Lectures on Machine Learning

Lecture 1: from artificial intelligence to parameter learning

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University of Milan and INFN Milan (UNIMI)

Why lectures on machine learning?

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- fast development of new tools and algorithms in the past years,
- nowadays it is a requirement in experimental and theoretical physics,
- large interest from the HEP community: *IML, conferences, grants*.

What expect from these lectures?

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- Learn the basis of machine learning techniques.
- Learn when and how to apply machine learning algorithms.

The talk is divided in two lectures:

Lecture 1 (today)

- Artificial intelligence
- Machine learning
- Model representation
- Metrics
- Parameter learning

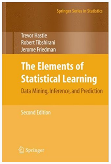
Lecture 2 (tomorrow)

- Non-linear models
- Beyond neural networks
- Clustering
- Cross-validation
- Hyperparameter tune

Some references

Books:

- *The elements of statistical learning*, T. Hastie, R. Tibshirani, J. Friedman.
- *An introduction to statistical learning*, G. James, D. Witten, T. Hastie, R. Tibshirani.
- *Deep learning*, I. Goodfellow, Y. Bengio, A. Courville.



Springer Series in Statistics

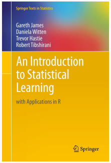
Trevor Hastie
Robert Tibshirani
Jerome Friedman

The Elements of Statistical Learning

Data Mining, Inference, and Prediction

Second Edition

Springer



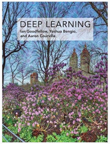
Springer Texts in Statistics

Gareth James
Daniela Witten
Trevor Hastie
Robert Tibshirani

An Introduction to Statistical Learning

with Applications in R

Springer



DEEP LEARNING

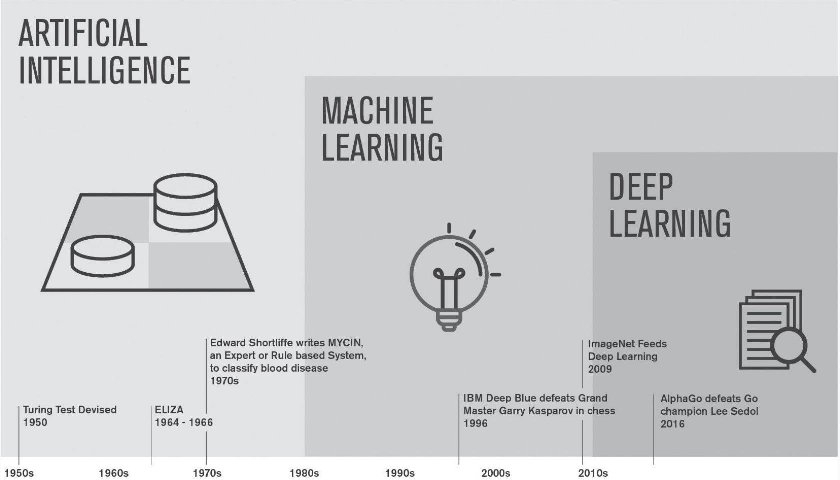
Ian Goodfellow, Yoshua Bengio, and Aaron Courville

Online resources:

- HEP-ML: `https://github.com/iml-wg/HEP-ML-Resources`
- Tensorflow: `http://tensorflow.org`
- Keras: `http://keras.io`
- Scikit: `http://scikit-learn.org`

Artificial Intelligence

Artificial intelligence timeline


ARTIFICIAL INTELLIGENCE
MACHINE LEARNING
DEEP LEARNING
Turing Test Devised 1950
ELIZA 1964 - 1966
Edward Shortliffe writes MYCIN, an Expert or Rule based System, to classify blood disease 1970s
IBM Deep Blue defeats Grand Master Garry Kasparov in chess 1996
ImageNet Feeds Deep Learning 2009
AlphaGo defeats Go champion Lee Sedol 2016
1950s
1960s
1970s
1980s
1990s
2000s
2010s

Defining A.I.

Artificial intelligence (A.I.) is *the science and engineering of making intelligent machines*. (John McCarthy ‘56)

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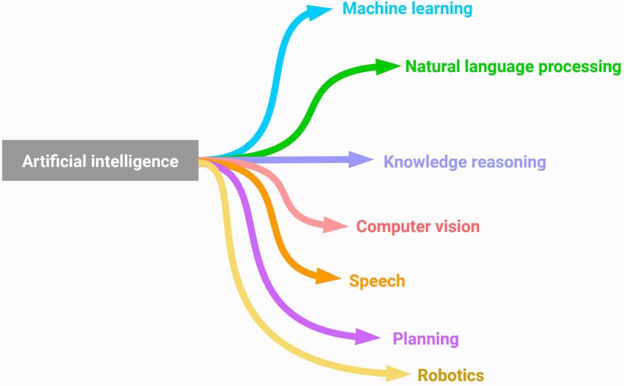
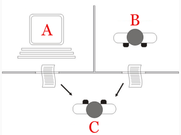


A.I. consist in the development of computer systems to perform tasks commonly associated with intelligence, such as *learning*.

A.I. and humans

There are two categories of A.I. tasks:

- **abstract and formal:** easy for computers but difficult for humans, *e.g.* play chess (IBM's Deep Blue 1997).
  → *Knowledge-based* approach to artificial intelligence.



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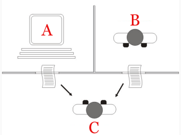

- **intuitive for humans but hard to describe formally:** *e.g.* recognizing faces in images or spoken words.
  → *Concept* capture and generalization

A.I. technologies

Historically, the *knowledge-based* approach has not led to a major success with intuitive tasks for humans, because:

- requires human *supervision* and hard-coded *logical inference rules*.
- lacks of *representation learning* ability.

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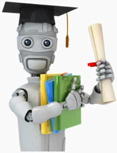
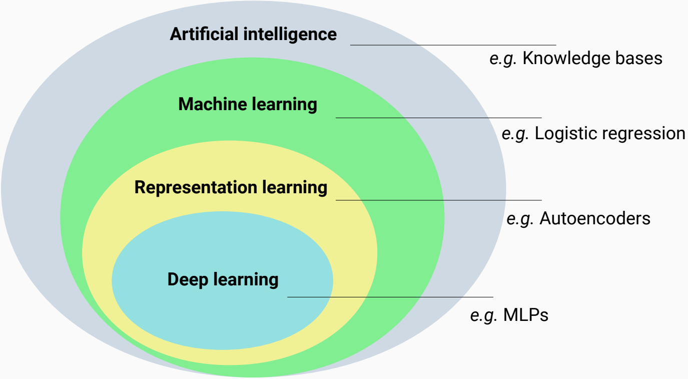
- lacks of *representation learning* ability.

Solution:

The A.I. system needs to *acquire its own knowledge*. This capability is known as **machine learning** (ML).
→ *e.g.* write a program which learns the task.



Venn diagram for A.I.



When a representation learning is difficult, ML provides **deep learning** techniques which allow the computer to build complex concepts out of simpler concepts, *e.g.* artificial neural networks (MLP).

Machine Learning

Machine learning definition

Definition from A. Samuel in 1959:
Field of study that gives computers the ability to learn without being explicitly programmed.

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Definition from T. Mitchell in 1998:
A computer program is said to *learn* from experience E with respect to some class of tasks T and performance measure P, if its performance on T, as measured by P, improves with experience E.

Machine learning examples

Thanks to work in A.I. and new capability for computers:

- **Database mining:**
  - Search engines
  - Spam filters
  - Medical and biological records

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    - Autonomous driving
    - Natural language processing
    - Robotics (reinforcement learning)
    - Game playing (DQN algorithms)

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- **Human learning:**
  - Concept/human recognition
  - Computer vision
  - Product recommendation

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Vitamin C and cancer cell metabolism pp. 1317 & 1391
In search of stem cells p. 1319
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sciencemag.org
AAAS
Machine intelligence
AI learns to read and write letters p. 1332

ML applications in HEP

ML in experimental HEP

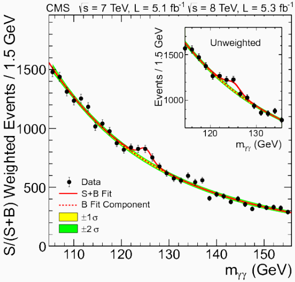
There are many applications in experimental HEP involving the **LHC measurements**, including the **Higgs discovery**, such as:

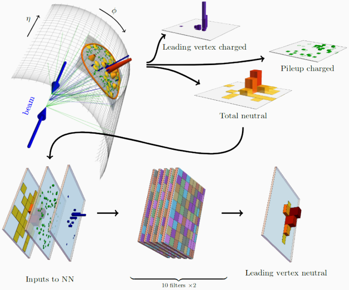
- Tracking
- Fast Simulation
- Particle identification
- Event filtering

ML in experimental HEP

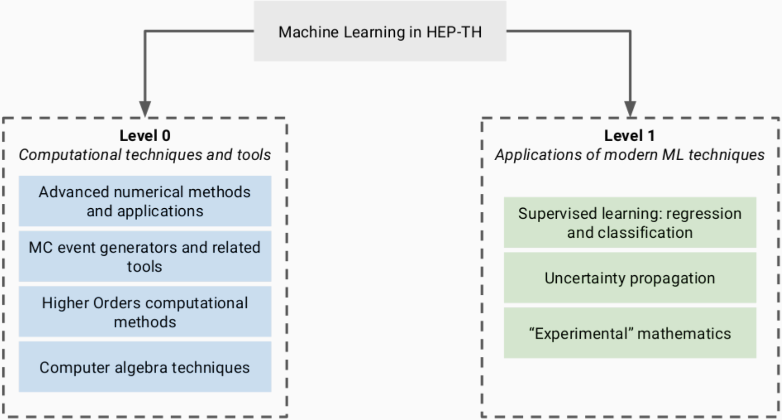
Some remarkable examples are:

- **Signal-background detection:**
  Decision trees, artificial neural networks, support vector machines.
- **Jet discrimination:**
  Deep learning imaging techniques via convolutional neural networks.
- **HEP detector simulation:**
  Generative adversarial networks, *e.g.* LAGAN and CaloGAN.





ML in theoretical HEP



Machine Learning in HEP-TH

Level 0
Computational techniques and tools

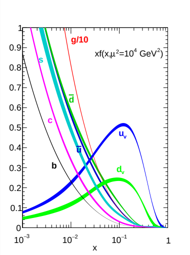
- Advanced numerical methods and applications
- MC event generators and related tools
- Higher Orders computational methods
- Computer algebra techniques

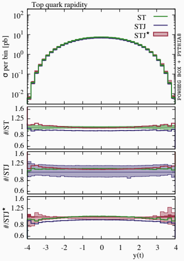
Level 1
Applications of modern ML techniques

- Supervised learning: regression and classification
- Uncertainty propagation
- "Experimental" mathematics

ML in theoretical HEP

- **Supervised learning:**
  - The structure of the proton at the LHC
    - parton distribution functions
  - Theoretical prediction and combination
  - Monte Carlo reweighting techniques
    - neural network Sudakov
  - BSM searches and exclusion limits
- **Unsupervised learning:**
  - Jet physics
    - GANs and CycleGANs for jet reconstruction
  - Clustering and compression
    - PDF4LHC15 recommendation
  - Density estimation and anomaly detection
    - Monte Carlo sampling
- **Reinforcement learning:**
  - Jet grooming

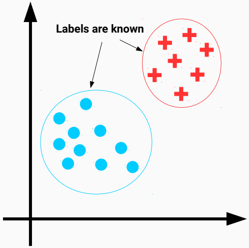


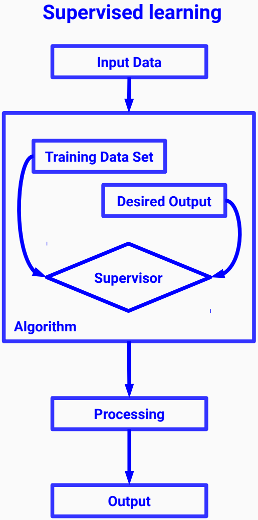


Machine learning algorithms

Machine learning algorithms:

- Supervised learning:
  regression, classification, ...

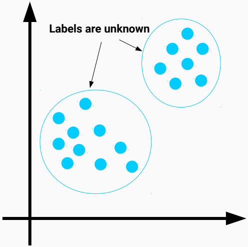




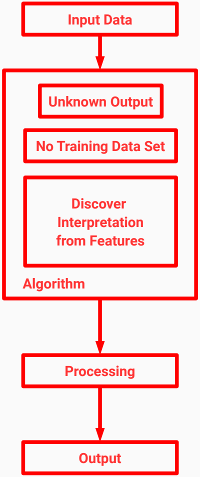
Machine learning algorithms

Machine learning algorithms:

- Supervised learning: regression, classification, ...
- Unsupervised learning: clustering, dim-reduction, ...



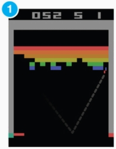
Unsupervised learning

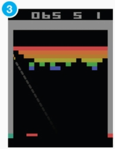


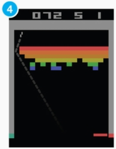
Machine learning algorithms

Machine learning algorithms:

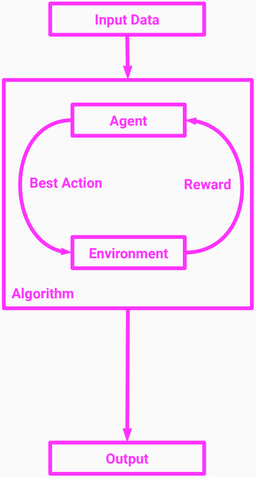
- Supervised learning:
  regression, classification, ...
- Unsupervised learning:
  clustering, dim-reduction, ...
- Reinforcement learning:
  real-time decisions, ...



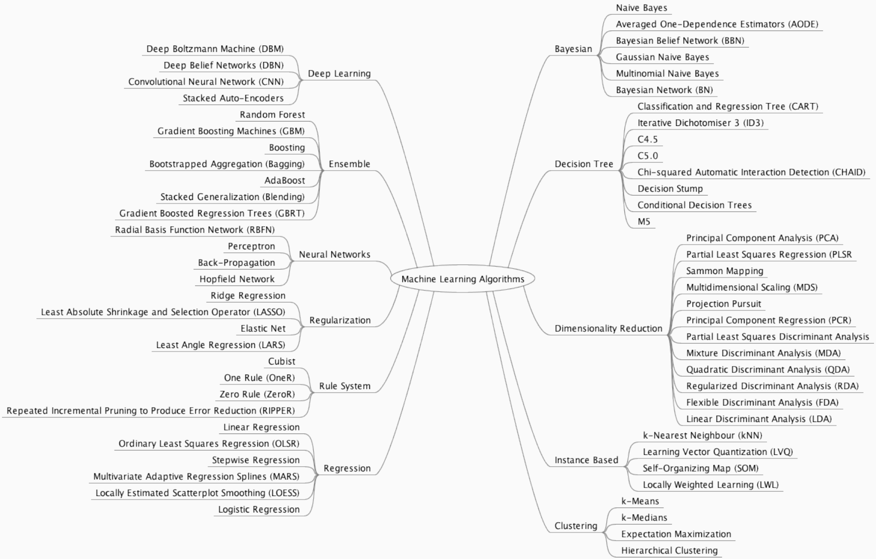




Reinforcement learning



Machine learning algorithms

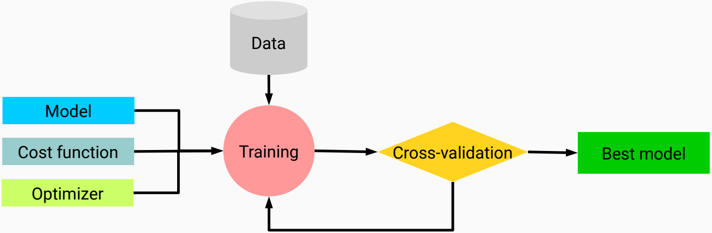


- Machine Learning Algorithms
  - Deep Learning
    - Deep Boltzmann Machine (DBM)
    - Deep Belief Networks (DBN)
    - Convolutional Neural Network (CNN)
    - Stacked Auto-Encoders
  - Ensemble
    - Random Forest
    - Gradient Boosting Machines (GBM)
    - Boosting
    - Bootstrapped Aggregation (Bagging)
    - AdaBoost
    - Stacked Generalization (Blending)
    - Gradient Boosted Regression Trees (GBRT)
  - Neural Networks
    - Radial Basis Function Network (RBFN)
    - Perceptron
    - Back-Propagation
    - Hopfield Network
  - Regularization
    - Ridge Regression
    - Least Absolute Shrinkage and Selection Operator (LASSO)
    - Elastic Net
    - Least Angle Regression (LARS)
  - Rule System
    - Cubist
    - One Rule (OneR)
    - Zero Rule (ZeroR)
    - Repeated Incremental Pruning to Produce Error Reduction (RIPPER)
  - Regression
    - Linear Regression
    - Ordinary Least Squares Regression (OLSR)
    - Stepwise Regression
    - Multivariate Adaptive Regression Splines (MARS)
    - Locally Estimated Scatterplot Smoothing (LOESS)
    - Logistic Regression
  - Bayesian
    - Naive Bayes
    - Averaged One-Dependence Estimators (AODE)
    - Bayesian Belief Network (BBN)
    - Gaussian Naive Bayes
    - Multinomial Naive Bayes
    - Bayesian Network (BN)
  - Decision Tree
    - Classification and Regression Tree (CART)
    - Iterative Dichotomiser 3 (ID3)
    - C4.5
    - C5.0
    - Chi-squared Automatic Interaction Detection (CHAID)
    - Decision Stump
    - Conditional Decision Trees
    - M5
  - Dimensionality Reduction
    - Principal Component Analysis (PCA)
    - Partial Least Squares Regression (PLSR
    - Sammon Mapping
    - Multidimensional Scaling (MDS)
    - Projection Pursuit
    - Principal Component Regression (PCR)
    - Partial Least Squares Discriminant Analysis
    - Mixture Discriminant Analysis (MDA)
    - Quadratic Discriminant Analysis (QDA)
    - Regularized Discriminant Analysis (RDA)
    - Flexible Discriminant Analysis (FDA)
    - Linear Discriminant Analysis (LDA)
  - Instance Based
    - k-Nearest Neighbour (kNN)
    - Learning Vector Quantization (LVQ)
    - Self-Organizing Map (SOM)
    - Locally Weighted Learning (LWL)
  - Clustering
    - k-Means
    - k-Medians
    - Expectation Maximization
    - Hierarchical Clustering

More than 60 algorithms.

Workflow in machine learning

The operative workflow in ML is summarized by the following steps:

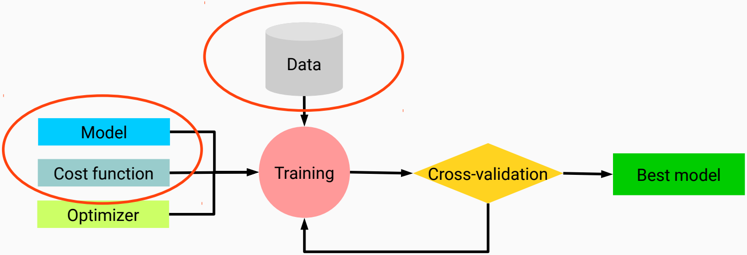


The best model is then used to:

- supervised learning: make predictions for new observed data.
- unsupervised learning: extract features from the input data.

Models and metrics

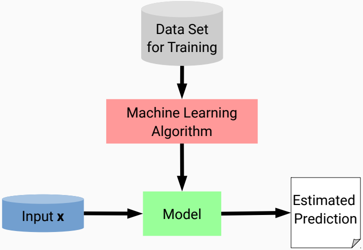
Models and metrics



Model representation in supervised learning

We define parametric and structure models for statistical inference:

- **examples:** linear models, neural networks, decision tree...



- Given a training set of input-output pairs $A = (x_1, y_1), \ldots, (x_n, y_n)$.
- Find a model $\mathcal{M}$ which:

$$\mathcal{M}(\boldsymbol{x}) \sim \boldsymbol{y}$$

where $\boldsymbol{x}$ is the input vector and $\boldsymbol{y}$ discrete labels in classification and real values in regression.

Model representation in supervised learning

Examples of models:

$\rightarrow$ linear regression we define a vector $\boldsymbol{x} \in \mathbb{R}^n$ as input and predict the value of a scalar $y \in \mathbb{R}$ as its output:

$$\hat{y}(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x} + b$$

where $\boldsymbol{w} \in \mathbb{R}^n$ is a vector of parameters and b a constant.

Model representation in supervised learning

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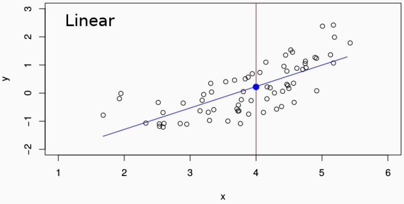
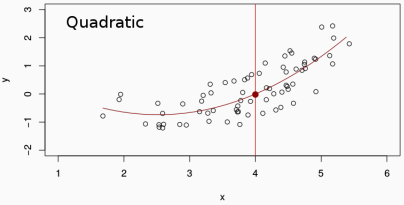
→ Generalized linear models are also available increasing the power of linear models:





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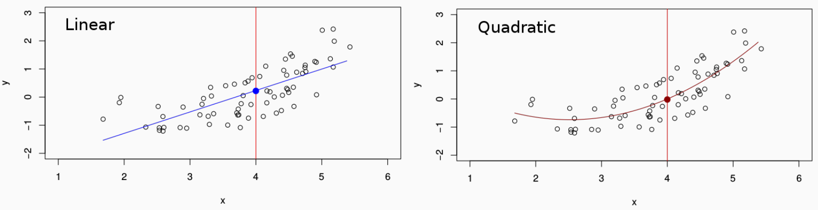
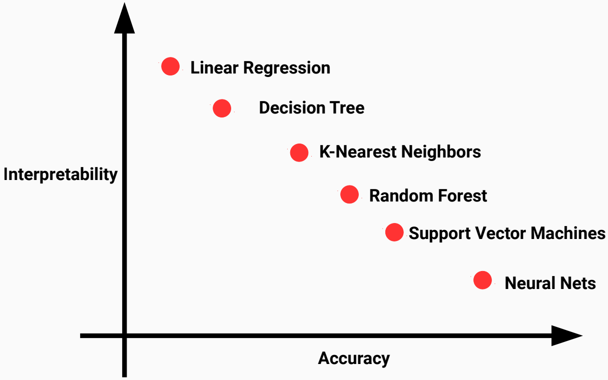


→ Non-linear models: neural networks (talk later).

Model representation trade-offs

However, the selection of the appropriate model comes with trade-offs:

- **Prediction accuracy vs interpretability**:
  → *e.g.* linear model vs splines or neural networks.



Model representation trade-offs

However, the selection of the appropriate model comes with trade-offs:

- **Prediction accuracy vs interpretability**:
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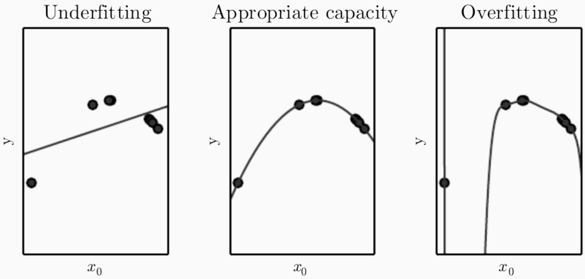
- **Optimal capacity/flexibility:** number of parameters, architecture
  → deal with overfitting, and underfitting situations



Assessing the model performance

How to check model performance?

→ define metrics and statistical estimators for model performance.

Examples:

- Regression: cost / loss / error function,
- Classification: cost function, precision, accuracy, recall, ROC, AUC

Assessing the model performance - cost function

To access the model performance we define a cost function $J(\boldsymbol{w})$ which often measures the difference between the target and the model output.

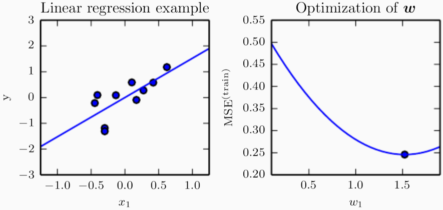
In a optimization procedure, given a model $\hat{y}_{\boldsymbol{w}}$, we search for:

$$\arg\min_{\boldsymbol{w}} J(\boldsymbol{w})$$

The mean square error (MSE) is the most commonly used for regression:

$$J(\boldsymbol{w}) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_{\boldsymbol{w}}(\boldsymbol{x}_i))^2$$

a quadratic function and convex function in linear regression.



Assessing the model performance - cost function

Other cost functions are depending on the nature of the problem.

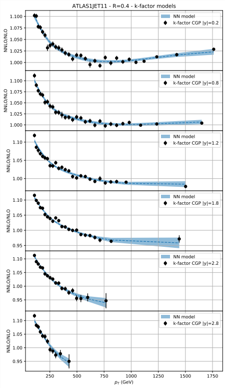
Some other examples:

- regression with uncertainties, chi-square:

$$J(\boldsymbol{w}) = \sum_{i,j=1}^{n} (y_i - \hat{y}_{\boldsymbol{w}}(\boldsymbol{x}_i))(\sigma^{-1})_{ij}(y_j - \hat{y}_{\boldsymbol{w}}(\boldsymbol{x}_j))$$

  where:

  - σ_{ij} is the data covariance matrix. *e.g.* for LHC data experimental statistical and systematics correlations.

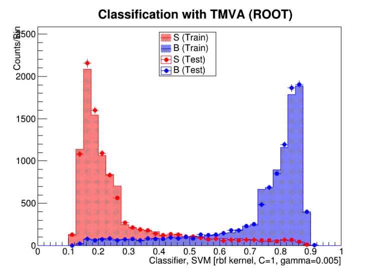


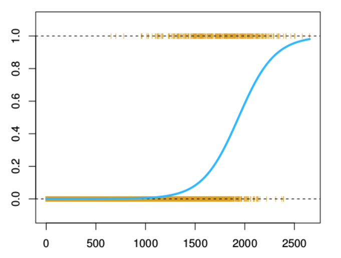
Assessing the model performance - cost function

- logistic regression (binary classification): cross-entropy

$$J(\boldsymbol{w}) = -\frac{1}{n}\sum_{i=1}^{n} y_i \log \hat{y}_{\boldsymbol{w}}(\boldsymbol{x}_i) + (1-y_i)\log(1-\hat{y}_{\boldsymbol{w}}(\boldsymbol{x}_i))$$

where $\hat{y}_{\boldsymbol{w}}(\boldsymbol{x}_i) = 1/(1+e^{-\boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{x}_i})$.

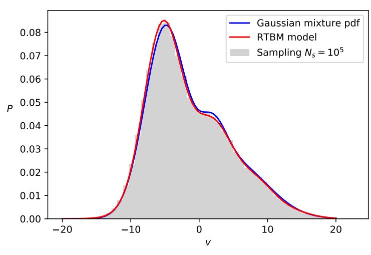


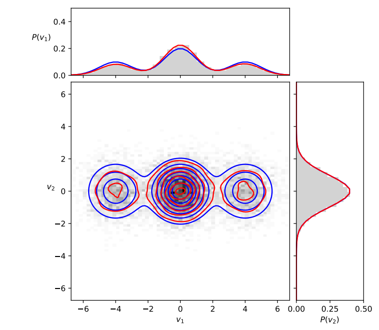


Assessing the model performance - cost function

- density estimate / regression: negative log-likelihood:

$$J(\boldsymbol{w}) = -\sum_{i=1}^{n} \log(\hat{y}_{\boldsymbol{w}}(\boldsymbol{x}_i))$$





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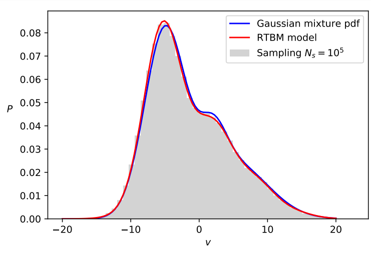

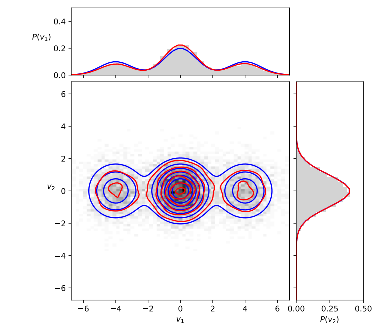

- Kullback-Leibler, RMSE, MAE, etc.

Training and test sets

Another common issue related to model capacity in supervised learning:

- The model should not learn **noise** from data.
- The model should be able to **generalize** its output to new samples.

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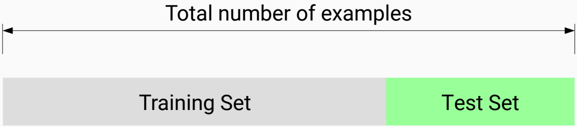
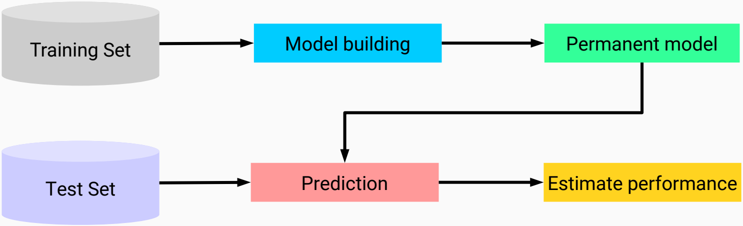
To observe this issue we split the input data in training and test sets:

- training set error, $J_{\mathrm{Tr}}(\boldsymbol{w})$
- test set/generalization error, $J_{\mathrm{Test}}(\boldsymbol{w})$



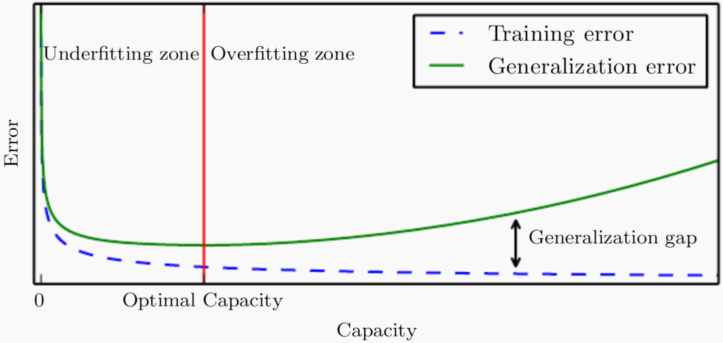
Training and test sets

The test set is independent from the training set but follows the same probability distribution.



Bias-variance trade-off

From a practical point of view dividing the input data in training and test:



The training and test/generalization error conflict is known as bias-variance trade-off.

Bias-variance trade-off

Supposing we have model $\hat{y}(\boldsymbol{x})$ determined from a training data set, and considering as the true model

$$Y = y(X) + \epsilon, \text{ with } y(x) = E(Y|X = x),$$

where the noise ϵ has zero mean and constant variance.

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If we take (x_0, y_0) from the test set then:

$$E[(y_0 - \hat{y}(x_0))^2] = \left(\mathrm{Bias}[\hat{y}(x_0)]\right)^2 + \mathrm{Var}[\hat{y}(x_0)] + \mathrm{Var}(\epsilon),$$

where

- $\mathrm{Bias}[\hat{y}(x_0)] = E[\hat{y}(x_0)] - y(x_0)$
- $\mathrm{Var}[\hat{y}(x_0)] = E[\hat{y}(x_0)^2] - \left(E[\hat{y}(x_0)]\right)^2$

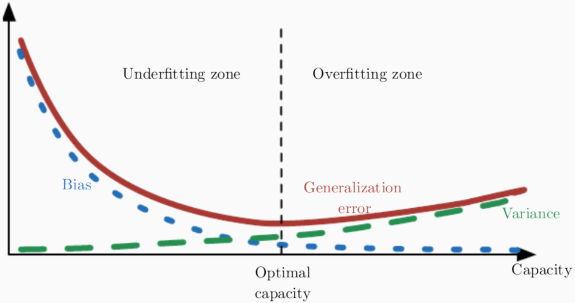
So, the expectation averages over the variability of y_0 (bias) and the variability in the training data.

Bias-variance trade-off

If $\hat{y}$ increases **flexibility**, its variance increases and its biases decreases.

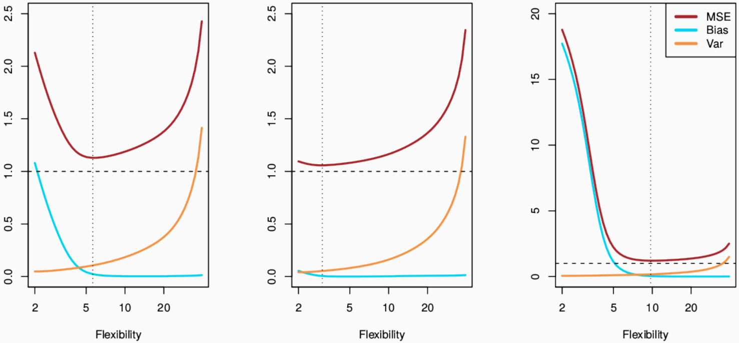
Choosing the flexibility based on average test error amounts to a bias-variance trade-off:

- **High Bias** → underfitting:
  erroneous assumptions in the learning algorithm.
- **High Variance** → overfitting:
  erroneous sensitivity to small fluctuations (noise) in the training set.



Bias-variance trade-off

More examples of bias-variance trade-off:



Bias-variance trade off

Regularization techniques can be applied to modify the learning algorithm and reduce its generalization error but not its training error.

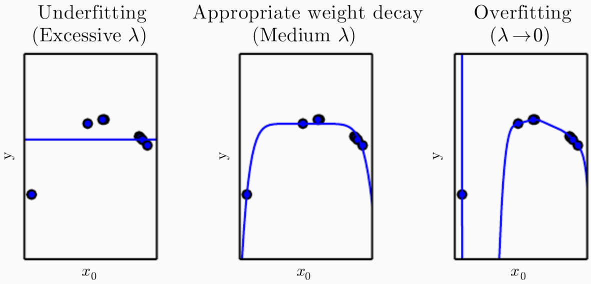
For example, including the weight decay to the MSE cost function:

$$J(\boldsymbol{w}) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_{\boldsymbol{w}}(\boldsymbol{x}_i))^2 + \lambda \boldsymbol{w}^T \boldsymbol{w}.$$

where λ is a real number which express the preference for weights with smaller squared L^2 norm.

Solution for the bias-variance trade off

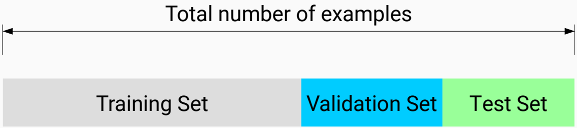
Tuning the hyperparameter λ we can regularize a model without modifying explicitly its capacity.



Solution for the bias-variance trade off

A common way to reduce the bias-variance trade-off and choose the proper learning hyperparamters is to create a validation set that:

- not used by the training algorithm
- not used as test set



Total number of examples

Training Set

Validation Set

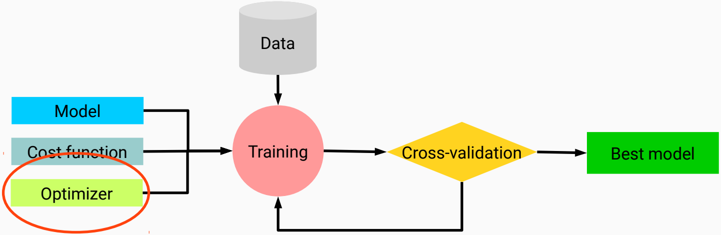
Test Set

- **Training set**: examples used for learning.
- **Validation set**: examples used to tune the hyperparameters.
- **Test set**: examples used only to access the performance.

Techniques are available to deal with data samples with large and small number of examples. (talk later)

Parameter learning

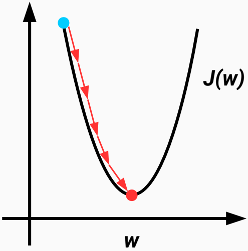
Parameter learning



Cost function minimization

Optimization algorithms **minimize an objective function**, $J(\boldsymbol{w})$, that depends on the model internal learnable parameters $\boldsymbol{w}$.

$$\arg\min_{\boldsymbol{w}} J(\boldsymbol{w})$$



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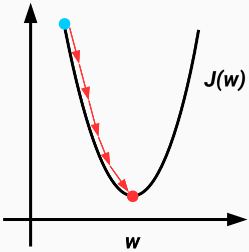

$$\arg\min_{\boldsymbol{w}} J(\boldsymbol{w})$$

The most popular techniques are:

- normal equations (least squares)
- derivative based optimization
- evolutionary algorithms

The choice of a technique depends on the model and problem employed.

Normal equations

The normal equation is a method to solve for $\boldsymbol{w}$ analytically.

- it is employed in linear and non-linear least squares optimization.
- it is fast for small models with few features, otherwise it can be computationally intensive and slow.

Normal equations example

Example: multivariate linear regression.

Suppose we have m training examples and n features in a matrix X, size (m, n), and the observed values $\boldsymbol{y}$ we have to solve the system:

$$X\boldsymbol{w} = \boldsymbol{y}$$

How to solve it when the system if overdetermined?

Normal equations example

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3. We obtain the solution:

$$\boldsymbol{w} = (X^T X)^{-1} X^T \boldsymbol{y} = X^+ \boldsymbol{y}$$

   with X^+ is the pseudoinverse of X.

Derivative based optimization

More general optimization algorithms based on derivatives:

- **First order optimization algorithms:** uses the gradient of the cost function with respect to the parameters in a iteractive procedure.
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In practice Gradient Descent is the most popular technique in ML.

Which method?

Q: normal equation or derivative based?

Suppose we have $\boldsymbol{m}$ training examples and $\boldsymbol{n}$ features.

Normal equation

- ✓ no parameters to tune
- ✓ no iterations
- ✗ slow if n is large
- ✗ requires $(X^T X)^{-1}, \mathcal{O}(n^3)$

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Normal equation

✓ no parameters to tune

✓ no iterations

✗ slow if n is large

✗ requires $(X^T X)^{-1}, \mathcal{O}(n^3)$

Gradient descent

✓ efficient when n is large

✓ easy to implement/use

✗ requires iterations

✗ requires parameter tune

Gradient descent idea

Basic idea:
Assuming we want to minimize $J(\boldsymbol{w})$ where $\boldsymbol{w}$ is a vector of parameters:

- select a initial solution vector $\boldsymbol{w}$,
- change the $\boldsymbol{w}$ to reduce $J(\boldsymbol{w})$

Repeat until a minimum of $J(\boldsymbol{w})$ is reached.

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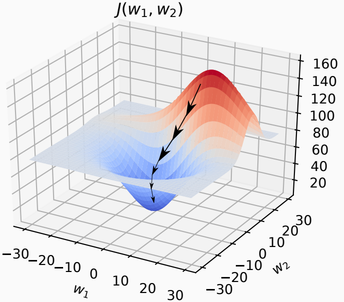

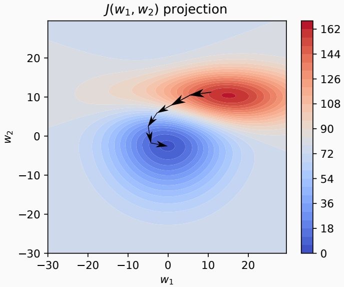

Gradient descent algorithm

Simultaneously for each parameter in $\boldsymbol{w}$ repeat until convergence:

$$w_i := w_i - \eta \frac{\partial}{\partial w_i} J(\boldsymbol{w})$$

where

- η is the learning rate.

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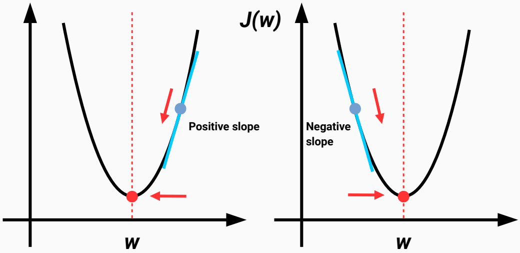
Why the negative sign in term $-\eta$? (example in 1D)

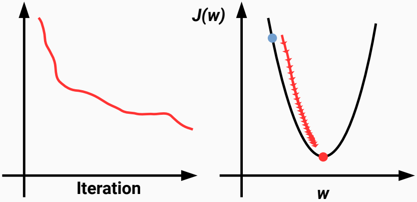


- if $\nabla_w J(w) > 0$ then w decreases
- if $\nabla_w J(w) < 0$ then w increases

Gradient descent and learning rate

The η is another example of hyperparameter which requires tune.

- if η is **too small**, gradient descent can be slow.



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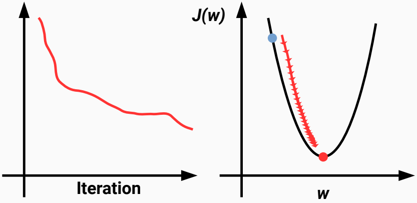

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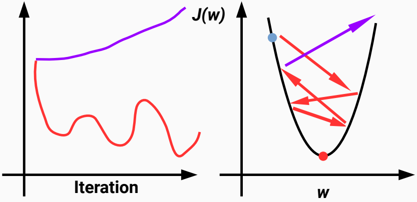

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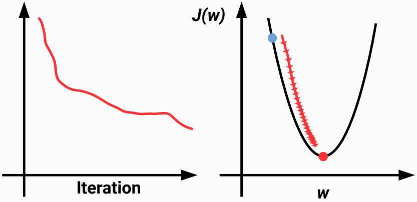

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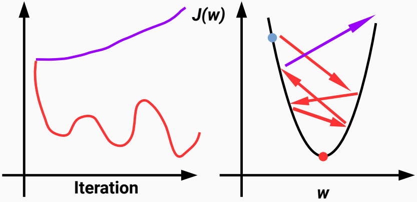


- Practical hint, start with small η values and then increase slowly.

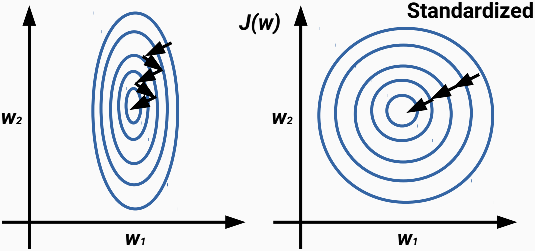
Gradient descent and feature scaling

Another practical hint: **feature scaling**.

Make sure the input features x_i are in a similar scale, *e.g.* standardization:

$$x_i := \frac{x_i - \mu_{x_i}}{\sigma_{x_i}}$$

where μ_{x_i} and σ_{x_i} are the mean and standard deviation respectively.



Gradient descent variants

When performing gradient descent the cost function $J(\boldsymbol{w})$ is evaluated over the training data, *e.g.* for the MSE cost function:

$$\frac{\partial}{\partial \boldsymbol{w}} J(\boldsymbol{w}) = \frac{\partial}{\partial \boldsymbol{w}} \left(\frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_{\boldsymbol{w}}(\boldsymbol{x}_i))^2 \right).$$

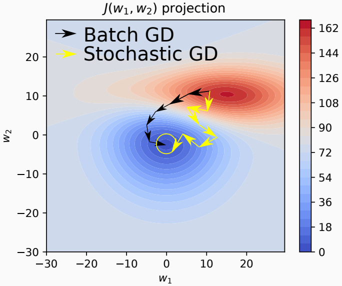
If the training data set is too large, there are gradient descent variations that may improve convergence in terms of speed and quality:

- Batch Gradient Descent: all training data points are evaluated in the cost function gradient at each iteration.

Gradient descent variants

- Stochastic Gradient Descent (SGD):
  1. randomly shuffle training examples,
  2. use 1 example at each iteration.

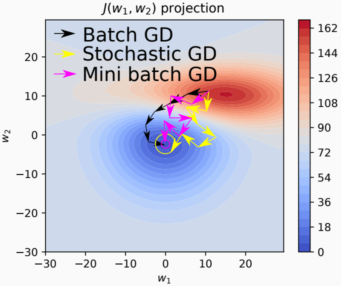
  Features:
  - parameters updates have high variance and cost function fluctuates.
  - helps to discover new and possibly better minima.
  - requires to slowly decrease the learning rate η to reduce fluctuations.



Gradient descent variants

- Mini Batch Gradient Descent:
  1. use a subset of size b (batch size) of examples in each iteration,
  2. use the batch set example at each iteration.

  Features:
  - takes the best from both previous methods,
  - reduces the variance in the parameter updates (stable convergence),
  - good for data parallelism, efficient for matrix operations



Gradient descent schemes

SGD has many improvements and extensions, for example:

- Momentum: it stores the update $\Delta \boldsymbol{w}$ at each iteration and update parameters following:

$$\boldsymbol{w} := \boldsymbol{w} - \eta \nabla_{\boldsymbol{w}} J(\boldsymbol{w}) + \alpha \Delta \boldsymbol{w}$$

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All these schemes and respective parameters can be considered as extra hyperparameters to tune.

Examples of second order optimization

Popular examples of second order optimization algorithms:

- Newton's method: an iterative method based on Taylor expansion.
  Example in 1D: consider the Taylor expansion

  $$J_T(w) = J_T(w_n + \Delta w) \approx J(w_n) + J'(w_n)\Delta w + \frac{1}{2}J''(w_n)\Delta w^2$$

  We aim to find Δw which satisfies:

  $$\nabla_{\Delta w} J_T(w_n + \Delta w) = J'(w_n) + J''(w_n)\Delta w = 0$$

  $$w_{n+1} = w_n + \Delta w = w_n - \frac{J'(w_n)}{J''(w_n)}$$

  $w_1, w_2, \ldots$ will converge to a stationary point w^* where $J'(w^*) = 0$.

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  $w_1, w_2, \ldots$ will converge to a stationary point w^* where $J'(w^*) = 0$.
  Generalization in N dimensions:

  $$(\boldsymbol{H} J(\boldsymbol{w_n}))\boldsymbol{\Delta w} = -\nabla J(\boldsymbol{w}_n)$$

  where $\boldsymbol{H}$ is the Hessian matrix.

Examples of second order optimization

Popular examples of second order optimization algorithms:

- Quasi-newton methods: *i.e.* methods which optimizes even if the Hessian matrix is expensive or not available. The Taylor's series is:

  $$J(\boldsymbol{w}_n + \Delta \boldsymbol{w}) \approx J(\boldsymbol{w}_n) + \nabla_{\boldsymbol{w}} J(\boldsymbol{w}_n)^T \Delta \boldsymbol{w} + \frac{1}{2} \Delta \boldsymbol{w}^T B \Delta \boldsymbol{w},$$

  where B is an approximation to the Hessian matrix and

  $$\nabla_{\boldsymbol{w}} J(\boldsymbol{w}_n + \Delta \boldsymbol{w}) \approx \nabla_{\boldsymbol{w}} J(\boldsymbol{w}_n) + B \Delta \boldsymbol{w},$$

  which produces the Newton step:

  $$\Delta \boldsymbol{w} = -B^{-1} \nabla_{\boldsymbol{w}} J(\boldsymbol{w}_n).$$

  Some methods: BFGS, L-BFGS, DFP, Broyden.

  - differ by the choice of the solution to update B.

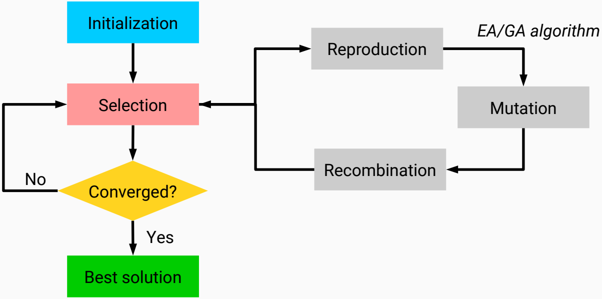
Popular in ML since the beginning of the deep learning era.

Evolutionary algorithms

Evolutionary algorithms (EA), inspired by biological evolution, is a generic population-based metaheuristic optimization algorithm.

Techniques in EA use mechanisms such as: reproduction, mutation, recombination, and selection.

Genetic algorithm is the most popular technique of EA.

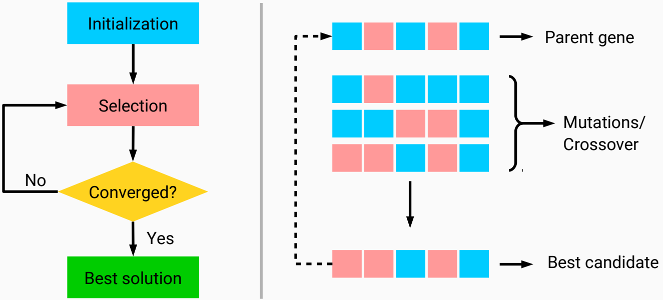


Genetic algorithm

Genetic algorithm is well suited when:

- gradients are not available,
- non parametric function,
- non homogeneous cost function along all training set points.

Example:



Questions?