Deep Learning Mechanics

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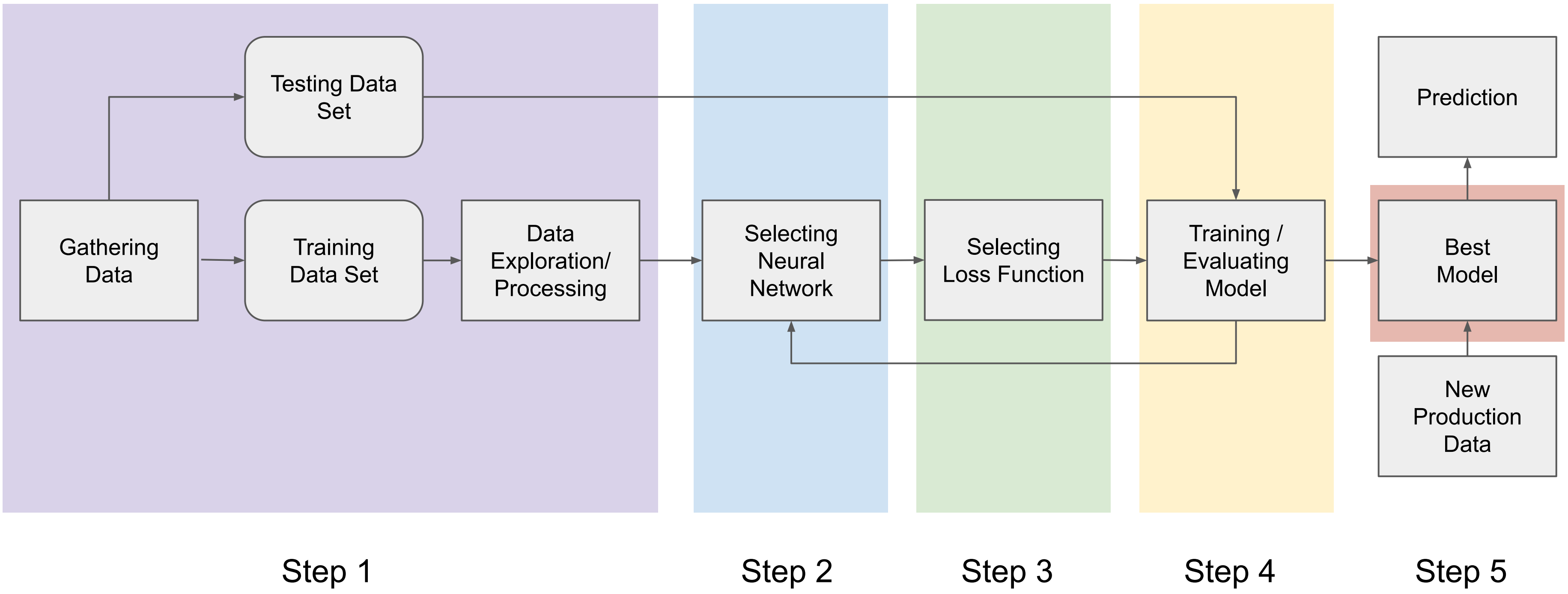
Simplified workflow for a deep learning project



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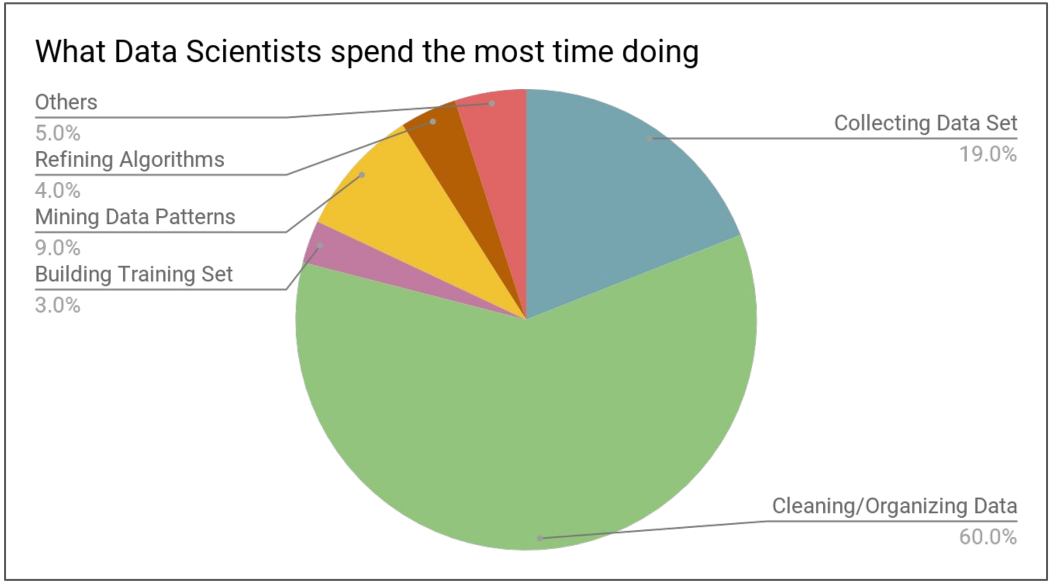
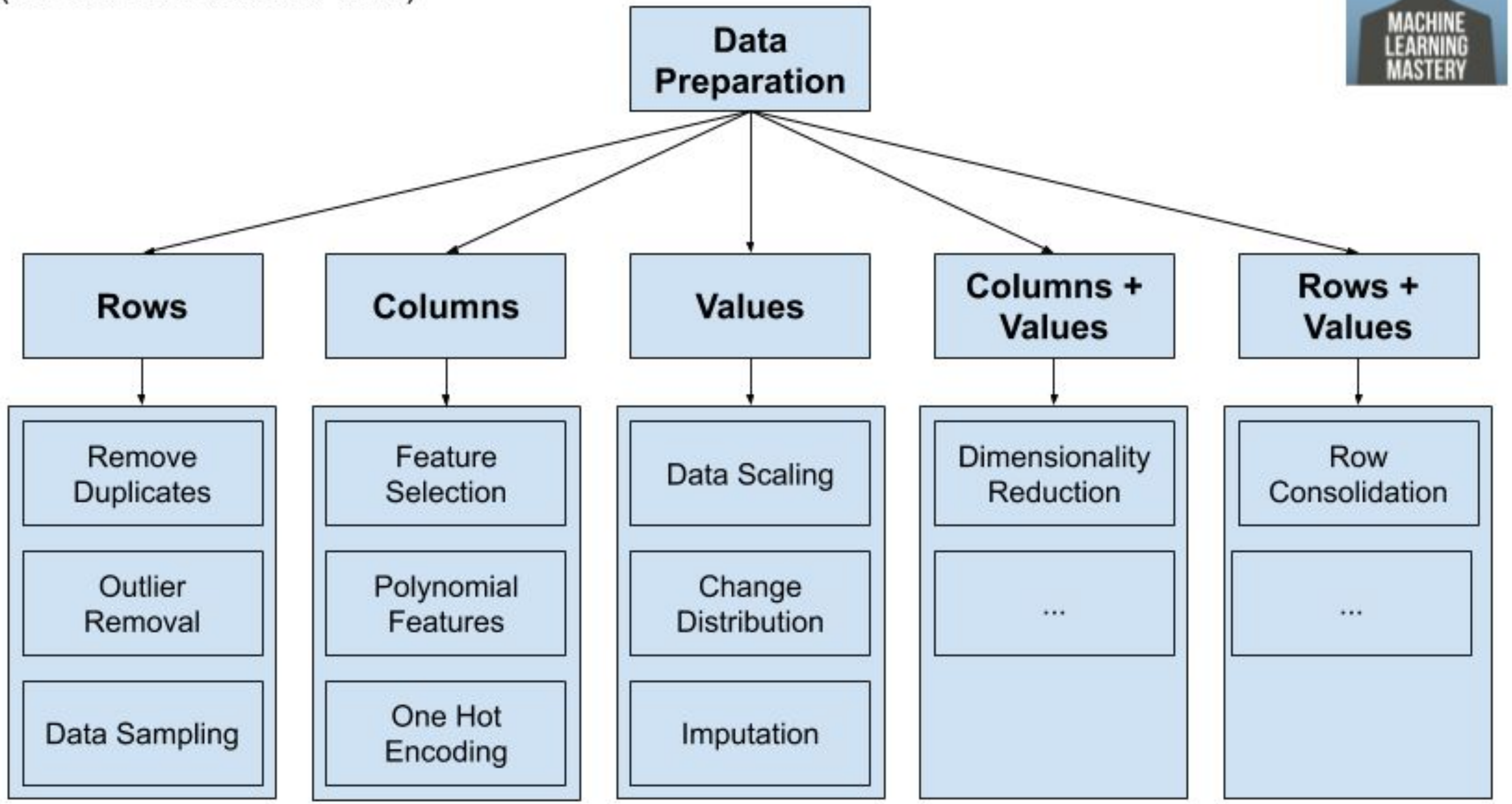
Step 1. Data Preparation and Processing

- The most time-consuming but the most *creative* job
  - Take > 80% time
  - Require experience
  - May need domain expertise
- Determines the upper limit for the goodness of DL
  - Models/Algorithms:
    just approach the upper limit



Survey from Forbes in 2017 (Data Source)

Data Preparation Framework
(*for structured/tabular data*)



Special deep learning tasks in data prep step

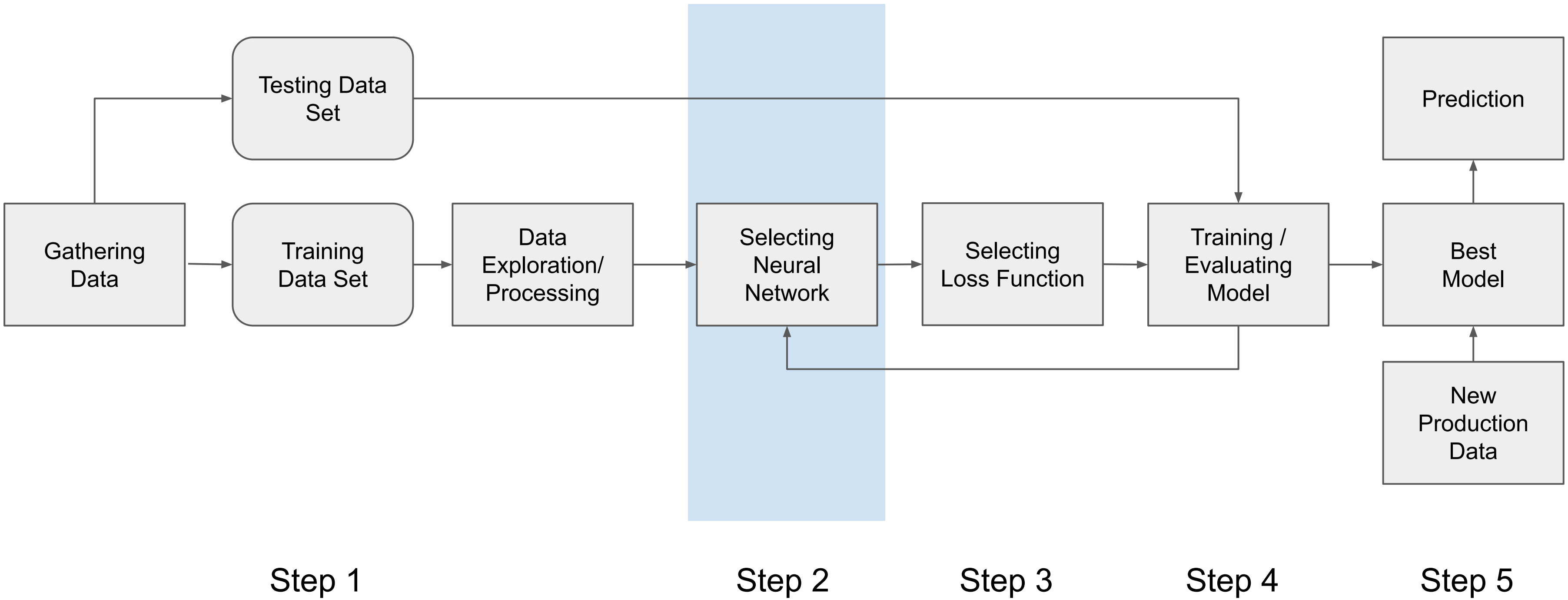
- Image Data Processing
  - Pixel scaling
  - Train-Time Augmentation
  - Test-Time Augmentation
  - Convolution and Flattening

- Data Tokenization
  - Breaking the sequence data into units
  - Mapping units to vectors
  - Aligning & padding sequences

- Data Embedding
  - Map data to lower-dim vectors
    - Sparse to dense
    - Merging diverse data
    - Preserve relationship
  - Techniques
    - Std Dimensionality Reduction
    - Word2Vec
    - Be part of the model training
  - *Representation Learning*

$$\text{Embedding Dims} \approx \sqrt[4]{\text{Possible Values}}$$

Workflow for a deep learning project



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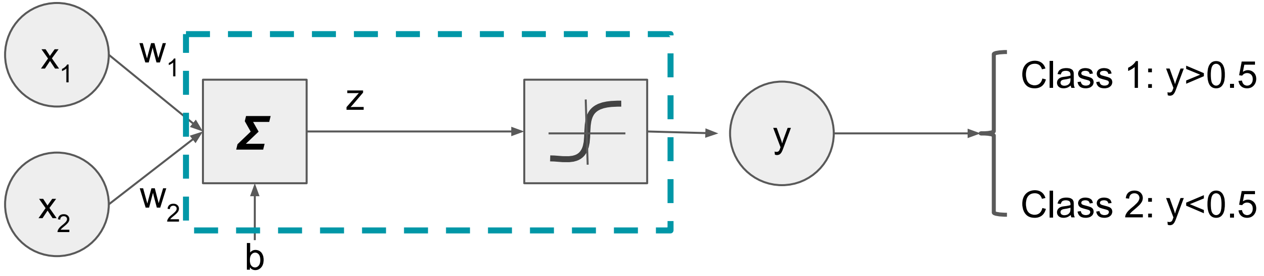
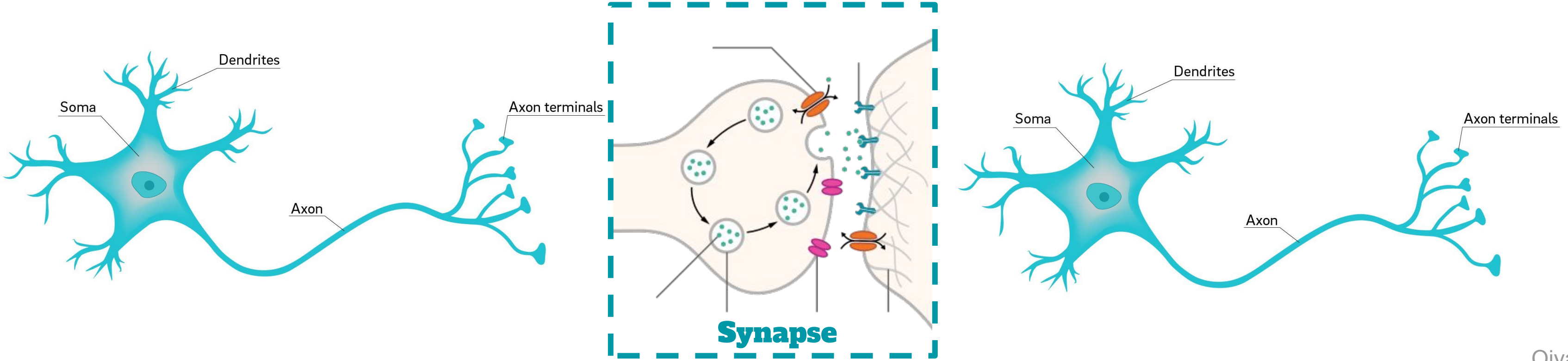
Recap: artificial neuron vs. biological neuron

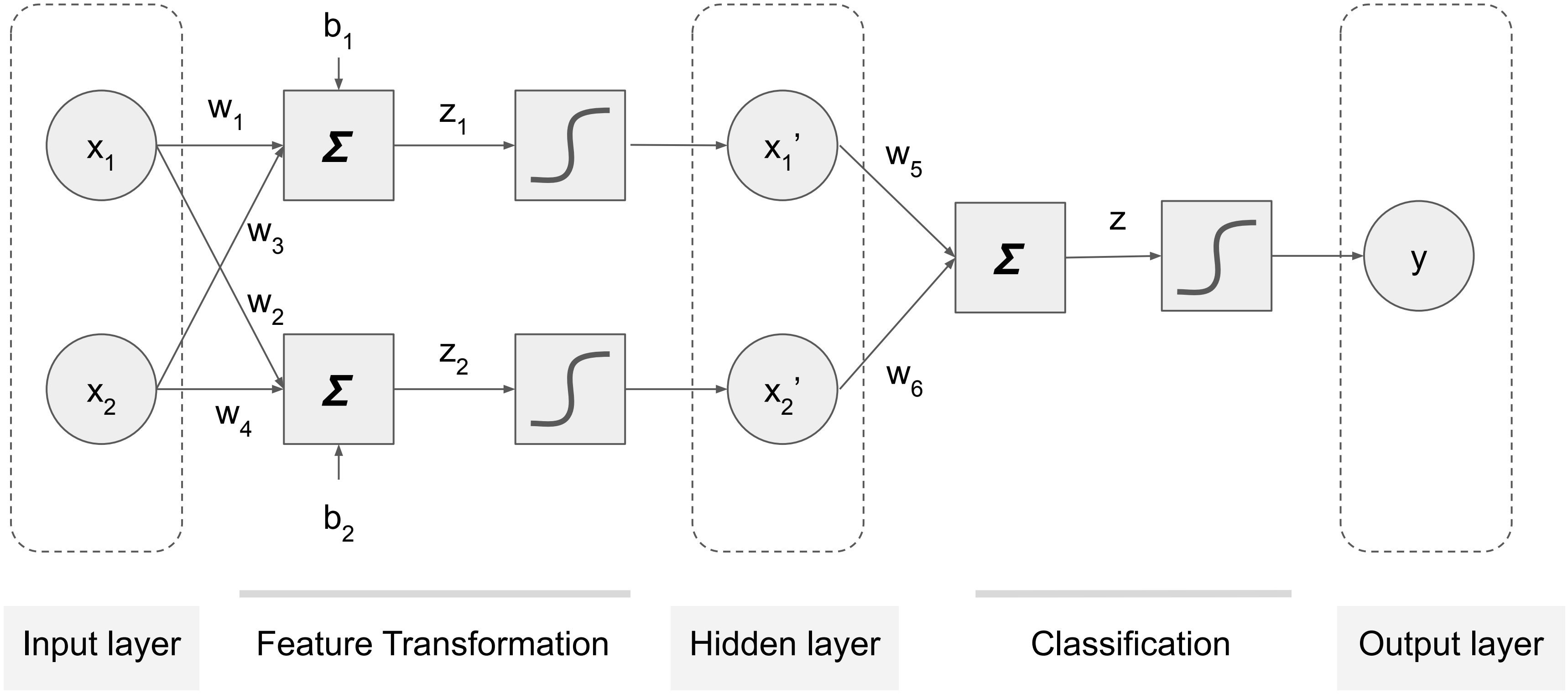
$$z = w_1 x_1 + w_2 x_2 + b \qquad y = \sigma(w_1 x_1 + w_2 x_2 + b)$$

McCulloch-Pitts (MCP) neuron model





(Deep) Neural Networks ~ piling/stacking logistic-regression classifiers



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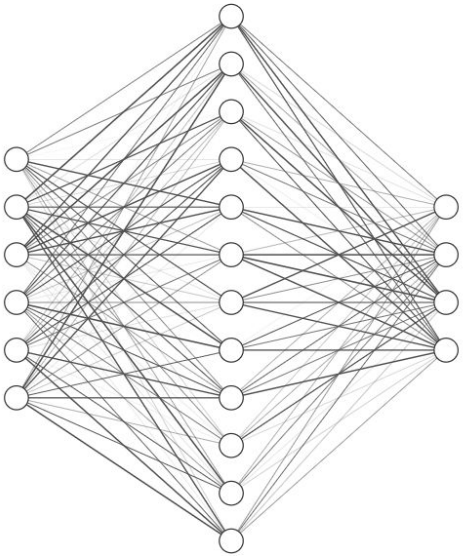
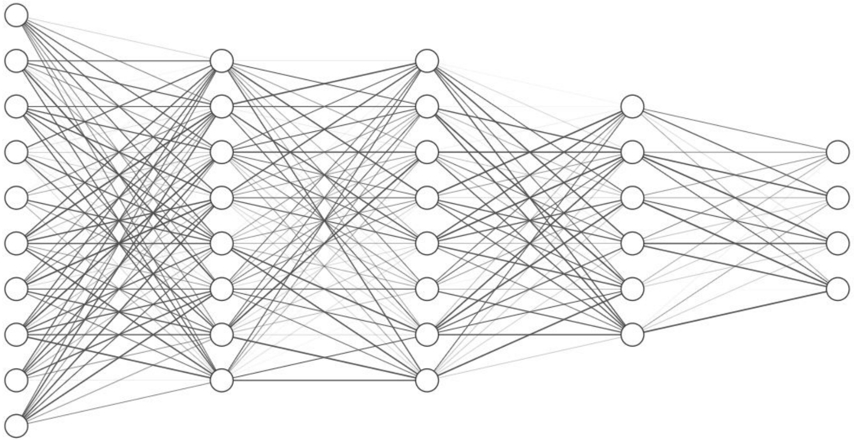
Why deep?

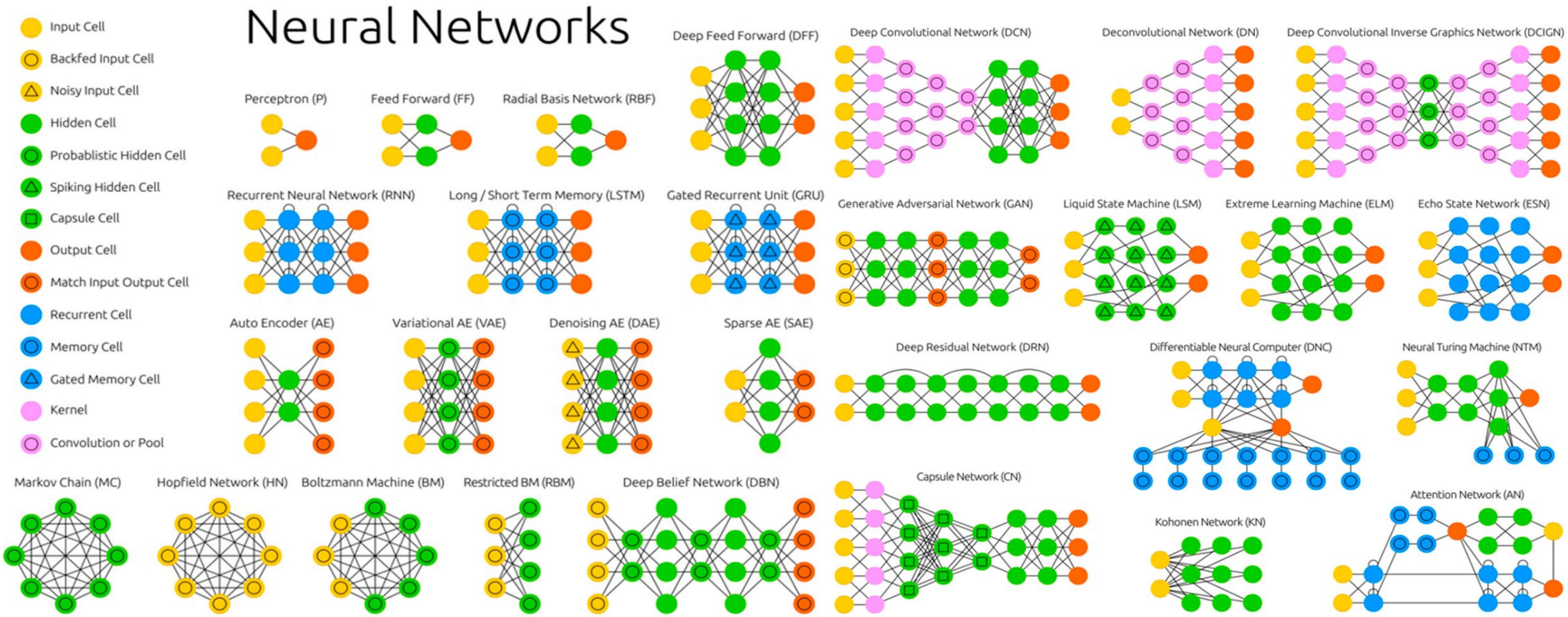
- Shallow network can fit any function
  - Has less number of hidden layers
  - Has to be really "fat"



- Deep network is more efficient.
  - Exponentially fewer parameters (2017)
  - It can extract/build better features



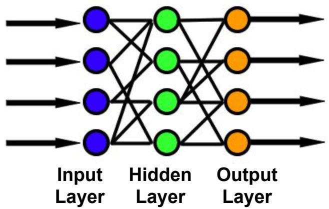
Types of Deep Learning Architectures



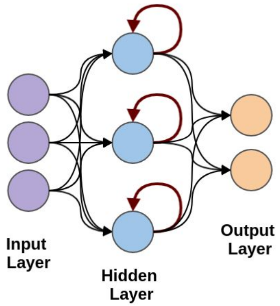
[Proceedings 2020, 47(1), 9]

A simpler classification of neural network types

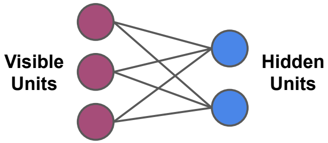
- Feed forward neural networks (No cycle in node connections)
  - Fully connected network
  - Convolutional networks (CNNs)



- Recurrent networks (w/ directed cycle in node connections)
  - Fully recurrent NN
  - Recursive NN
  - Long short-term memory (LSTM)
  - Hopfield network (w/o hidden nodes)

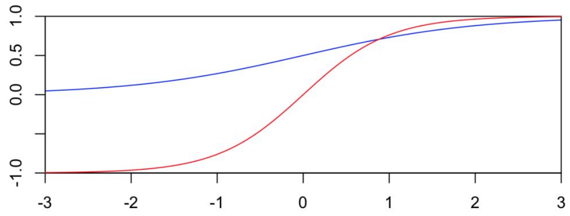


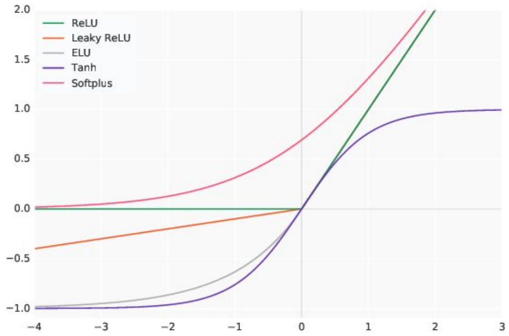
- Symmetric networks (no directions in node connections)
  - Boltzmann Machines
    - RBM, DBM, SOM



Activation Function

- Sigmoid function: $$\sigma(z) = \frac{1}{1 + \exp(-z)}$$
- tanh function: $$tanh(z) = \frac{\exp(z) - \exp(-z)}{\exp(z) + \exp(-z)}$$
- Rectified linear unit (ReLU) $$f(x) = x^+ = \max(0, x)$$
  - Softplus
  - Leaky ReLU
  - Exponential LU (ELUs)
  - GELU
  - Dynamic ReLU
- Softmax function: $$y_i = \frac{e^{z^{(i)}}}{\sum_{j=0}^{K} e^{z^{(j)}}}$$
- Maxout Network:
  - *Learnable* activation function





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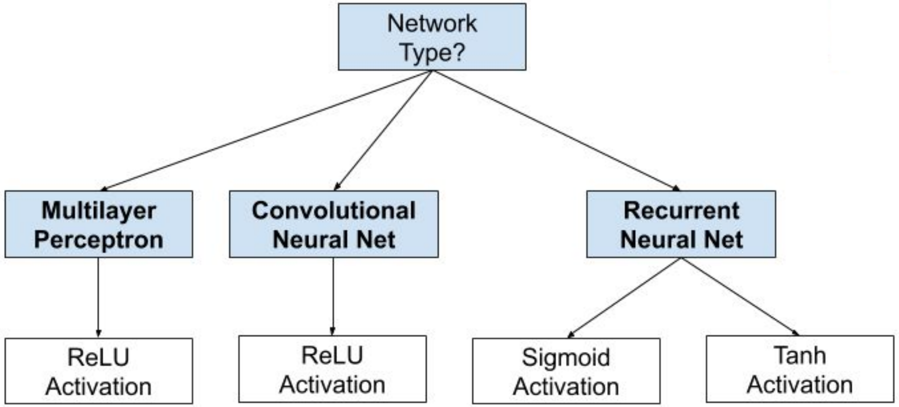
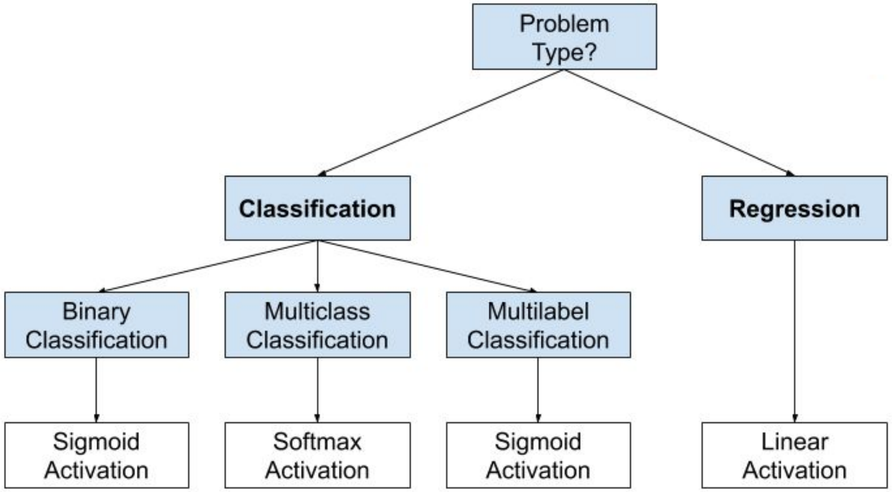
How to choose activation functions?

For hidden layers

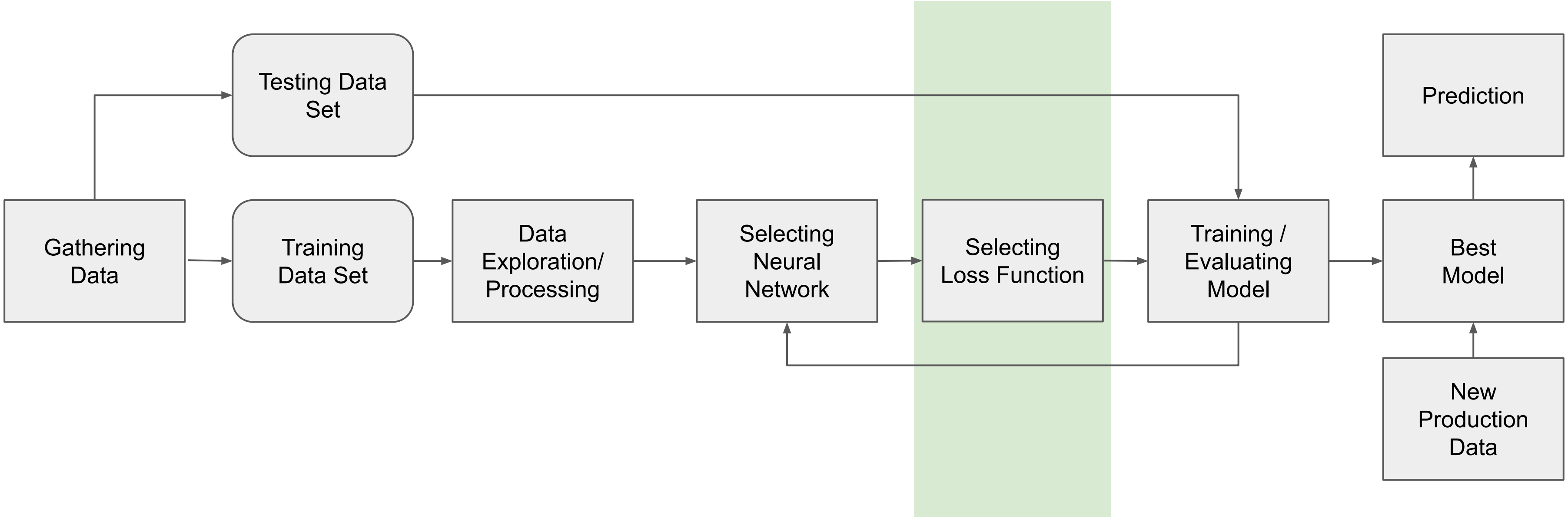


For output layers



From [Machine Learning Mastery Blog Post]

Workflow for a deep learning project



Step 1 Step 2 Step 3 Step 4 Step 5

How to measure the performance of the model?

- General name: objective function

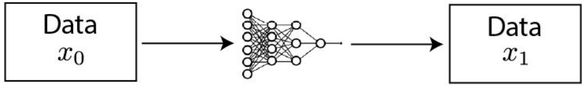
- Measure the misfit of the model as a function of parameters
  - Criterion is to *minimize* the error functions
  - Loss Function, Cost Function: a penalty on difference between predictions and labels

- Evaluate the probability of *generating* training set
  - Criterion is to *maximize* the distribution likelihood as a function of parameters
  - Maximum (log)-likelihood estimation: minimize the divergence of distributions

- Regression losses and classification losses

Loss functions

- Generative/Predictive:



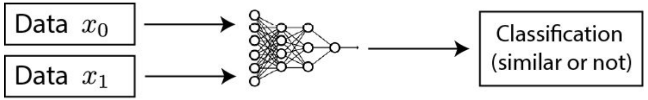
  - Regression Loss
    - Mean Square Error / Quadratic Loss / L2 Loss:
    - Mean Absolute Error / L1 Loss:
  - "Physics-informed" residuals
  - Cross-Entropy Loss and variations
    - Softmax Loss / Log Loss / Negative Log Likelihood
    - Weighted CE / Balanced CE / Focal Loss
    - Dice Loss / IOU Loss / Tversky Loss

$$L_{MSE} = \frac{1}{n}\sum_{i}^{n}(t_i - s_i)^2$$

$$L_{MAE} = \frac{1}{n}\sum_{i}^{n}|t_i - s_i|$$

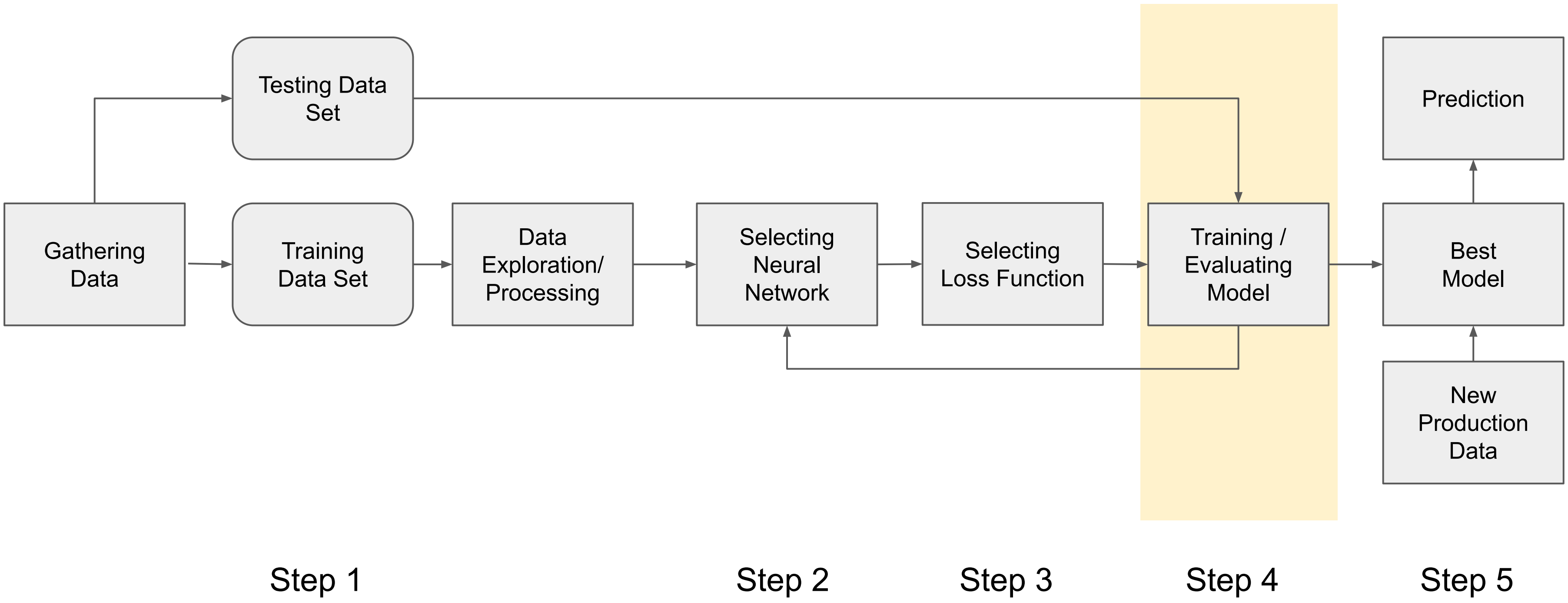
$$L_{CE} = -\sum_{i}^{C} t_i \log(s_i)$$

- Contrastive:

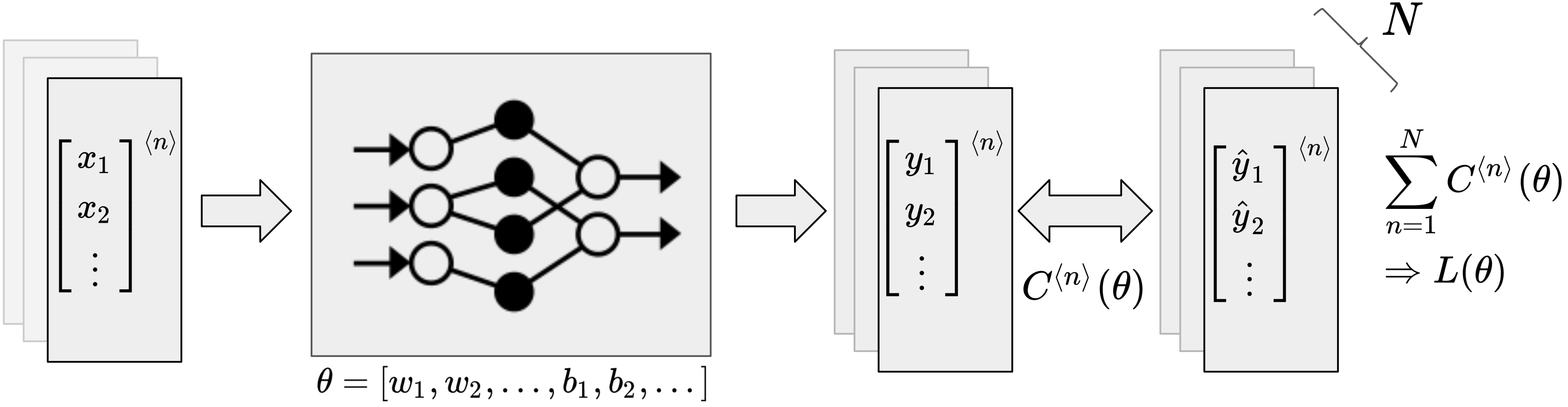


  - Ranking Loss/Margin Loss/Contrastive Loss/Triplet Loss

Workflow for a deep learning project



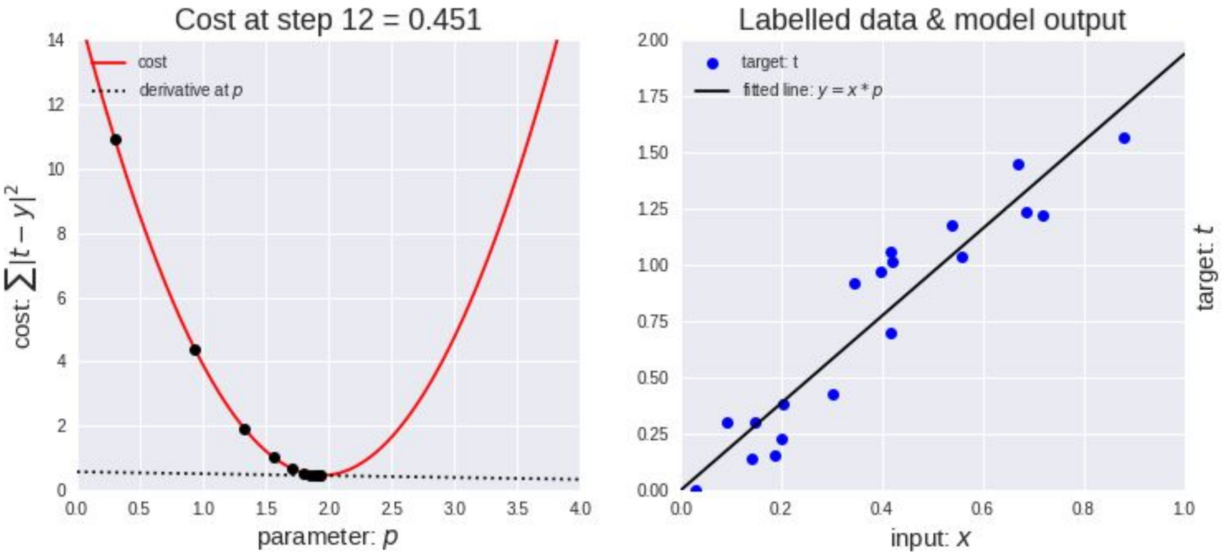
Training a DNN is an optimization problem



- We know how to compute *L(θ)*, analytically or numerically.
- Start from an arbitrary initialization of θ_0, and get an initial $L_0(\theta)$
- Apply optimization algorithm to minimize *L(θ)*

DL Optimization Algorithm

- Gradient Descent (a 1st-order approach) $\theta \longleftarrow \theta - \eta \nabla L(\theta)$
  - Most popular algorithm
    - Pros: simple and fast
    - Cons: sometimes hard to tune



Source Link

Gradient-Descent Optimizers

- Stochastic GD / Mini-Batch GD
- Adding momentum:
  - Classical Momentum (CM)
  - Nesterov's Accelerated Gradient (NAG)
- Adaptive learning rate:
  - AdaGrad, AdaDelta, ...
  - RMSprop
- Combining the two
  - **ADAM** (as **default** in many libs)
- Beyond Adam:
  - Lookahead (2019), RAdam (2019)
  - AdaBound/AmsBound (ICLR 2019)
  - Range (2019)
  - AdaBelief (NeurIPS 2020 Spotlight)

Gradient descent vs Momentum vs AdaGrad vs RMSProp vs Adam

(Source)

Higher Order Optimization Algorithms

- Newton-like methods (2nd-order methods)

$$\theta \longleftarrow \theta - \frac{\ell'(\theta)}{\ell''(\theta)}$$

    - Prons: **fewer** iterations, fewer hyperparameters
    - Cons: much more **costly** in each iteration, more storing
  - DFP/Broyden/BFGS/L-BFGS: a quasi-newton one
    - Good for low dimensional models
  - Conjugate gradient (CG): between GD and Newton
    - moderately high dimensional models

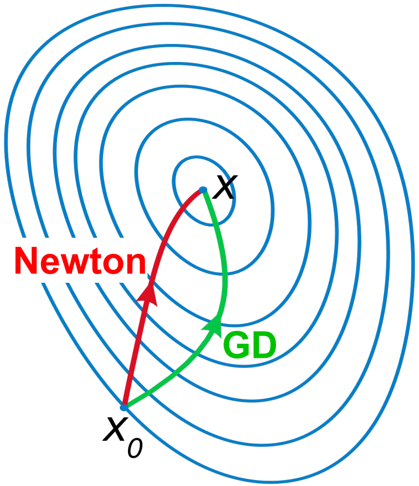
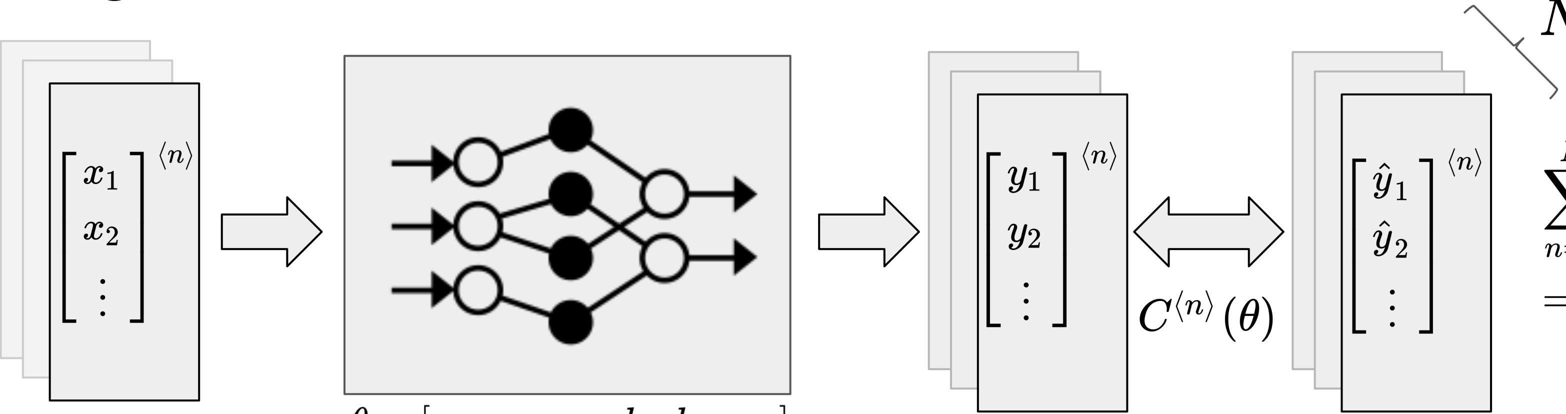


Figure from Wikipedia

- Natural gradient descent methods $\tilde{\nabla}_\theta L(\theta) = F^{-1} \nabla_\theta L(\theta)$
  - K-FAC (Martens and Grosse, 2015)
  - Shampoo (Gupta, et al., 2018)
  - K-BFGS (Goldfarb, et al., NeurIPS 2020)

Using Gradient Descent to train DNN



$$\sum_{n=1}^{N} C^{\langle n \rangle}(\theta)$$
$$\Rightarrow L(\theta)$$

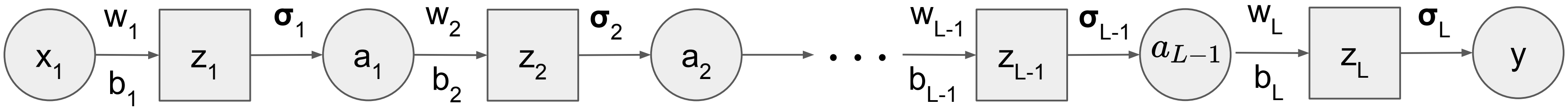
$$\theta = \underbrace{[w_1, w_2, \ldots, b_1, b_2, \ldots]}_{\text{Millions of parameters!}}$$

$$\theta_0 \rightarrow \nabla L(\theta_0) \rightarrow \theta_1 \rightarrow \nabla L(\theta_1) \rightarrow \theta_2 \rightarrow \cdots$$
$$\theta_1 = \theta_0 - \eta \nabla L(\theta_0)$$
$$\theta_2 = \theta_1 - \eta \nabla L(\theta_1)$$
$$\vdots$$

$$\nabla L(\theta) = \sum_{n=1}^{N} \begin{bmatrix} \frac{\partial C^{\langle n \rangle}(\theta)}{\partial w_1} \\ \frac{\partial C^{\langle n \rangle}(\theta)}{\partial w_2} \\ \vdots \\ \frac{\partial C^{\langle n \rangle}(\theta)}{\partial b_1} \\ \vdots \end{bmatrix}$$

How to compute the gradient vector with millions of elements **efficiently?**

Backpropagation: a game of chain rule



$$y = \sigma_L\Big(w_L \cdot \sigma_{L-1}\big(\cdots w_2 \cdot \underbrace{\sigma_1(\underbrace{w_1 \cdot x + b_1}_{z_1})}_{a_1} + b_2\big) + b_L\Big)$$

$$\frac{\partial C\big(y(w)-\hat{y}\big)}{\partial w} = \frac{\partial z}{\partial w}\frac{\partial C}{\partial z} = \frac{\partial z}{\partial w}\left[\frac{\partial a}{\partial z}\frac{\partial C}{\partial a}\right] = \frac{\partial z}{\partial w}\left[\sigma' \cdot \left(\frac{\partial z_{(+1)}}{\partial a}\frac{\partial C}{\partial z_{(+1)}}\right)\right]$$

① Forward Pass

$$\frac{\partial z_1}{\partial w_1} = x_1 \longrightarrow \frac{\partial z_2}{\partial w_2} = a_1 \longrightarrow \cdots \longrightarrow \frac{\partial z_{L-1}}{\partial w_{L-1}} = a_{L-2} \longrightarrow \frac{\partial z_L}{\partial w_L} = a_{L-1}$$

② Backward Pass

$$\frac{\partial C}{\partial z_1} = \sigma_1'\left[w_2\frac{\partial C}{\partial z_2}\right] \longleftarrow \cdots \longleftarrow \frac{\partial C}{\partial z_{L-1}} = \sigma_{L-1}'\left[w_L\frac{\partial C}{\partial z_L}\right] \longleftarrow \frac{\partial C}{\partial z_L} = \sigma_L'\frac{\partial C}{\partial y} \longleftarrow \frac{\partial C}{\partial y}$$

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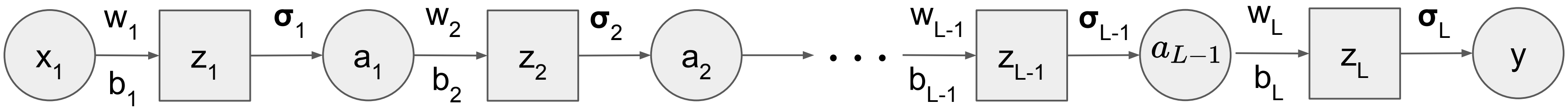
Gradient vanishing/exploding in DL training

- Causes



$$y = \sigma_L\Big(w_L \cdot \sigma_{L-1}\big(\cdots w_2 \cdot \sigma_1(w_1 \cdot x + b_1) + b_2\big) + b_L\Big)$$

After backprop

  - Gradients in initial layers = Multiplication of Gradients at prior layers
  - Small variation around 1 results in vanishing/exploding

- Techniques to resolve:
  - General: adjusting learning rate, dropout, batch normalization, layer normalization
  - For gradient exploding: gradient clipping, weight regularization
  - For gradient vanishing: activation function, proper initialization parameters, LSTM, skip connections

Backprop Beyond Deep Learning

- A different way to calculate the differentiation of iterative math expressions
  - Not approximate, unlike numerical differentiation
  - Exact, like manual or symbolic differentiation, but with constant overhead
- Automatic differentiation (algorithmic differentiation)
  - Problems constructed by differentiable directed graphs (e.g. NN)
  - General functional blocks (FF, conv, recurrent blocks, etc)
  - Modularized optimization: differentiable optimizations in layer levels
- Differentiable physics
  - Physics problems represented by a sequence of differentiable operators
  - Differentiable programming
    - Enables classical numerical algorithms
    - Beyond simple chained transformations to include more complex control structures

Workflow for a deep learning project

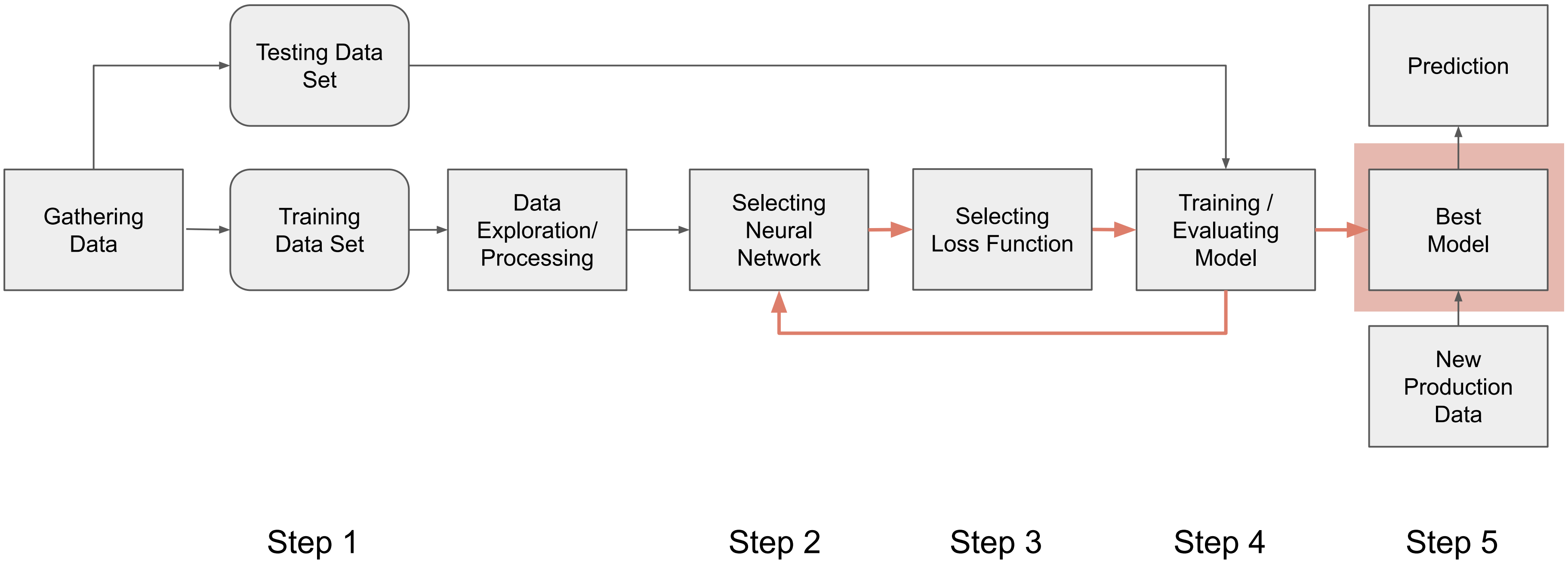


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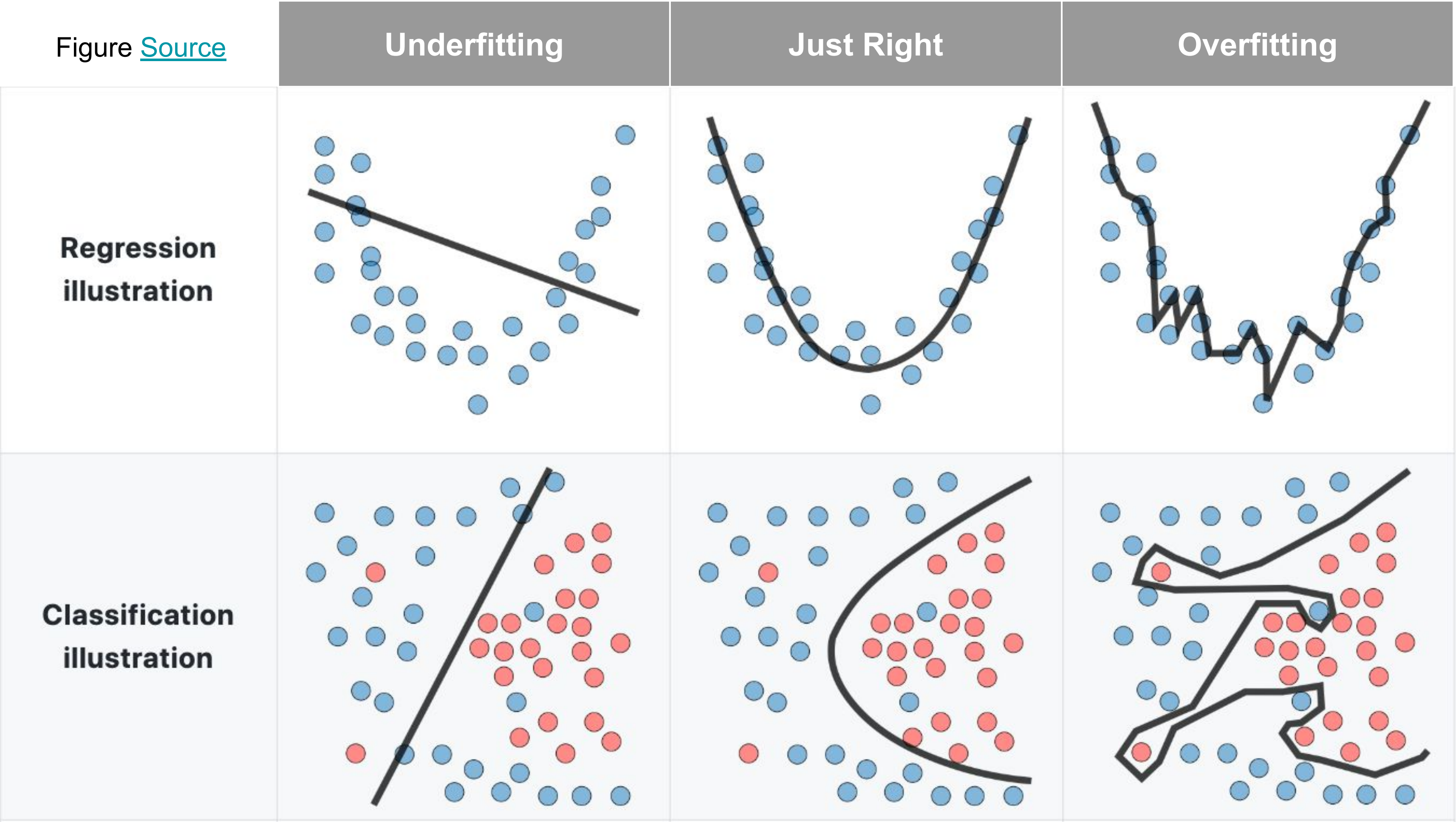
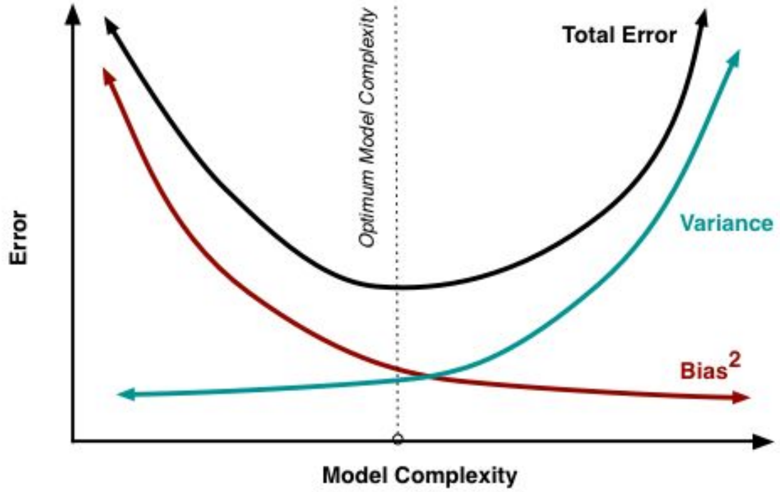
Figure [Source]

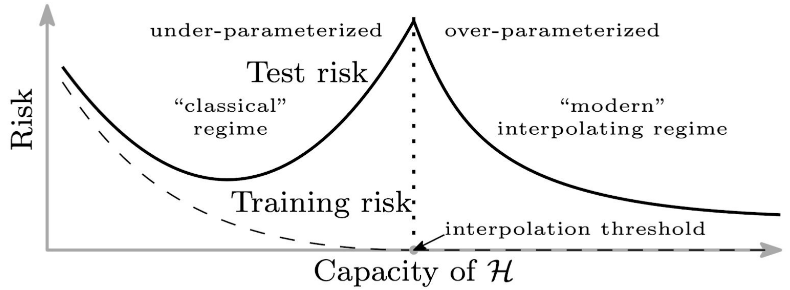


Underfitting and Overfitting

- Underfitting: model too simple:
  - Diagnose:
    - cannot even fit the training data
    - training error ~ testing error
  - Ignore the variance in training data
  - Higher prediction bias

- Overfitting: model too complex
  - Diagnose:
    - well-fit for training data
    - large error for testing data
  - Over-interpret training data
  - More deviation from new data





From Belkin's 2018 paper

How to prevent underfitting?

- Redesign the model
- Increase model's complexity
- Add more features as input
- Training longer
- More data will <u>not</u> help

How to prevent overfitting?

- Get more data
  - Collect more data
  - Data augmentation

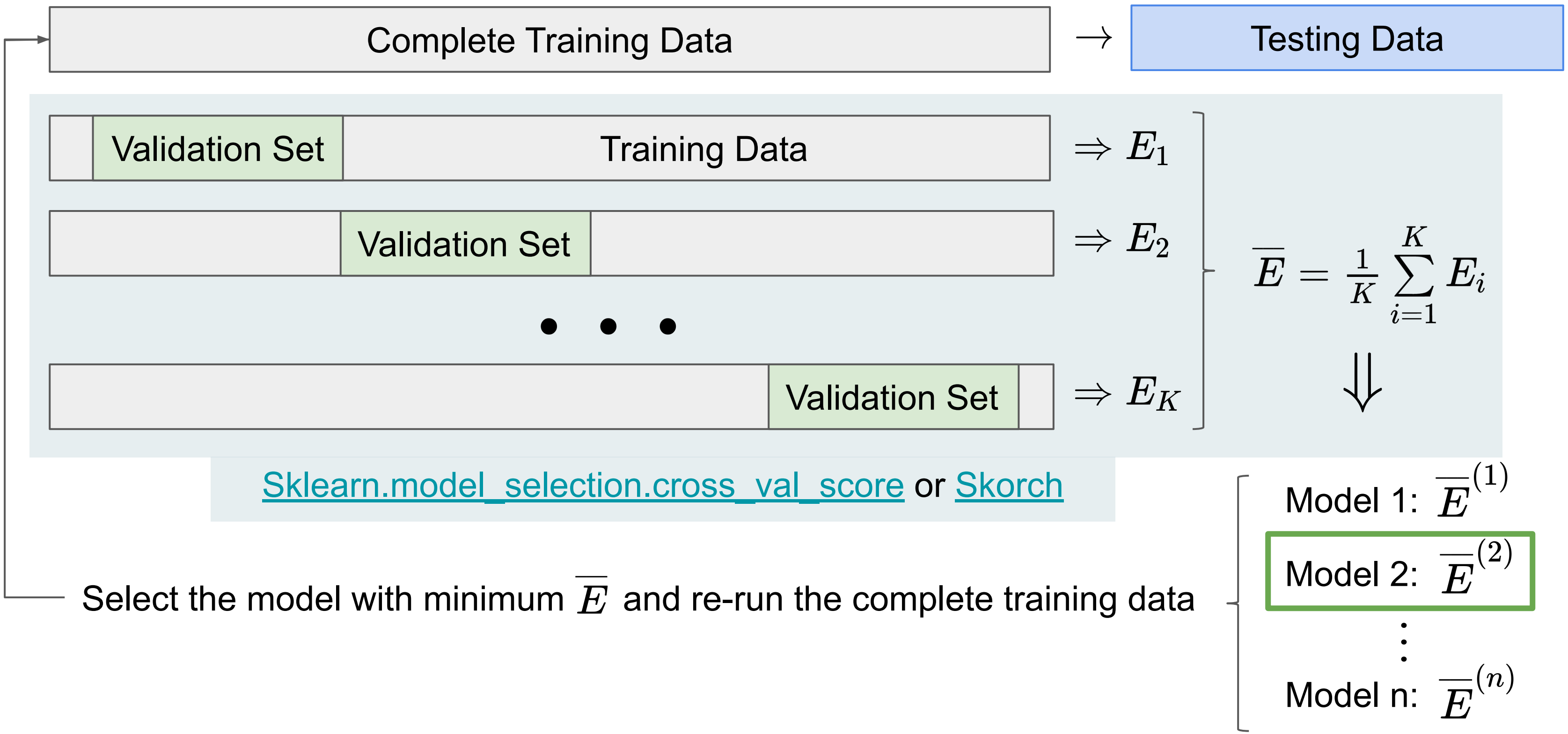
- Reduce the model’s complexity

- Regularization
  - Weight Regularization to make the model smoother (L1, L2, Elastic net)

$$\hat{L}(x, y) = L(x, y) + \lambda \sum_{i=1}^{n} \theta_i^2$$

  - Early stopping

Model Selection: K-fold Cross Validation



Errors/scores in practice

Training Set	Validation Set		Public Testing Set	Private Testing Set

Error: $E^{val} < E^{Pub} < E^{Pri}$

Score: $S^{val} > S^{Pub} > S^{Pri}$

OARC Workshop Survey

https://forms.gle/nbWgNP45qCwZhLRh9