Introduction to Deep Learning

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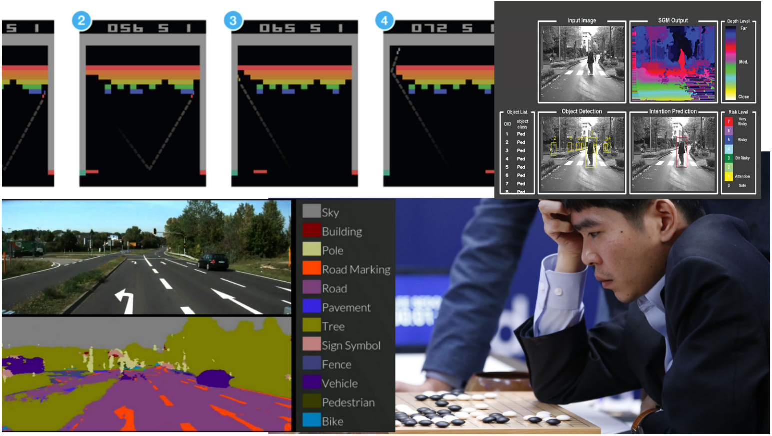
Deep Learning: A Breakthrough in AI?



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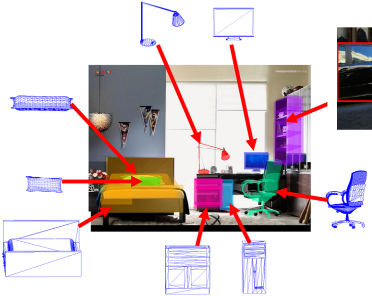

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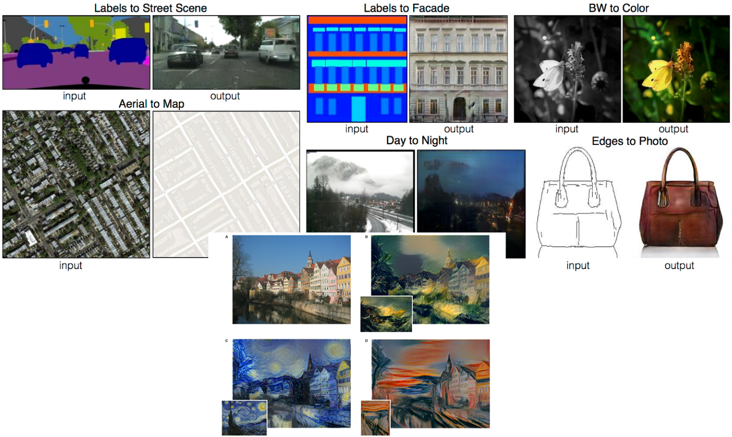

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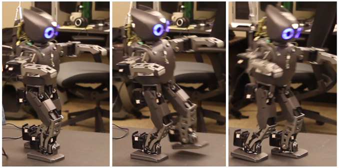

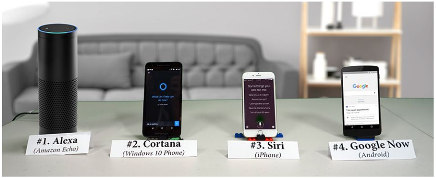

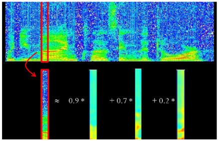

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Deep learning approach for active classification of electrocardiogram signals

M.M. Al Rahhal[a], Yakoub Bazi[a,*], Haikel AlHichri[a], Naif Alajlan[a], Farid Melgani[b], R.R. Yager[c,1]

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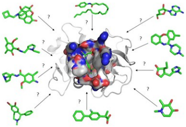

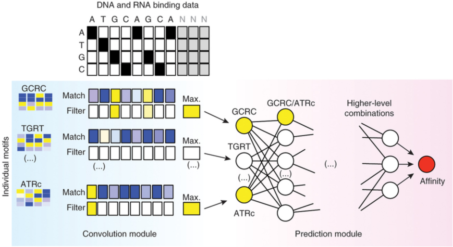

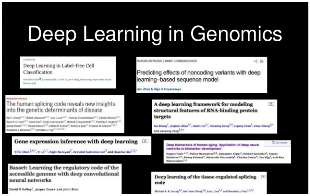

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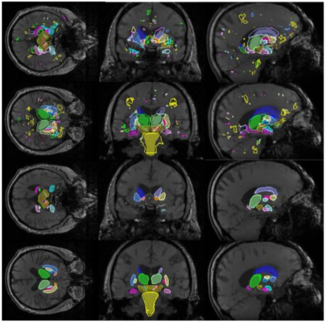

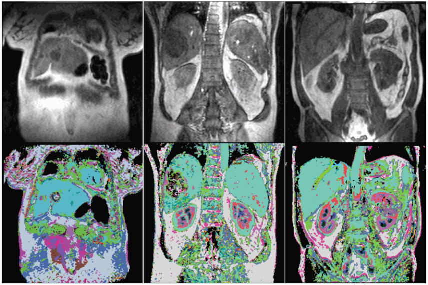

(a) (b) (c)

Machine Learning (ML) very summarized

A diagram of what AI/ML does after all

How's the input data of a ML system?

- Data types: attributes, signal/sound, image (2D/3D), video...

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  - What's that?: Reinforcement Learning (RL)

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1. Data normalization ✓

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   - Image: moments, SIFT, HOG, SURF...
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   - Solution 2: use the whole data (*sensory* data)

Desired output: ML tasks

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- RL: game playing, auto driving, robotics
- Structured data generation (image, text, translations...)

What's inside the AI/ML box?

Machine learning

Train on some data, build a model, apply it on new data

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PCA, SVM, K-means, logistic regression, LME, tSNE............

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Deep learning

- Evolution of neural networks
- Big family of methods, applications and architectures
- "Component" philosophy

ML concepts: supervised case

Train/validation/test protocol

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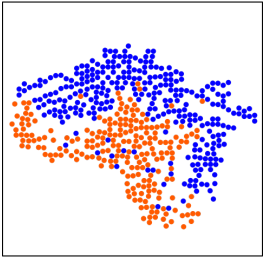
Error types



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TRAIN	VALID.	TEST

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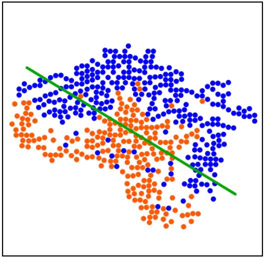
- Train error (underfitting)



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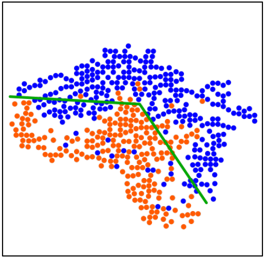

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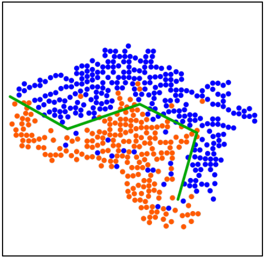

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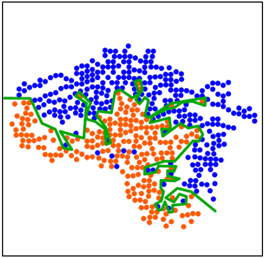

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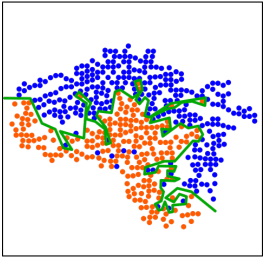

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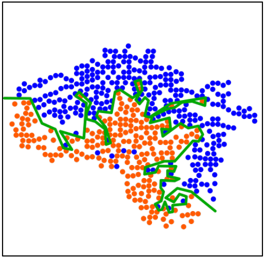
- Human error :o

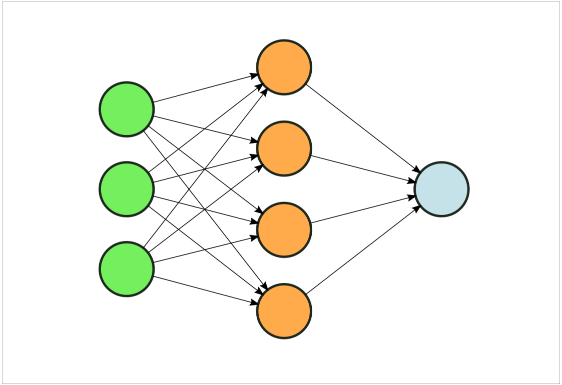


Deep learning concepts

- Neural networks (metaphor)
- Now we have huge datasets
- Now we have powerful hardware
- Deep architectures deliver much better performance
- Theoretical improvements (optimization)

Not extensively exploited in Bioinfo!

A simple (but complete) example neural network



Inputs $*$ *weights* capture interactions between input variables.
Enough hidden units allow to model any Borel-measurable function.
Not deep yet!

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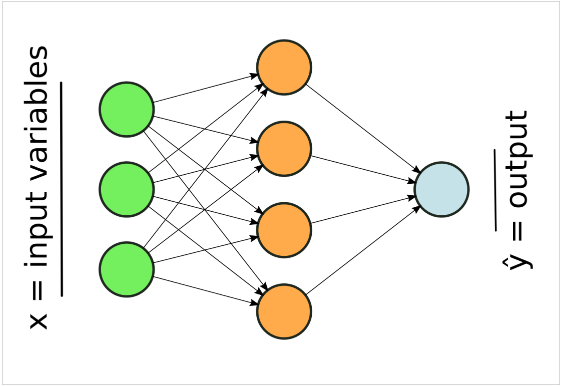

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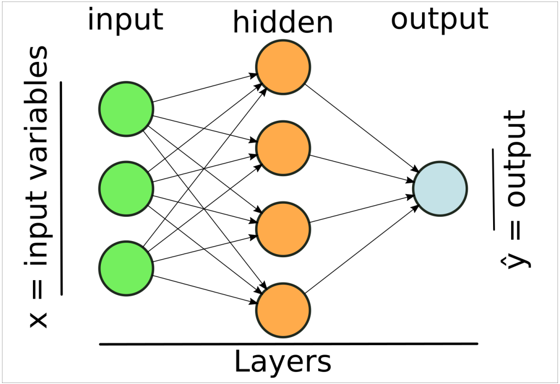

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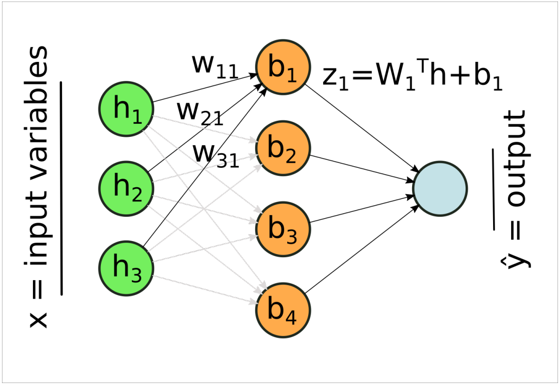

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7. Compute the activation function of each output unit $g_2(z)$

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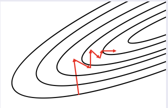

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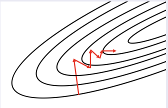

4. Possibly re-run the NN with new or shuffled train data (**epoch**)

Gradient Descent (GD): considerations

Learning rate: yet another hyperparameter

Tradeoff: large step (overstepping) vs small step (slow learning)

- Decreasing η
- Momentum / Nesterov momentum
- Adagrad / RMSProp / ADAM

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Granularity of gradient updates

- **Batch** GD. All train examples per update. *Expensive*
- **Stochastic** GD. One (random) example per update. *High variance*
- **Mini-batch** GD. Some (power of 2) examples per update. *Best option*

Output units

General considerations

- Type depends on the task type
- Must not saturate easily (i.e. give meaningful gradients)
- Easy to optimize (≈linear), compatible with cost function
- Cost function: **cross-entropy**

$$C = -\frac{1}{|x|}\sum_{x}(y \ln \hat{y} + (1-y)\ln(1-\hat{y}))$$

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- Regression (Gaussian) → **linear** unit
- Binary classification (Bernoulli) → **sigmoid** unit
- Multiclass classif. (Multinoulli) → **softmax** units (one unit per class, outputs sum 1, initially fuzzy)

Hidden and input units

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- Basically hidden $\equiv$ input
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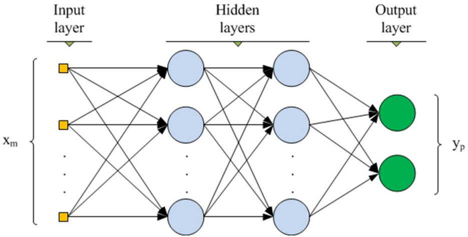
- Logistic sigmoid / hyperbolic tangent $\rightarrow$ *deprecated**
- Rectified Linear Unit (ReLU) $\rightarrow$ **best**: $g(z) = \max\{0, z\}$
- Maxout $\rightarrow$ good for some problems
  - Split input in blocks
  - Pick the highest input as output

How can we reduce the validation error?

- Use more train data (I wish I had it!)
- Data augmentation
  - Data synthesis
  - Add noise: input data, weights of hidden layers, outputs
- Parameter normalization (L_1 or L_2)
- Early stopping (train error stable, validation error grows)
- Dropout: randomly deactivate units

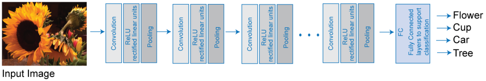
Multi-layer perceptron / feed-forward NN

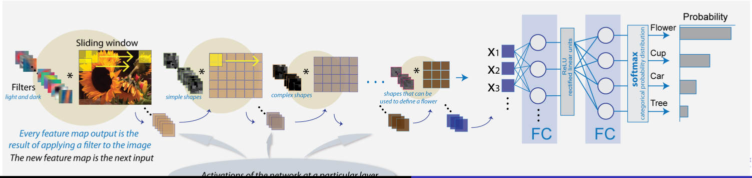
- Tasks: **regression**, **classification**
- The outputs of one layer are the inputs of the next (no loops)
- Totally connected (dense) layers by default
- Efficient, easy to optimize



Convolutional neural networks

- Tasks: **image processing** (locally-structured data)
- Convolutional layers: specialized filters
- Pooling layers: reduce size (can be maxout)
- Parameter sharing: same filters applied to whole input (dim. reduction, no overfitting)





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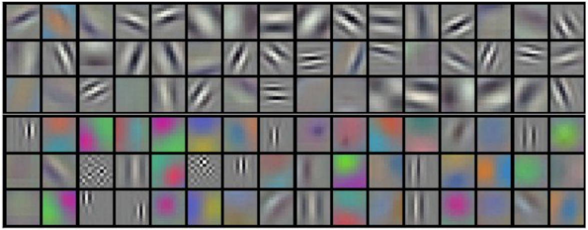
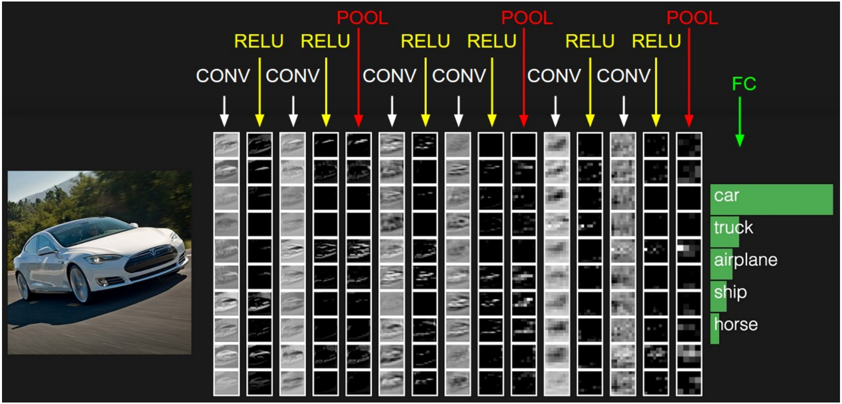
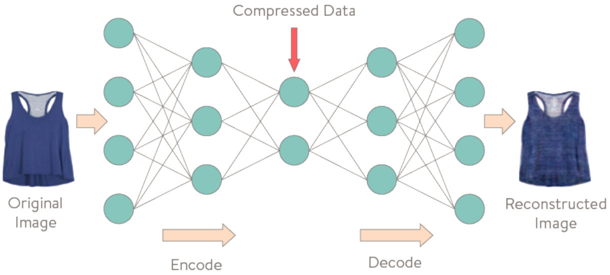


CNN filters in action

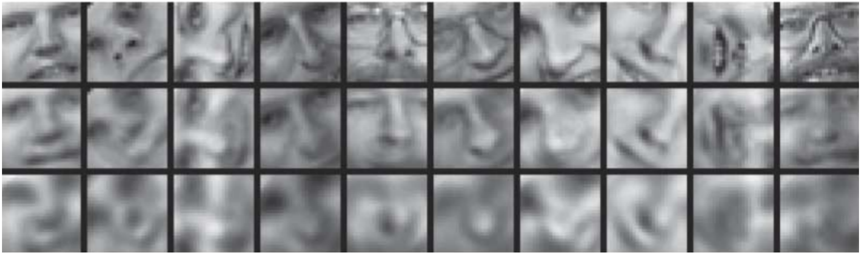


Autoencoders

- Tasks: dimensionality reduction, noise filtering
- Output = input. Weird!!
- Trick: middle layer(s) are smaller than input, so a "compressed" representation is forced



Autoencoder vs PCA



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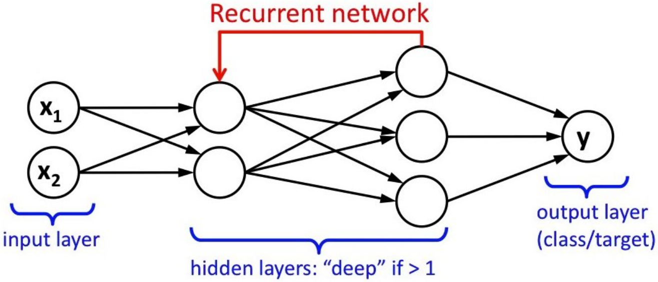
First row: original image; second row: autoencoder representation; third row: PCA reconstruction

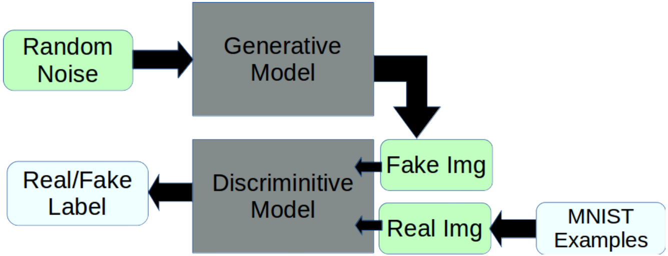
Recurrent neural networks

- Tasks: sequence (signal) processing
- There are loops and/or units with memory
- Harder to optimize/computationally more expensive
- Long-short term memory (LSTM): very effective



Generative adversarial networks

- Tasks: data generation
- One network (generative) trying to *cheat* the other (discriminative)
- Can create lifelike images/others



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- How to decide? (This is an art)
  - Train error: increase width and depth
  - Validation error: increase depth

DL libraries

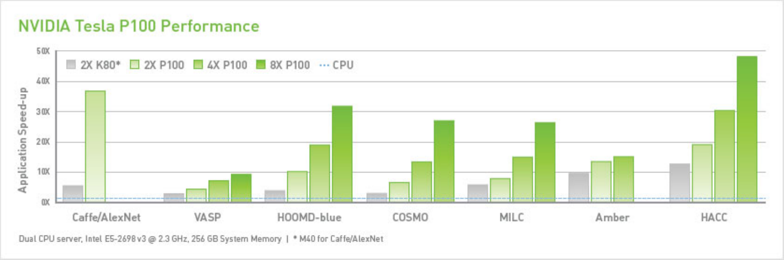
- Theano
- Tensorflow
- Caffe
- Lasagne*
- Keras*
- CNTK
- dl4j
- ...

Example: CNN on MNIST using Keras

```
model = Sequential()

model.add(Convolution2D(nb_filters, kernel_size[0], kernel_size[1],
                        border_mode='valid',
                        input_shape=input_shape))
model.add(Activation('relu'))
model.add(Convolution2D(nb_filters, kernel_size[0], kernel_size[1]))
model.add(Activation('relu'))
model.add(MaxPooling2D(pool_size=pool_size))
model.add(Dropout(0.25))

model.add(Flatten())
model.add(Dense(128))
model.add(Activation('relu'))
model.add(Dropout(0.5))
model.add(Dense(nb_classes))
model.add(Activation('softmax'))

model.compile(loss='categorical_crossentropy',
              optimizer='adadelta',
              metrics=['accuracy'])

model.fit(X_train, Y_train, batch_size=batch_size, nb_epoch=nb_epoch,
          verbose=1, validation_data=(X_test, Y_test))
score = model.evaluate(X_test, Y_test, verbose=0)
print('Test score:', score[0])
print('Test accuracy:', score[1])
```

Where do you train your DL experiments?

- CPU: slooooow
- GPU: mainstream, really fast
- FPGA: ???
- Multi-core CPUs: ???



About to finish, so...

Any questions?