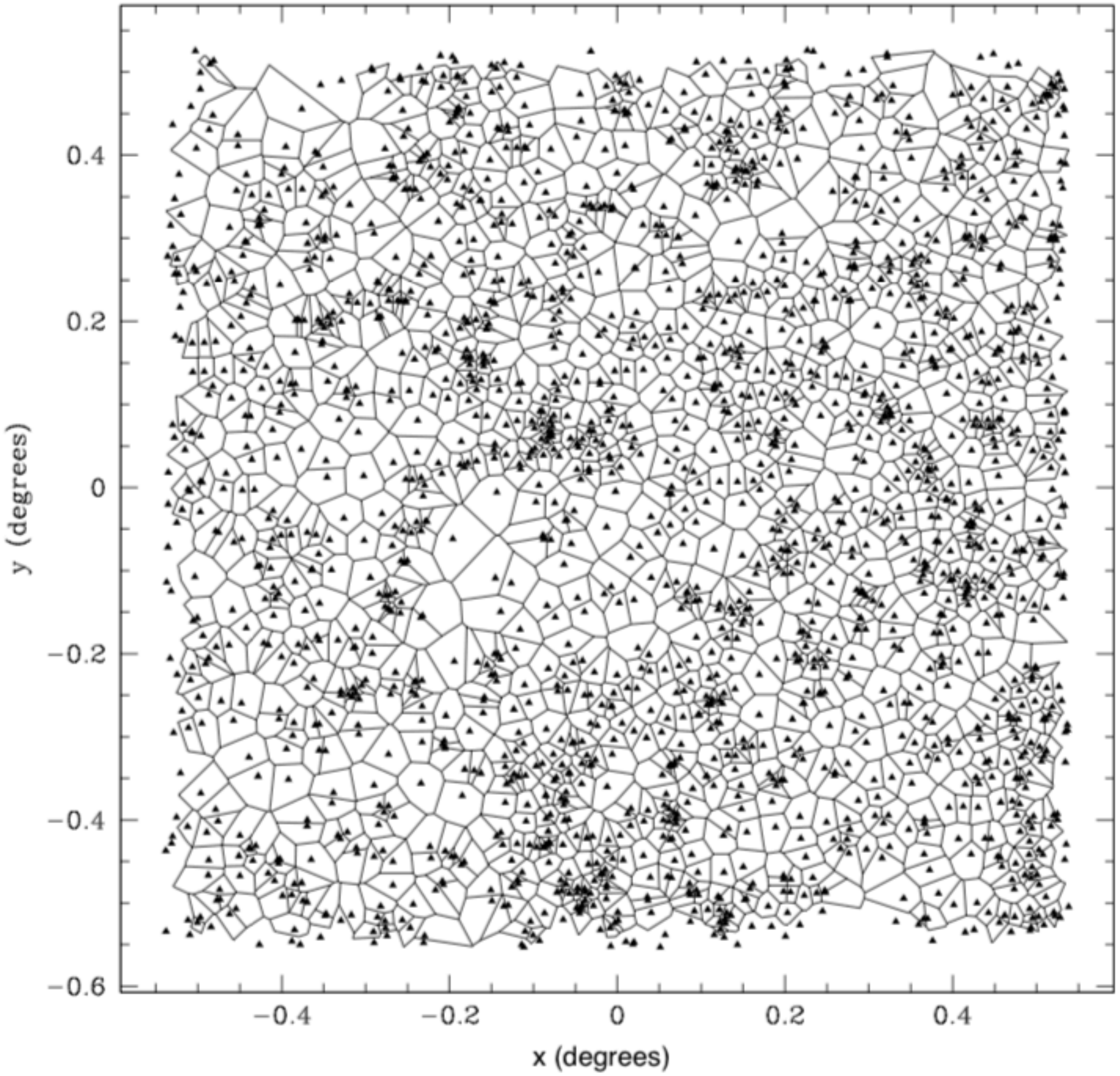


Fig. 1. Voronoi tessellation of a galaxy field

Clustering

- Example: Finding hadronic jets (The Anti-kT Jet Clustering Algorithm)
- http://inspirehep.net/record/779080

- Hierarchical clustering with various metrics