Third dimension: Data x Space Complexity

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Outline and Structure

1. Handling of NP-Hardness
2. Data space properties and Space complexity
3. Function Approximation and Approximate Representation
4. External penalty method

Motivations: Why do we need to understand Complexity ?

- The performance of an algorithm influences the execution of the program. Hence, understanding the complexity of an algorithm is significant
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  - Estimate space complexity or storage : memory required for the algorithm
    $\Rightarrow$ Execute the algorithm with the optimized data resources
  - Estimate time complexity : running time taken by the algorithm to produce the output (results)
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Two criteria to evaluate performance of algorithms (wrt approximation ratio): complexity in space vs. time

- **Space Complexity** of an algorithm : amount of memory it needs to run to completion.
- **Time Complexity** of an algorithm : amount of CPU time it needs to run to completion

Space complexity

Memory space S(P) needed by a program P, consists of two components

1. A fixed part: fixed elements/components

   $\rightarrow$ fixed space requirements (C) : Independent of the characteristics of the inputs and outputs

   - needed for instruction space (byte code)
   - space for simple variables, fixed-size structured variable, constants
     $\Rightarrow$ comprises variables, and constants used in the program

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2. A variable part : changeable elements/components

   → variable space (Sp): dependent on a particular instance (I)

   - Number, size, values of inputs and outputs associated with instance I
   - Refers to the program size: recursive stack space, formal parameters, local variables, return address

$$\boxed{S(P) = c + Sp(instance)}$$

Time complexity

Time required T(P) to run a program P also consists of two components:

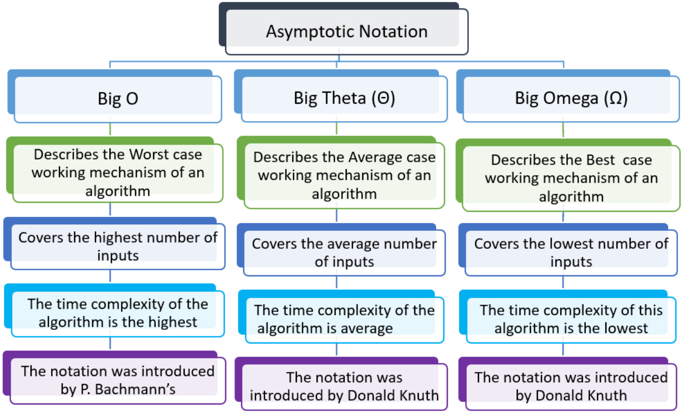
1. A fixed part (c): compile time which is independent of the problem instance
2. A variable part (Tp): run time which depends on the problem instance

$$\boxed{T(P) = c + Tp(instance)}$$

Asymptotic notation

Asymptotic notation

- analytical tool used to describe the execution of an algorithm considering its input values
- facilitate the comparative analysis of algorithms without considering their constants and input variables


Asymptotic Notation
Big O
Big Theta (Θ)
Big Omega (Ω)
Describes the Worst case working mechanism of an algorithm
Describes the Average case working mechanism of an algorithm
Describes the Best case working mechanism of an algorithm
Covers the highest number of inputs
Covers the average number of inputs
Covers the lowest number of inputs
The time complexity of the algorithm is the highest
The time complexity of the algorithm is average
The time complexity of this algorithm is the lowest
The notation was introduced by P. Bachmann's
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Source: https://www.scholarhat.com/tutorial/datastructures/complexity-analysis-of-data-structures-and-algorithms

Relation to TIME Complexity Theory (1)

Time Complexity classes

- DTIME : amount of computation time (or number of computation steps) that a computer would take to solve a certain computational problem using a certain algorithm

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  In terms of DTIME : $\text{PTIME} = \bigcup_{k \in \mathbb{N}} \text{DTIME}(n^k)$

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- NTIME : set of all problems that can be solved by a **nondeterministic Turing machine** in time $O(f(n))$

  Complexity class NP defined in terms of NTIME : $\text{NP} = \bigcup_{k \in \mathbb{N}} \text{NTIME}(n^k)$

  where NTIME(n^k) : set of problems that can be solved by a NTM in polynomial time $O(n^k)$

Relation to TIME Complexity Theory (2)

- EXPTIME : set of all problems that are solvable by a **deterministic TM** in exponential time, i.e., in $O(2^{p(n)})$ time, where $p(n)$ is a polynomial function of n

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Relationship to NP-HARDness ?

- Warning
  - There are problems in EXPTIME that are not NP-hard
  - There are NP-hard problems that are not in EXPTIME
- Relates to **NP (class) problems**: computational problems that can be solved in polynomial time by NTM (and can be verified in polynomial time by DTM)
- A problem C is NP-complete if (1) C is in NP, and (2) Every problem in NP is reducible to C in polynomial time
- A problem X is NP-hard if only (2)
  - If C is NP-complete; then C is NP-hard (not vice-versa)
  - A problem is **NP-complete** if it is both NP and NP-hard

NP-Hard CO

NP-Hard Combinatorial Optimization (CO) problems

- MCF : Min-cost (unsplittable) flow problem
- MCP : Multi-constrained (single) path problem
- QAP : Quadratic assignment problem
- . . .

In general: math.program with integer/binary variables ($\Rightarrow$ nonconvex) $\Rightarrow$ NP-Hardness

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NP-Hard CO: Classes

Approximation Scheme (AS): ALG solves OP with input instance I of size *n*

Polynomial Time AS (PTAS): $(1 \pm \varepsilon)$ approximation ratio

- For min.OP: ALG/OPT $\leq (1 + \varepsilon)$, for $\varepsilon > 0$
- For max.OP: OPT/ALG $\leq (1 - \varepsilon)$, for $\varepsilon > 0$
- Time complexity: polynomial in the size *n* of input instance I (PTIME) for any fixed > 0
- Example: min. partitioning, multiple knapsack
- Sub-class **Fully-Polynomial Time AS (FPTAS)**
  - Time complexity: polynomial in both input size *n* **and** $1/\varepsilon$
  - Example: 0-1 knapsack problem

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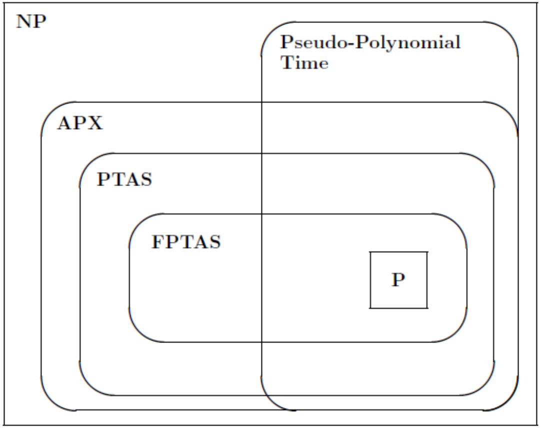
APX

- all min.OP that admit PTIME approximation algorithm with some finite worst case approx. ratio (constant-factor c approximation algorithms): ALG/OPT $\leq c$
- all max.OP that admit PTIME approximation algorithm with some positive worst case approx. ratio: OPT/ALG $\leq c$
- Example: metric-TSP, MIS, min.vertex cover
- Note: $f(n)$-APX: approximation by a factor of $f(n)$

NP-Hard CO: Approximation

Strict inclusion: $\mathrm{P} \subsetneq \mathrm{FPTAS} \subsetneq \mathrm{PTAS} \subsetneq \mathrm{APX} \subsetneq \mathrm{NP}$



A **pseudo-polynomial time** (numeric) algorithm : worst-case time complexity is polynomial in the numeric value of input (the largest integer present in the input) but not necessarily in the length of the input (the number of bits required to represent it),

Source: Lectures on Scheduling, edited by R.H. Moehring, C.N. Potts, A.S. Schulz, G.J. Woeginger, L.A. Wolsey, 2009.

NP-Hard CO: Involvement of ML ?

Involvement of (machine/statistical) learning-based methods

- Combining: NP-Hard (often) $\times$ NP-Hard CO
- Q: Does it help ?
- Yes

  ...it may help in reducing search space for NP-Hard CO problem solving schemes

Examples from CO

How can it help ?

Example: **Path-enumeration problem**

- k-shortest simple (no cycle) path problem (kSSP)
  - Directed graphs: $O(kn(m + nlog(n)))$ [Yen1971]
    Note: for undirected graphs: $O(k(m + nlog(n)))$ [Katoh1982]
  - **How to set k ?**

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  - **How to set k ?**
- Exhaustive search (simple paths)

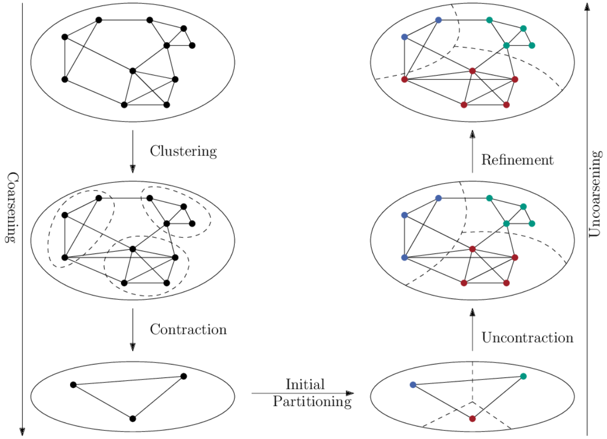
$$O((n-1) \times (n-2) \times \ldots \times n - (n-2) \times n - (n-1)) \tag{1}$$
$$= O((n-1) \times (n-2) \times \ldots \times 2 \times 1) \tag{2}$$
$$= O((n-1)!) \tag{3}$$

per vertex !

- Fundamental to identify "size" of search space itself

Examples from CO

- Many techniques to reduce (or characterize) search space
  - Graph sparsification: clustering - coarsening (by edge contraction) - partitioning
  - Dimensionality reduction: (input) $\mathbb{R}^n \rightarrow \mathbb{R}^d$ (data), $n \gg d$
  - ...



Source: Parallel and External High Quality Graph Partitioning Yaroslav Akhremtsev, 2019, Computer Science

Examples from CO

But then what about **strongly** NP-Hard CO ? (no FPTAS)

- strongly NP-Hard : still NP-hard even when all numbers in the input are bounded by some polynomial in the length of the input) ?
- Ex: subset-sum partition, bin-packing, etc. are strongly NP-Hard problems
- In layman terms: still intractable on small instances

Dealing with NP-Hardness

Approximation: Compromise on exactness (bound on quality of solution)

- Find an efficient algorithm running in $O(n^c)$ time that may not return the exact solution but something "close" (approximate solution) with guarantees of performance
- Example: instead of finding a k-clique, maybe will find a k/2-clique or k vertices that are "almost" a clique

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Restriction/Reduction: Compromise on generality

- Restriction to Class P (PTIME transform)
- Sometimes possible to work with restricted classes of inputs.
- Example: 3-SAT to 2-SAT $\in$ P

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Heuristics: Compromise on efficiency

- Some problems have algorithms that run in exponential time in worst-case but worst-case does not seem to happen often in practice
- Producing feasible solution in reasonable time, improving expected runtime on large subset of instances
- Example: matheuristics, greedy heuristic, neural networks

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$\Rightarrow$ Learning from examples implies either Sampling or Selection

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- Complexity of learning tasks (not atomic)
  - Tradeoff between learning error (bias of model) and generalization error (variance of model)
  - Lack of automated/online training: end-to-end model (feature extraction + classification/regression) still involves domain knowledge/human intervention
  - Cost/gain ratio vs. (added functionality and) performance

Applicability of Statistical (Learning) methods

1. **Descriptive**: what has happened ? why has it happened (explanatory: root cause analysis, diagnostics)

   Techniques

   - Statistical methods: quantitative/qualitative data analysis
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3. **Prescriptive**: what would happen, what could happen if (which decision/action should be taken ? What should be done) ?

   Techniques

   - Structured learning
   - Math.programming models to optimize a set of decisions for directing a given "objective", for achieving desired outcome
   - Physics: none

Importance of IID Assumption

- IID Assumption: **critical assumption** in statistics, machine learning, etc.
  - Formally: tuples of set $\{(x_i, y_i)\}_{i=!}^{N}$ are drawn independently from the same joint distribution $P(x, y) = \mathbf{P}(\mathbf{y}|\mathbf{x})P(x)$

    Note: $P(y|x)$ relationship to capture by mean learning algorithm (directly or indirectly)
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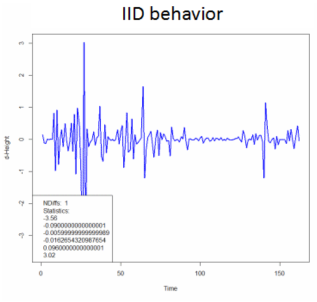
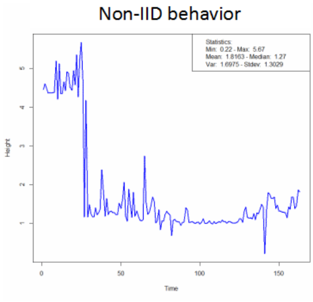




Importance of IID Assumption

Stationary process $\not\Rightarrow$ IID process

- Stationary process: joint probability distribution of the RVs invariant to time shifts but RVs may be dependent over time (thus, not IID)

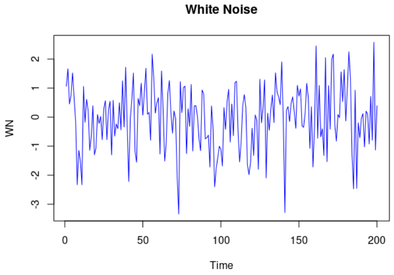
$$P(X_t|X_{1:t-1};\theta,t) = P(X_t|X_{1:t-1};\theta)$$

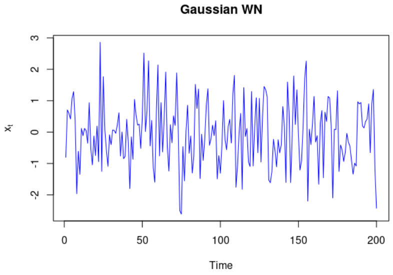
  - Stationary process of IID RVs: $P(X_t|X_{1:t-1};\theta,t) = P(X_t;\theta)$
- Note: IID $\not\Rightarrow$ Stationary process
  - Ex: process where each RV has a different probability distribution depending on the time step is IID but not stationary
- Consequence: can't use common stationarity tests ADF, PP or KPSS (for testing IIDness, in particular, checking mutual independence is far from trivial)

Importance of IID Assumption: facts

White noise process $\nRightarrow$ IIDness

- Zero expectation: $E[X_t] = 0$
- Finite variance: $Var[X_t] < \infty$
- Elements are uncorrelated: $Cor(X_t, X_s) = 0$
- Consequence: can't use (classical) white noise tests
- Notable exception: Gaussian white noise $\Rightarrow$ IIDness





Implications

IID Assumption Holds

Common memoryless generative process

- Independent draws from same JPD
- Data distribution at training time $\equiv$ at testing and generalization time

Linear regression $y = f(X, \beta) + \varepsilon$, with f linear in parameters vector β

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- Uncorrelated $E[\varepsilon_i \varepsilon_j | X] = 0$
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- Equal var. $E[\varepsilon^2 | X] = \sigma^2$ (homoskedastic)

Then Gauss-Markov theorem holds: BLUE (min.var) = least-square estimator

- (data) Normally distributed: error decreases by aggregating measures (over long time periods)
- (data) Not normally distributed: large datasets (invoke CLT)

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In practice

Non-IIDness

- Coupling/relationship (not independent) and/or heterogeneity (not identical)
- Data distribution at training $\neq$ at testing and generalization time $\Rightarrow$ Poor generalization (re-training)

Error uncorrelated, unequal variance (heteroskedastic)

- Different values of response var. y have different variance in their errors
- Gauss-Markov theorem does not apply: OLS estimators still unbiased but not efficient (not least variance)
- Weighted LS –possibly- at rescue (exact weights)

Error correlated, unequal variance

- Error distribution known (independently of data): Generalized LS
- Variance not completely known: Iterative Reweigthed LS

Comparison against classical regression/inversion methods

Stat. method: regression problems

- Given (x, y_{obs}), find parameters β such that $y_{obs} \approx f(x; \beta)$ i.e. such that f estimates relationship between dependent (y) and independent var (x)
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Indirect method: inverse problems

- Given (y_{obs}, m), model identification step to find g s.t. $y_{obs} \approx g(m)$
- Then, inversion method: $m \approx g^{-1}(y_{obs})$
- For nonlinear inverse problems: $y = g(m)$
  - If $g(m)$ well-behaved: first-order approx: $\Delta y = y - y_{est} = J_g \Delta m$

    Thus, $\Delta m = (J_g^{\intercal} J_g + \lambda \mathcal{I})^{-1} J_g^{\intercal} \Delta y$, where $(J_g)_{ij} = \frac{\partial g(m)_i}{\partial m_j}$
  - Otherwise, transformation to well-posed problem (second-order variational methods)

Comparison against classical regression/inversion methods

Stat. method: regression problems

- Given (x, y_{obs}), find parameters β such that $y_{obs} \approx f(x; \beta)$ i.e. such that f estimates relationship between dependent (y) and independent var (x)
- Then, predict $y_{pre} = f(x; \beta)$

Indirect method: inverse problems

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Direct/algorithmic method: NN approximates g^{-1}

- Given (y_{obs}, m), find g^{-1} such that $m \approx g^{-1}(y_{obs})$
- Then, predict $y_{pre} = g(m)$
- How (forward process): Invertible Neural Networks (INNs), Bayesian NN

Outline and Structure

1. Handling of NP-Hardness
2. Data space properties and Space complexity
3. Function Approximation and Approximate Representation
4. External penalty method

Space Complexity Theory: DSPACE

In computational complexity theory

- DSPACE: defines the set of all problems that can be solved by Turing machines using $O(f(n))$ space for some function f of the input size n
  - Represents the total amount of computational resource (memory space) for a deterministic Turing machine to solve a given computational problem with a given algorithm
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- Measure DSPACE is used to define complexity classes, sets of all of the decision problems that can be solved using a certain amount of memory space

- For each function $f(n)$, there is a complexity class SPACE(f(n)), the set of decision problems that can be solved by a deterministic Turing machine using space $O(f(n))$

- There is no restriction on the amount of computation time that can be used, though there may be restrictions on some other complexity measures (like alternation)

Space Complexity Theory: PSPACE

In computational complexity theory, PSPACE is the set of all decision problems which can be solved by a Turing machine using a polynomial amount of space.

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Formal definition: PSPACE

- **If** DSPACE($t(n)$) denotes the set of all problems that can be solved by Turing machines using at most $t(n)$ space for some function t of the input size n
- **Then** PSPACE can be formally defined as

$$\mathrm{PSPACE} = \bigcup_{k \in \mathbb{N}} \mathrm{SPACE}(n^k)$$

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Examples

- Finite horizon POMDPs (Partially Observable Markov Decision Processes)
- Canadian traveller problem (CTP): generalization of SP problem to graphs that are partially observable
- Plan existence problem in automated planning and scheduling

Space Hierarchy Theorem

In computational complexity theory

- **Space hierarchy theorems** are separation results that show that both deterministic and nondeterministic machines can solve more problems in (asymptotically) more space, subject to certain conditions.
  - For example, a deterministic Turing machine can solve more decision problems in space "n" log "n" than in space "n"
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- The foundation for the hierarchy theorems lies in the intuition that with either more time or more space comes the ability to compute more functions (or decide more languages)

- The hierarchy theorems are used to demonstrate that the time and space complexity classes form a hierarchy where classes with tighter bounds contain fewer languages than those with more relaxed bounds.

Space Hierarchy Theorem

Space hierarchy theorems rely on the concept of space-constructible functions

Formally: function $f : \mathbb{N} \rightarrow \mathbb{N}$ is space constructible if

- $f(n) \geq log(n)$
- and there exists a Turing machine which computes the function $f(n)$ in space $O(f(n))$ when starting with an input 1^n, where 1^n represents a string of n 1's

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Note: common functions are space-constructible, including polynomials, exponents, and logarithms.

Statement: For every space constructible function $f : \mathbb{N} \rightarrow \mathbb{N}$, there exists a language L that is decidable in space $O(f(n))$ but not in space $o(f(n))$

Space Complexity Theory: Classes

The above theorem implies the necessity of the space-constructible function assumption in the space hierarchy theorem

- $\mathrm{L} = \mathrm{DSPACE}(O(log(n)))$
- $\mathrm{PSPACE} = \bigcup_{k \in \mathbb{N}} \mathrm{DSPACE}(n^k)$
- $\mathrm{EXPSPACE} = \bigcup_{k \in \mathbb{N}} \mathrm{DSPACE}(2^{n^k})$

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Note: the complements of all problems in PSPACE are also in PSPACE, meaning that Co-PSPACE = PSPACE

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Consequences

- Adding non-determinism to the TM does not take up any more space

  Even though it may take up more time

- We can simulate a NTM on a DTM without needing more than a polynomial increase in space

  Even though there is a (potentially) exponential increase in the number of states

Relation to TIME Complexity Theory (1)

Time Complexity classes

- DTIME : amount of computation time (or number of computation steps) that a computer would take to solve a certain computational problem using a certain algorithm

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- PTIME (or P): set of all problems that can be solved by a deterministic Turing machine using a polynomial amount of computation time, or polynomial (amount of computation) time

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- NTIME : set of all problems that can be solved by a nondeterministic Turing machine in $O(n^k)$ time

  $$\mathrm{NP} = \bigcup_{k\in\mathbb{N}} \mathrm{NTIME}(n^k)$$

Relation to TIME Complexity Theory (2)

Time Complexity classes (cont'd)

- EXPTIME : set of all problems that are solvable by a deterministic Turing machine in exponential time, i.e., in $O(2^{p(n)})$ time, where $p(n)$ is a polynomial function of n.

  In terms of DTIME : $\text{EXPTIME} = \bigcup_{k \in \mathbb{N}} \text{DTIME}\left(2^{n^k}\right)$

- NEXPTIME : the set of decision problems that can be solved by a non-deterministic Turing machine using time $2^{n^{O(1)}}$

  In terms of NTIME : $\text{NEXPTIME} = \bigcup_{k \in \mathbb{N}} \text{NTIME}(2^{n^k})$

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By time hierarchy theorem and space hierarchy theorem:

$$\mathrm{P} \subsetneq \mathrm{EXPTIME}, \mathrm{NP} \subsetneq \mathrm{NEXPTIME} \text{ and } \mathrm{PSPACE} \subsetneq \mathrm{EXPSPACE}$$

PSPACE complete

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It turns out that some of these problems are essentially as hard as any such problem can be: such problems are called **PSPACE complete**.

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in complexity theory, a decision problem is PSPACE-complete IF

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in complexity theory, a decision problem is PSPACE-complete IF

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- and every problem in PSPACE can be reduced to it in polynomial time.

- The problems that are PSPACE-complete can be thought of as the hardest problems in PSPACE.
- These problems are widely suspected to be outside of P and NP, but that is not known. It is known that they lie outside of NC.

PSPACE-complete vs. NP-complete

PSPACE-complete problems take **exponential time** to deterministically compute the result

- Just like NP-complete problems
- Either the decision or functional problem versions

PSPACE-complete vs. NP-complete

PSPACE-complete problems take **exponential time** to deterministically compute the result

- Just like NP-complete problems
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But PSPACE-complete problems take **exponential time** to deterministically verify the result $><$ NP-complete can verify a solution in polynomial time

Outline and Structure

Characterizing (Artificial) Neural Networks

- **Expressivity**: what class(es) of functions $\mathcal{F}$ can be represented/approximated by neural network Φ cf. Universal approximation Theorem [Cybenko1989], [Hornik1991], [Leshno1993]

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- **Effectiveness** vs. **Efficiency**: how many layers (depth) and units per layer (width) are needed to compute functions $f(\in \mathcal{F}) : \mathbb{R}^d \to \mathbb{R}$

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- **Learnability/Trainability**: given structure (nbr of layers, neurons per layer), activation function σ, and labeled data points (x, y), find parameters w for the best fitting function $f \in F \to$ curse of non-convexity and dimensionality

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  Note: low complexity $f \not\Rightarrow$ highly trainable model (low training resources/time)

- **Generalization**: learn a neural model that minimizes the difference between the expected and the empirical risk (generalization error on previously unseen (x, y))

  Note: deep relationship with bias vs. variance tradeoff and stability property

Expressive power of Neural Networks

Universal approximation property: neural network with finite number of neurons can uniformly approximate arbitrarily well any continuous function on compact subsets of $\mathbb{R}^d$ when given appropriate parameters

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- Generalizes Hornik's Theorems (1989,1991) by dropping assumptions of continuity, monotonicity, and boundedness on activation function
- Establishes NSC on activation functions to ensure universal approximation property
- **Th**: standard multilayer feedforward network with a locally bounded, piecewise continuous activation function can approximate any continuous function to any degree of accuracy **iff** activation function σ is not polynomial almost everywhere

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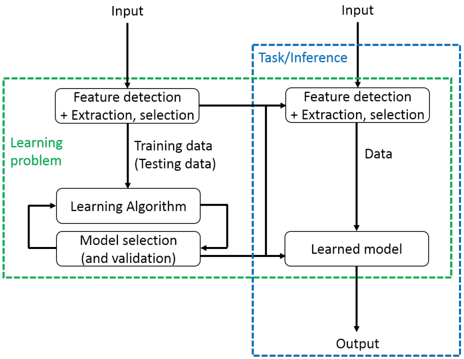
Intuition

- Neural network universality **iff** if σ does not coincide with polynomial (almost everywhere)
- Necessary condition: assume
    - σ: polynomial of degree N
    - Φ: neural network of depth L (hidden layers) and activation σ_L

$\Rightarrow$ Each function implemented by Φ polynomial of degree at most N^L irrespective of width W

Neural networks as ML problems solver

- Pro's: Compelling arguments for using NNs as general template (matching input to outputs) for solving machine learning (ML) problems including nonlinear regression
- Con's: BUT **designing** and **training** the right NN for given learning task coins many theoretical gaps and practical concerns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Model selection (and validation)
Learned model
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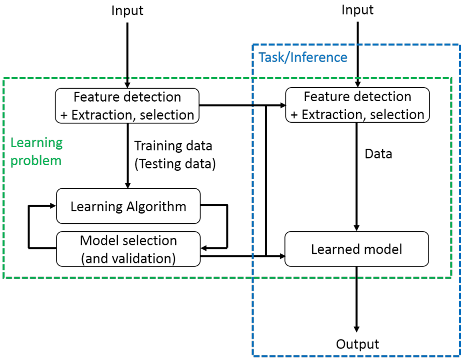
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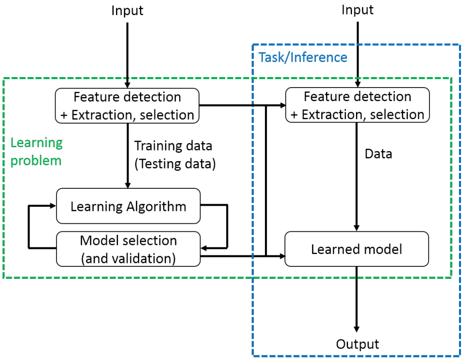
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Quality of **training** and its properties: performance bounds/guarantees, robustness, etc.

$\rightarrow$ Parameters of learned model (parameter learning)

$\Rightarrow$ Computational/Optimization methods for machine learning

Learning Problem

Assumptions

- Training set $\{X, Y\}$ of n random independent and identically distributed (i.i.d.) observations/labeled data points $(x_i, y_i) \in \{\mathcal{X}, \mathcal{Y}\}, i \in \{1, \ldots, n\}$
- Learning machine capable of implementing set of prediction functions $\{p(w, x) : \mathbb{R}^d \times \mathbb{R}^{d_x} \rightarrow \mathbb{R}^{d_y}\}$ parameterized by parameter vector $w \in W \subseteq \mathbb{R}^d$

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- Find vector w^* such that function $p(w^*, x)$ obtained from any given input $x \in \mathcal{X}$ is best at predicting the appropriate label $y \in \mathcal{Y}$ corresponding to x

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Optimization Problem

- Loss function: given pair (x, y), parameter vector w and predicted output $p(w, x)$

$$\ell : \mathbb{R}^{d_x} \times \mathbb{R}^{d_y} \to \mathbb{R} : (x, y) \to \ell(p(w, x), y) \tag{4}$$

Measures discrepancy between true output y (supervisor response) to a given input x and predicted output $p(w, x)$ (learning machine response)

$\Rightarrow$ Find parameter vector w^* which minimizes loss incurred from any input-output pair

Learning Problem: Expected and Empirical risk

Expected Risk $R(w)$

- Expected risk: $\mathcal{L}(w) = \int \ell(p(w,x),y)dP(x,y) = \mathbb{E}_{(x,y)}[\ell(p(w,x),y)]$ (5)

  $P(x,y) : \mathbb{R}^{d_x} \times \mathbb{R}^{d_y} \to [0,1]$ unknown joint probability distribution representing true relationship between inputs and outputs $\to$ **Stochastic optimization** with unknown P
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Empirical Risk $R_n(w)$

- Empirical risk: $\hat{\mathcal{L}}(w) = \frac{1}{n}\sum_{i=1}^{n} \ell(p(w,x_i),y_i)$ (7)

  Measures error on given training set $\{X,Y\} = \{(x_i,y_i) : i = 1,\ldots,n\}$ with each (x_i,y_i) selected independently at random from $\{\mathcal{X},\mathcal{Y}\})$ $\to$ **Sample average approximation**
- Empirical risk minimization: $\hat{w} = \arg\min_{w \in W} \hat{\mathcal{L}}(w) = \frac{1}{n}\sum_{i=1}^{n} \ell(p(w,x_i),y_i)$ (8)

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Empirical Risk $R_n(w)$

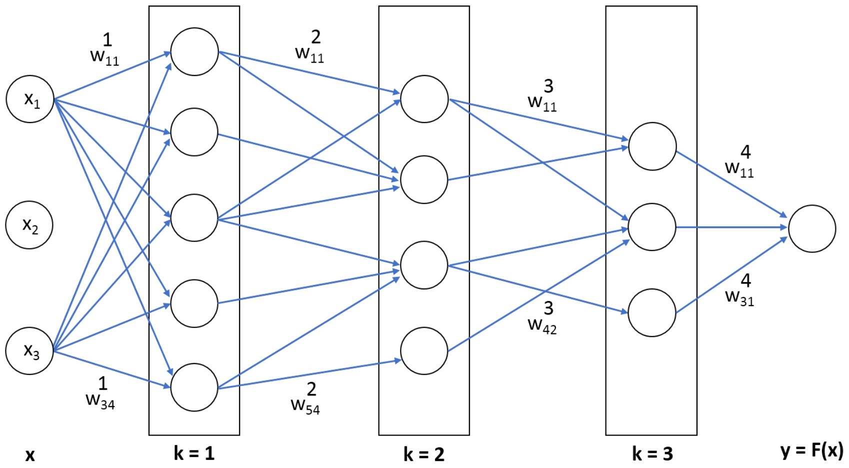
- Empirical risk: $\hat{\mathcal{L}}(w) = \frac{1}{n}\sum_{i=1}^{n} \ell(p(w,x_i),y_i)$ (7)

  Measures error on given training set $\{X,Y\} = \{(x_i,y_i) : i = 1,\dots,n\}$ with each (x_i,y_i) selected independently at random from $\{\mathcal{X},\mathcal{Y}\})$ $\rightarrow$ **Sample average approximation**
- Empirical risk minimization: $\hat{w} = \arg\min_{w \in W} \hat{\mathcal{L}}(w) = \frac{1}{n}\sum_{i=1}^{n} \ell(p(w,x_i),y_i)$ (8)

Empirical Risk Minimization (ERM principle): **induction principle**

Approximate the function which minimizes the expected risk (the problem we **want to solve**) by the function which minimizes empirical risk (the problem we **can solve**)

Neural Networks: Example



Learning Problem for Neural Networks

For an unknown target function $f \in \mathcal{F}$ and given training data set $\{X, Y\}$ (randomly selected from distribution $\{\mathcal{X}, \mathcal{Y}\}$)

1. **Selection of NN structure**: depth L and width W
   Interconnection between neurons arranged in one or multiple layers
   Transformation functions each neuron/unit j at layer k performs:
   - **Transfer potential**: weighted sum of input vector $x^{(k-1)}$ ($= x^{(0)}$ for the first layer) which is passed by unit i at layer $k-1$ to neuron/unit j at layer k

$$\sum_{i=1}^{L_{k-1}} w_{ij}^{(k)} x_i^{(k-1)} \tag{9}$$

   - **Activation function** σ: non-/linear function applied to the transfer potential by each neuron j at layer k to produce

$$x_j^{(k)} = \sigma\Big(\sum_{i=1}^{L_{k-1}} w_{ij}^{(k)} x_i^{(k-1)}\Big) \tag{10}$$

   - Output $p^{(k)}(w_j^{(k)}, x_j^{(k)})$ of neuron/unit j in layer k defines input vector $x^{(k+1)}$ for next layer $k+1$
2. Minimization of empirical loss $\hat{\mathcal{L}}$ on given training data set $\{X, Y\}$ from distribution $\{\mathcal{X}, \mathcal{Y}\} \rightarrow \hat{w}$
3. Estimation of generalization ability (testing loss) $\hat{\mathcal{L}}(\hat{w})$ on test data set $\{X^t, Y^t\}$ (randomly selected from the same distribution $\{\mathcal{X}, \mathcal{Y}\}$)

Representational capacity of neural networks

UAT characterizes **representational capacity** of neural networks: set of hypotheses a given model is capable of expressing when assigning some value to its parameters

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Main focus

i) Existence of approximations without explicit constructive method or explicit construction methods involving activation functions that are unusable in practice due to their complexity cf. [Maiorov-Pinkus,1999]

ii) Properties of approximations by analyzing their error for certain classes of functions provided that sufficiently many hidden units (N) are available

$\Rightarrow$ Characterizing W and L simultaneously in approximation rate remains open and challenging

iii) Asymptotic estimates have limited applicability when properties of fixed neural structure of finite size need to be understood;

$\Rightarrow$ Very few results address quantitative and non-asymptotic approximation rate of neural networks

iv) Characterizing which functions (class of) NNs can express over entire domain instead of determining their representational capacity for a finite sample of size n

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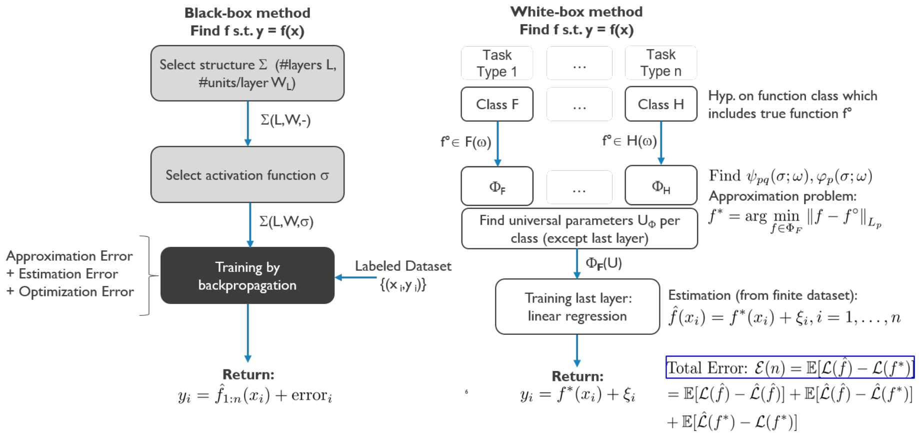
UAT neither address learnability of neural structure (depth, width) nor trainability of its parameters

Black-box vs. White-box Method


Black-box method
Find f s.t. y = f(x)
Select structure Σ (#layers L, #units/layer W$_L$)
Σ(L,W,-)
Select activation function σ
Σ(L,W,σ)
Approximation Error
+ Estimation Error
+ Optimization Error
Training by backpropagation
Labeled Dataset {(x$_i$,y$_i$)}
Return:
$y_i = \hat{f}_{1:n}(x_i) + \mathrm{error}_i$
White-box method
Find f s.t. y = f(x)
Task Type 1
…
Task Type n
Class F
…
Class H
Hyp. on function class which includes true function f°
f°∈ F(ω)
f°∈ H(ω)
Φ$_F$
…
Φ$_H$
Find $\psi_{pq}(\sigma;\omega), \varphi_p(\sigma;\omega)$
Approximation problem:
$f^* = \arg\min_{f\in\Phi_F} \|f - f^\circ\|_{L_p}$
Find universal parameters U$_Φ$ per class (except last layer)
Φ$_F$(U)
Training last layer: linear regression
Estimation (from finite dataset):
$\hat{f}(x_i) = f^*(x_i) + \xi_i, i = 1, \ldots, n$
Return:
$y_i = f^*(x_i) + \xi_i$
$\boxed{\text{Total Error: } \mathcal{E}(n) = \mathbb{E}[\mathcal{L}(\hat{f}) - \mathcal{L}(f^*)]}$
$= \mathbb{E}[\mathcal{L}(\hat{f}) - \hat{\mathcal{L}}(\hat{f})] + \mathbb{E}[\hat{\mathcal{L}}(\hat{f}) - \hat{\mathcal{L}}(f^*)]$
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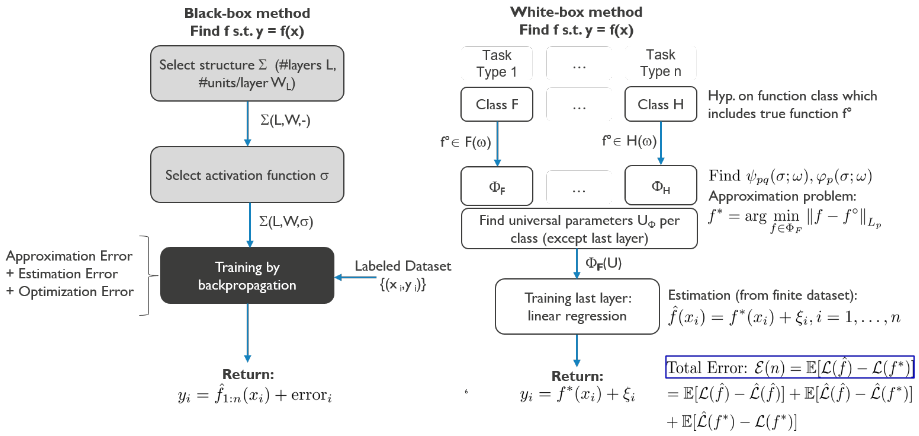
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Main motivations

- Constructive function approximation-based
- Training procedure with tight-error control
- Performance guarantees and verifiable models

Back box Gradient-based Methods: Error

Suppose

- Expected risk minimizer: $w^\star = \arg\min_{w \in W} \mathcal{L}(w) = \mathbb{E}_{(x,y)}[\ell(p(w,x),y)]$
- Empirical risk minimizer: $\hat{w} = \arg\min_{w \in W} \mathcal{L}_n(w) = \frac{1}{n}\sum_{i=1}^{n} \ell(p(w,x_i),y_i)$

Compute minimizer $\hat{w}_\epsilon$ (accuracy ϵ) over n datapoints

- Approximation error: $E_{app} = \mathcal{L}(w^\star)$
- Estimation error: $E_{est}(n) = \mathbb{E}[\mathcal{L}(\hat{w}) - \mathcal{L}(w^\star)]$
- Optimization error: $E_{opt}(n,\epsilon) = \mathbb{E}[\mathcal{L}(\hat{w}_\epsilon) - \mathcal{L}(\hat{w})]$

Goal: $\min_{n,\epsilon} \mathbb{E}[\mathcal{L}(\hat{w}_\epsilon) - \mathcal{L}(w^\star)]$

- Objective function: $\mathbb{E}[\mathcal{L}(\hat{w}_\epsilon) - \mathcal{L}(w^\star)]$

$$= \mathbb{E}[\mathcal{L}(\hat{w}_\epsilon) - \mathcal{L}_n(\hat{w})] + \mathbb{E}[\mathcal{L}_n(\hat{w}) - \mathcal{L}_n(w^\star)] + \mathbb{E}[\mathcal{L}_n(w^\star) - \mathcal{L}(w^\star)]$$

Kolmogorov Representation Theorem

Kolmogorov Representation Theorem (1959)

Every continuous function $f : [0,1]^n \subset \mathbb{R}^n \to \mathbb{R}$ defined on $n-$dimensional space ($n \geq 2$) can be completely determined by sums and superpositions[a] of continuous functions φ_q ($q = 1, \ldots, 2n+1$) of one variable and ψ_{pq} ($p = 1, \ldots, n$, $q = 1, \ldots, 2n+1$) of variable x_p

$$f(x_1, \ldots, x_n) = \sum_{q=1}^{2n+1} \varphi_q \Big(\sum_{p=1}^{n} (\psi_{pq}(x_p) \Big) \tag{11}$$

with

$2n+1$ continuous outer functions $\varphi_q : \mathbb{R} \to \mathbb{R}$ (dependent of f)

$2n^2 + n$ continuous inner functions $\psi_{pq} : [0,1] \to \mathbb{R}$ (independent of f)

$\Rightarrow$ only outer functions φ_q specific for given function f

[a] Thus, this theorem is often referred to as the Superposition Theorem

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Applicability to Neural Networks ?

A priori attractive: representation of function requires a fixed number of nodes, polynomially increasing with dimensions of the input space n

Kolmogorov Representation Theorem: Variants

- Lorentz (1962):

  Outer functions $\varphi_q := \varphi$ for all q

  Inner functions $\psi_{pq} := \lambda_p \psi_q$ for rationally independent constants $\lambda_p \leq 1$

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- Sprecher (1972):

  Inner functions $\psi_{pq}(x_p) := \lambda^{p-1} \psi(x_p + \epsilon q)$ with ψ Holder continuous

Relation to Neural Networks

[Hecht-Nielsen, 1987]: interpretation of Kolmogorov theorem as three-layer NN

To represent $f : \mathbb{R}^n \to \mathbb{R}^m : (x_1, \ldots, x_n) \to f(x_1, \ldots, x_n) = \sum_{q=1}^{2n+1} \varphi\Big(\sum_{p=1}^{n} (\psi_{pq}(x_p)\Big)$

i) n units (processing elements) in the first ($x-$input) layer: fanout units to distribute input x-vector components to the processing elements of next layer

ii) $2n+1$ units in the hidden / middle layer with transfer function ψ_q independent of f (except dim. n)

$$z_q = \sum_{p=1}^{n} \lambda^q \psi(x_p + \epsilon q) + q \tag{12}$$

where λ real constant, $\epsilon > 0$ rational number ψ continuous real monotonic increasing functions belonging to satisfy Lipschitz condition $|\psi(x) - \psi(y)| \leq c\,|x - y|^{\alpha}$ for any $0 < \alpha \leq 1$.

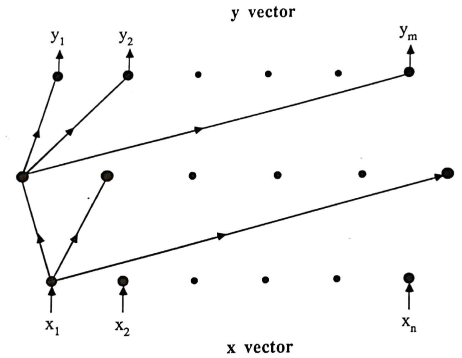
iii) m top layer/output units with transfer function φ dependent of f

$$y_i = \sum_{q=1}^{2n+1} \varphi_i(z_q), i = 1, 2, \ldots, m \tag{13}$$

where functions $\varphi_i, i = 1, 2, \ldots, m$ are real and continuous (dependent on f)

Example

Topology of the Kolmogorov Network[1]



[1] R. Hecht-Nielsen, Kolmogorov's mapping neural network existence theorem, Proc. of Int'l Conf. on Neural Networks, vol.III, pp.11-14, New York: IEEE Press

Limited applicability

Girosi & Poggio (1989)

Interpretation inapplicable for two main reasons

- Inner functions ψ highly nonsmooth $\Rightarrow$ ψ at least as difficult to approximate as f
- Outer functions φ dependent on specific f $\Rightarrow$ not representable in parameterized form

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1. Kolmogorov's Theorem cannot be used in any constructive way in neural learning context
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However... finding good and well founded **approximate representations** was left open

Approximation of Representation Theorem

Kurkova's Approximation Theorem [Kurkova 1992]

- Derived from Kolmogorov's Representation Theorem
- NB: original proof of Kolmogorov's theorem is not constructive, i.e. shows existence of a representation but cannot be used in an algorithm for numerical calculations

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Main idea

Relaxing exactness by an approximation of f (thus, approximate representation) enables estimating number of hidden units as a function of i) desired accuracy and ii) rate of increase of function f (modulus of continuity) being approximated

- One variable functions ϕ replaced by finite linear combinations of affine transformations of a single arbitrary sigmoidal function
- From UAT: sigmoidal functions can approximate any continuous function on any closed interval with arbitrary accuracy

Approximation of Representation: Kurkova Theorem

Let $S(\sigma)$ denote set of all staircase-like functions defined by $x \mapsto \sum_{i=1}^{k} a_i \sigma(b_i x + c_i)$

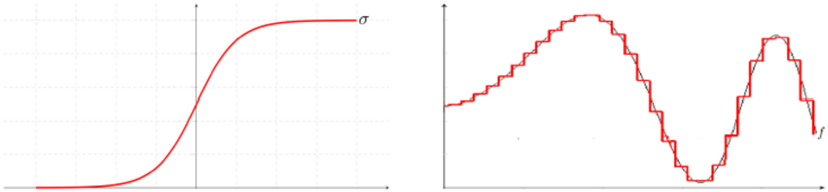

Figure 1: On the left, an activation function $\sigma : \mathbb{R} \to [0,1]$ and on the right a staircase-like function of a type σ which approximates f for the one dimensional case.

Kurkova Approximation Theorem

Let a continuous function $f : [0,1]^n \to \mathbb{R}$ and sigmoidal function $\sigma(\in S) : \mathbb{R} \to [0,1]$

Then, for any $\varepsilon > 0$ there exist $k \in \mathbb{N}$ and functions $\varphi_q; \psi_{pq} \in S(\sigma)$ such that for any $(x_1, \ldots, x_n) \in [0,1]^n$

$$\left| f(x_1, \ldots, x_n) - \sum_{q=1}^{k} \varphi_q \left(\sum_{p=1}^{n} \psi_{pq}(x_p) \right) \right| < \varepsilon \tag{14}$$

Approximation of Representation: Method

Constructive method: two-hidden layer networks with

- Universal set of weights for approximations of functions within a certain continuity class (Lipschitz, $\alpha-$Holder, etc.)

  $\Rightarrow$ Only weights from second hidden layer to output units are specific for the function f being approximated

- These weights appear linearly in parameterized expression

  $\Rightarrow$ **Training** becomes Linear regression problem

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Guaranteed method: Kurkova Th. provides upper estimates of number of hidden units needed for $\varepsilon-$approximation of continuous functions

- For every $m \in \mathbb{N}$ such that $m \geq 2n+1$, $n/(m-n) + v < \varepsilon / \|f\|_\infty$ for some $v > 0$
- Function f can be approximated with accuracy ε by two hidden layer neural network with activation function σ and
  - Number of units in first hidden layer: $nm(m+1)$
  - Number of units in second hidden layer: $m^2(m+1)^n$

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Note: number of hidden units (2nd layer) needed for good approximations of general continuous functions exponential in n.

Exercise

Finding good algorithms for constructing function approximators with

- (at least) two-hidden layer structure
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ii) Input dimensionality n

iii) Smoothness properties of f being approximated (start from Holder class or even stronger Lipschitz continuous)

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Goal

Construction procedure to provide neural structure capable of approximating all functions from a certain class with given accuracy where only weights corresponding to output units should be learned

Exercise: Tasks

1. Upper estimates of number of hidden units needed for good approximations of general continuous functions remain very large. For particular classes of functions, better estimates could be obtained

   Identifying classes of functions (smoothness class: Lipschitz, Holder, Sobolev, etc.) to obtain better estimates remains to be formalized

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   Evaluate and compare different regression methods to solve it depending on the properties of the problem

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   Evaluate and compare different regression methods to solve it depending on the properties of the problem

4. Compare resulting models in particular their complexity vs. accuracy

   Guaranteeing performance should not come at the detriment of inflexible or over-constraining models; tradeoff between *Tractable but bad model or Intractable but good model*

Outline and Structure

1. Handling of NP-Hardness
2. Data space properties and Space complexity
3. Function Approximation and Approximate Representation
4. External penalty method

External penalty method: Nonlinear ADM

Composite minimization problem

$$\min_{x\in\mathcal{X}} \varphi(x) = f(x) + h(x) + g(c(x) - b)$$

- $(\mathcal{X}, \langle\cdot,\cdot\rangle)$ and $(\mathcal{Y}, \langle\cdot,\cdot\rangle)$ real Hilbert spaces, $b \in \mathcal{Y}$
- $c\colon \mathcal{X} \to \mathcal{Y}$ is a **nonlinear**, differentiable mapping
- $h\colon \mathcal{X} \to \mathbb{R}$ is a differentiable nonconvex function
- $f\colon \mathcal{X} \to]-\infty, +\infty]$ and $g\colon \mathcal{Y} \to]-\infty, +\infty]$ are proper lsc convex functions

Properties algorithmic scheme

- **Full-splitting method**: at each iteration evaluates separately
  - nonsmooth components f, g via their proximity operators
  - smooth component h via its gradient
  - nonlinear operator c via its values
- **No subsolver** (primal) $\Rightarrow$ Lower computational cost
- Various OP can be reformulated as special cases of this generic model

Comparison: nonlinear ADM vs. alternatives

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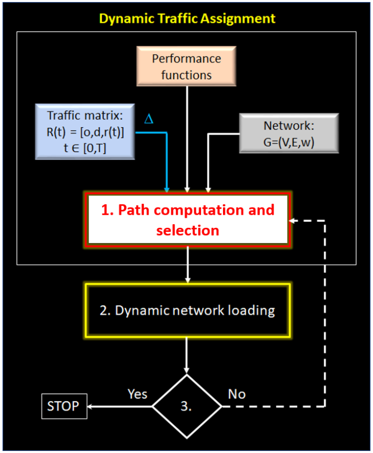
- $f \colon \mathcal{X} \to]-\infty, +\infty]$ and $g \colon \mathcal{Y} \to]-\infty, +\infty]$ are proper lsc convex functions

Method	**f**	**g**	**h**	**c**	**Splitting**	**Det.**	**Sto.**	**Subsolver**
Nonlinear ADM	cv	cv	nc-s	NL	yes	yes	yes	no
Valkonen 2014	cv	cv	0	NL	yes	yes	no	no
Bolte et al. 2018	0	cv	nc-s	NL	no	yes	no	yes
Linearized ADMs*	cv	cv	nc-s	L	yes	yes	yes	no
Prox-Linear*	cv	cv	0	NL	no	yes	yes	yes
iALMs*	0	cv	0	NL	no	yes	yes	yes

Legend: cv = convex, nc(-s) = non-convex (smooth), (N)L = (Non)Linear

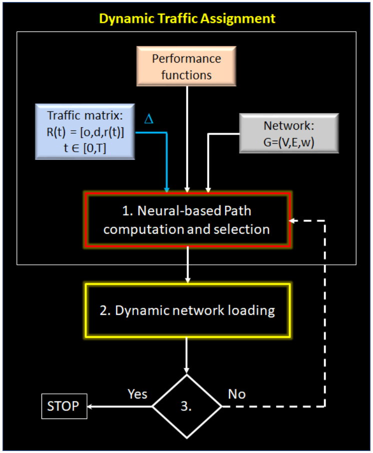
Use case: multi-constrained Dynamic Traffic Assignment (DTA)

1. Method to compute network path-dependent throughput, delay, etc. **by means of neural network**
2. Method to determine how path flows induce time-dependent arc-load, load-induced delay, etc.
3. Determine if/when performance criteria are met


Dynamic Traffic Assignment
Performance functions
Traffic matrix: R(t) = [o,d,r(t)] t ∈ [0,T]
Δ
Network: G=(V,E,w)
1. Path computation and selection
2. Dynamic network loading
STOP
Yes
3.
No

Use case: multi-constrained Dynamic Traffic Assignment (DTA)

1. Method to compute network path-dependent throughput, delay, etc. **by means of neural network**
2. Method to determine how path flows induce time-dependent arc-load, load-induced delay, etc.
3. Determine if/when performance criteria are met


Dynamic Traffic Assignment
Performance functions
Traffic matrix: R(t) = [o,d,r(t)] t ∈ [0,T]
Δ
Network: G=(V,E,w)
1. Neural-based Path computation and selection
2. Dynamic network loading
Yes
No
3.
STOP

1. Multi-constrained Dynamic Traffic Assignment (DTA)

Given $\varphi_a := \varphi(\ell_a)$ load-dependent utility function (nonconcave)

- S-shaped utility function: risk seeking then after certain threshold risk averse
- Bandwidth utility function: inelastic real-time and delay-/rate-adaptive services

Graph $G = (V, A)$, Path set $P = \cup_{k=1}^{n} P_k$, and Demand set $K = \{s_k, t_k, d_{st,k}, \tau_k\}_{k=1}^{n}$

Problem

$$\max \sum_{a \in A} \int_0^{\ell_a} \varphi_a(s) ds \tag{15}$$

s.t.

$$\sum_{p \in P_k} x_{stp} = d_{st} \qquad \forall d_{st} : (s,t) \in K \tag{16}$$

$$\sum_{(s,t) \in K} \sum_{p \in P_k} \delta_{stpa} x_{stp} = \ell_a \qquad \forall a \in A \tag{17}$$

$$0 \le \ell_a \le \kappa_a \qquad \forall a \in A \tag{18}$$

$$\sum_{a \in A} \delta_{stpa} \left(\frac{1}{\kappa_a - \ell_a} + t_a \right) \le \tau_k \qquad \forall k \in K, p \in P_k, x_{stp} > 0 \tag{19}$$

$$(d_{st} \ge)\, x_{stp} \ge 0 \qquad \forall (s,t) \in K, p \in P \tag{20}$$

Numerical Method

Reformulation

- Define variable

$$y_a = \frac{\kappa_a}{\kappa_a - \ell_a}, \ \forall a \in A \tag{21}$$

- Load variable ℓ_a becomes

$$\ell_a = \kappa_a \left(1 - \frac{1}{y_a}\right), \forall a \in A \tag{22}$$

- Constraints reformulated as

$$\begin{aligned}
&\sum_{p \in P_k} x_{stp} = d_{st} && \forall d_{st} : (s,t) \in K \\
&y_a \left(\sum_{(s,t) \in K} \sum_{p \in P_k} \delta_{stpa} x_{stp} - \kappa_a \right) = -\kappa_a && \forall a \in A \\
&\sum_{a \in A} \delta_{stpa} \left(\frac{y_a}{\kappa_a} + t_a \right) \leq \tau_k && \forall k \in K, p \in P_k : x_{stp} > 0 \\
&x_{stp} \geq 0 && \forall (s,t) \in K, p \in P \\
&y_a \geq 1 && \forall a \in A
\end{aligned}$$

S-shaped utility function

Nonconvex (S-Shaped) disutility function: measures disutility (φ_a) of using given arc $a \in A$ as function of carried traffic flow or load $\ell_a = \kappa_a(1 - \frac{1}{y_a}), \forall a \in A$

$$\varphi_a(s) = \frac{1}{2}\Big(1 - \frac{((s - \kappa_a/2)/\sigma_a}{\sqrt{1/2 + ((s - \kappa_a/2)/\sigma_a)^2}}\Big) \tag{23}$$

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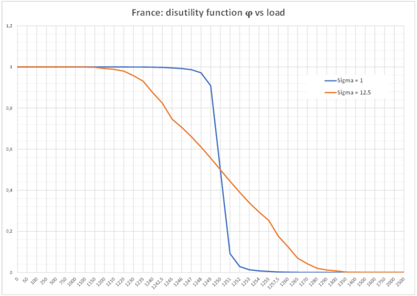
Topology	Scaling factor σ	Objective Function
austria	1108.00	$\frac{1}{2}\Big(1 - \frac{(s-5544000)/1108}{\sqrt{1/2+((s-5544000)/1108)^2}}\Big)$
atlanta	20.00	$\frac{1}{2}\Big(1 - \frac{(s-2000)/20}{\sqrt{1/2+((s-2000)/20)^2}}\Big)$
cost266	604.80	$\frac{1}{2}\Big(1 - \frac{(s-60480)/604.80}{\sqrt{1/2+((s-60480)/604.80)^2}}\Big)$
france	12.50	$\frac{1}{2}\Big(1 - \frac{(s-1250)/12.5}{\sqrt{1/2+((s-1250)/12.5)^2}}\Big)$
germany50	1	$\frac{1}{2}\Big(1 - \frac{(s-20)}{\sqrt{1/2+((s-20)^2}}\Big)$
giul39	3.20	$\frac{1}{2}\Big(1 - \frac{(s-320)/3.20}{\sqrt{1/2+((s-320)/3.20)^2}}\Big)$
india35	3.00	$\frac{1}{2}\Big(1 - \frac{(s-300)/3.00}{\sqrt{1/2+((s-300)/3.00)^2}}\Big)$
norway	20.00	$\frac{1}{2}\Big(1 - \frac{(s-2000)/20}{\sqrt{1/2+((s-2000)/20)^2}}\Big)$
pioro40	3.11	$\frac{1}{2}\Big(1 - \frac{(s-311)/3.11}{\sqrt{1/2+((s-311)/3.11)^2}}\Big)$



Instances

Network Topologies and Properties
SNDLibhttp://sndlib.zib.de/problems.overview.action

Topology	**Nodes**	**Arcs**	**Min, Max, Avg Degree**	**Diameter**	**Demands**
austria	65	216	1, 10, 3.32	9	1868
atlanta	15	44	2, 4, 2.93	5	210
cost266	37	114	2, 5 3.08	8	1332
france	25	90	2, 10, 3.60	5	300
germany50	50	176	2, 5, 3.52	9	662
giul39	39	172	3, 8, 4.41	6	1471
india35	35	160	2, 9, 4.57	7	595
norway	27	102	2, 6, 3.78	7	702
pioro40	40	178	4, 5, 4.45	7	780
zib54	54	81	1, 10, 3.00	8	1501

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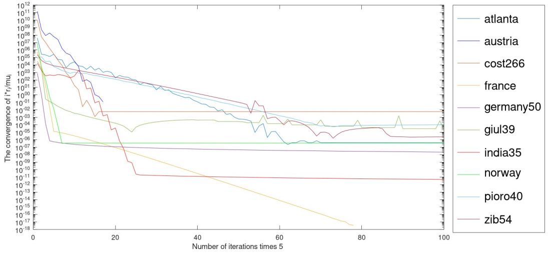
- Traffic demands (synthetic): variable size d_{st} and max.delay τ_k
- Path classes : for each demand $\{s_k, t_k, d_{st,k}, \tau_k\} \in K$ obtain set P_k of candidate paths

  Example: a) shortest path (hop-count), b) min.weight/least cost path, c) max.available bandwidth/least loaded path, and d) min.residual/unused bandwidth

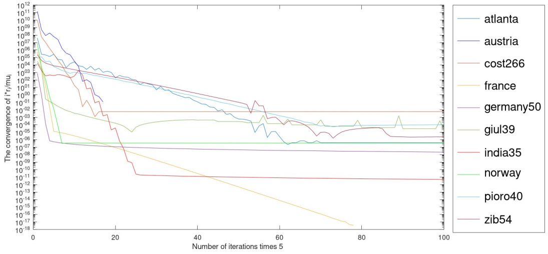
Numerical Method

Nonlinear ADM: convergence vs. number of iterations



Numerical Method

Nonlinear ADM: convergence vs. number of iterations



Comparison with commercial **MILP solver**

- RLT-based CR with variable $z_{stpa} = x_{stp} y_a$ such that bilinear constraints

$$\kappa_a y_a - y_a \left(\sum_{(s,t)\in K} \sum_{p \in P_k} \delta_{stpa} x_{stp} \right) = \kappa_a \rightarrow \quad \kappa_a y_a - \sum_{(s,t)\in K} \sum_{p \in P_k} \delta_{stpa} z_{stpa} = \kappa_a (\forall a \in A)$$

- PWL approx. of disutility function

Numerical Results

Disutility minimization - Nonlinear ADM (32GB/4)				
Topology	**Minimum Obj. value**	**Feasibility**	**Null Load Arcs**	**Computation Time (s)**
austria	2099892	7	15	3935
atlanta	**55404**	34	0	198
cost266	**234019**	0.009966	0	913
france	79662	2	0	298
germany50	1478	0.0015	1	**129**
giul39	46001	5	0	1821
india35	**32507**	5	1	471
norway	43623	8	0	679
pioro40	198780	95	1	890
zib54	128756	9	19	1038

Disutility minimization - MILP Solver (32GB/4)					
Topology	**Minimum Obj. value**	**Gap Optimal.**	**Null Load Arcs**	**Comp. Time (s)**	**Total Time (s)**
austria	**1641854**	0.000%	15	16.54	412.03
atlanta	63887	0.000%	0	59.07	60.56
cost266	317153	0.000%	0	58.44	153.95
france	**69115**	0.000%	0	31.80	38.20
germany50	**1448**	0.005%	4	**6790.86**	6911.11
giul39	**42472**	0.000%	0	851.81	948.17
india35	32969	0.250%	3	60.72	90.45
norway	**42455**	0.000%	0	538.37	563.24
pioro40	**156362**	0.160%	2	136.05	188.38
zib54	**105080**	0.000%	19	105.45	331.31