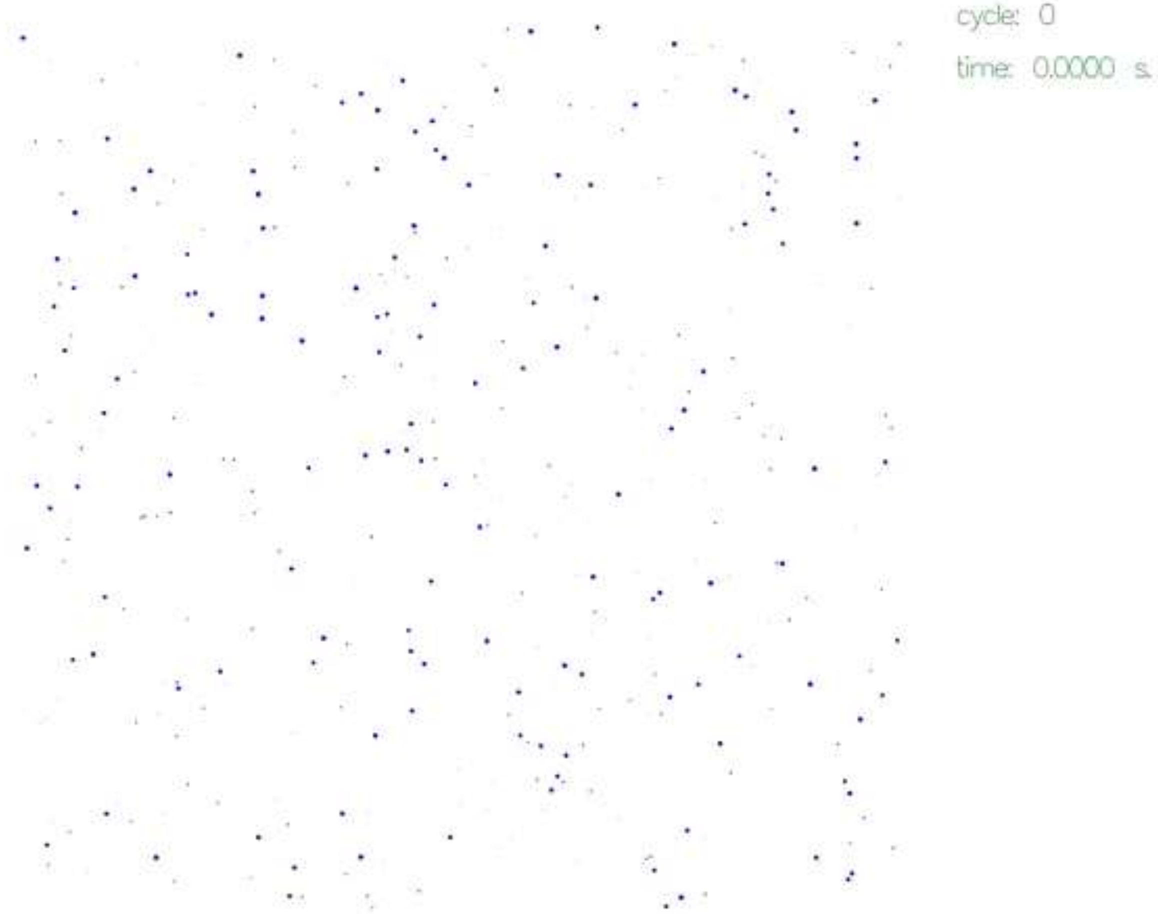
Multiple GPU Support

- CUDA_VISIBLE_DEVICES
- cudaError_t cudaSetDevice (int device)
- __host__ _device__ cudaError_t cudaMalloc (void** devPtr, size_t size)
- __host__ cudaError_t cudaMemcpyPeer (void* dst, int dstDevice, const void* src, int srcDevice, size_t count)
- __host__ cudaError_t cudaMemcpyPeerAsync (void* dst, int dstDevice, const void* src, int srcDevice, size_t count, cudaStream_t stream = 0)

Cluster Computing

N-Body Problem

- Given N objects
  - Mass
  - Velocity
- Compute the status of each object
- Universal Gravitation
  - O(N^2) forces

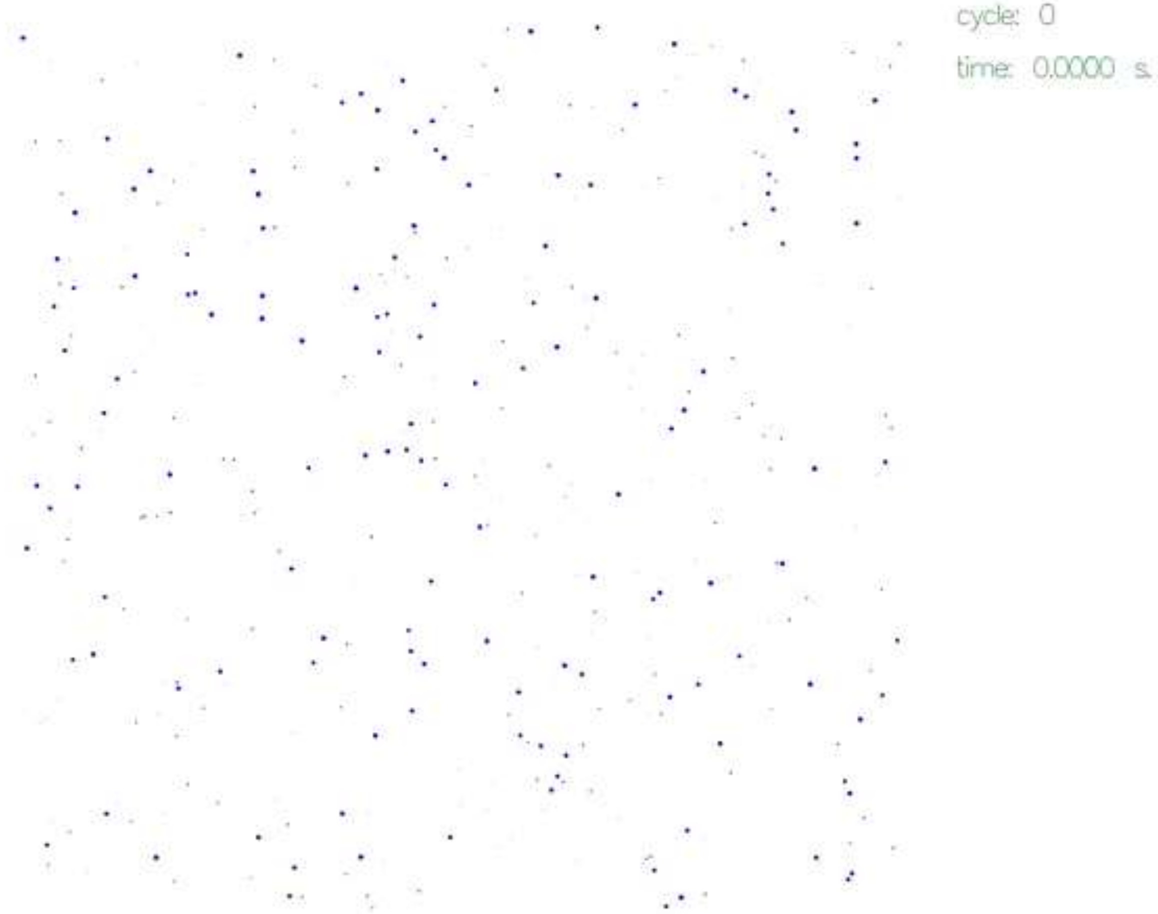


https://en.wikipedia.org/wiki/N-body_simulation

N-Body Problem

- Given N objects
  - Mass
  - Velocity
- Compute the status of each object
- Universal Gravitation
  - O(N^2) forces

- We need to scale!
- (Or have a better algorithm)



https://en.wikipedia.org/wiki/N-body_simulation

Cluster Computing

- Putting many (cheap) computers in a cluster
  - The computers in the same cluster do not have to be the same
  - Communication topology
    - All nodes are fully connected
    - Hubs
- Eventually, the communication will be the bottleneck
- For most cases, a network filesystem is employed

Message Passing Interface (MPI)

- Introduced in early 90’s
- Each process may have multiple threads
- Each process has its own address space
- Inter-process communication

MPI Example

```
#include <stdio.h>
#include <mpi.h>
int main(int argc, char *argv[])
{
    MPI_Init(&argc, &argv);
    printf(“hello world!\n");
    MPI_Finalize();
    return 0;
}
```

MPI Example

```
#include <stdio.h>
#include <mpi.h>
int main(int argc, char *argv[])
{
    int rank, size;
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Comm_size(MPI_COMM_WORLD, &size);
    printf(“hello world from %d of %d!\n", rank, size);
    MPI_Finalize();
    return 0;
}
```

MPI Communications

```
int MPI_Send(
    void* data,
    int count,
    MPI_Datatype datatype,
    int destination,
    int tag,
    MPI_Comm communicator)
int MPI_Recv(
    void* data,
    int count,
    MPI_Datatype datatype,
    int source,
    int tag,
    MPI_Comm communicator,
    MPI_Status* status)
```

MPI Communications

```
int MPI_Probe(
    int source,
    int tag,
    MPI_Comm comm,
    MPI_Status* status)
int MPI_Get_count(
    MPI_Status* status,
    MPI_Datatype datatype,
    int* count)
```

MPI Communications

```
int MPI_Isend(
        const void *buf,
        int count,
        MPI_Datatype datatype,
        int dest,
        int tag,
        MPI_Comm comm,
        MPI_Request *request)
```

MPI Communications

```
int MPI_Wait(
        MPI_Request *request,
        MPI_Status *status)

int MPI_Test(
        MPI_Request *request,
        int *flag,
        MPI_Status *status)
```

Communicator

```
int MPI_Comm_split(
        MPI_Comm comm,
        int color,
        int key,
        MPI_Comm * newcomm)

int MPI_Comm_free(MPI_Comm *comm)
```

Compilation and Execution

- MPICH, OpenMPI
- mpicc, mpiCC, mpic++
- mpiexec, mpirun
- mpiexec -np 4 ./a.out
- mpiexec --showme

- SLURM
  - sbatch
  - srun

MPI Configuration

- For each node, create a user that can ssh to all other nodes
- Install MPICH/OpenMPI
- mpirun -np 4 --hostfile myhost_file ./a.out
    - node1 slots=2 max_slots=10
    - node2 slots=2 max_slots=10

- mpirun -np 4 --hostfile myhost_file --byslot ./a.out
- mpirun -np 4 --hostfile myhost_file --bynode ./a.out

MPI Collective Communications

- MPI_Barrier(MPI_Comm communicator)
- MPI_Bcast(void* data, int count, MPI_Datatype datatype, int root,
  MPI_Comm communicator)
- MPI_Reduce(const void *sendbuf, void *recvbuf, int count,
  MPI_Datatype datatype, MPI_Op op, int root, MPI_Comm comm)
  - MPI_MIN, MPI_MAX, MPI_MINLOC, MPI_MAXLOC, MPI_BOR, MPI_BXOR, MPI_LOR, MPI_LXOR, MPI_BAND, MPI_LAND, MPI_SUM and MPI_PROD
- MPI_Allreduce(const void* send_buffer, void* receive_buffer, int count,
  MPI_Datatype datatype, MPI_Op operation,
  MPI_Comm communicator)

Cluster Computing

- MPI
  - Inter-node communication
  - High-performance computing
- Node failure
  - Broken hardware
  - Software bugs
  - Insufficient resources
- Node failure happens commonly for clusters with 1,000+ nodes
  - (1 - p)^1000

Cluster Computing

- MPI
  - Inter-node communication
  - High-performance computing
- Node failure
  - Broken hardware
  - Software bugs
  - Insufficient resources
- Node failure happens commonly for clusters with 1,000+ nodes
  - (1 - p)^1000

We need a system to handle these failures!

Distributed File System

- Decouple data and computing resources
- Replication to take care of node/disk failures
- HDFS
  - Name node
  - Data node

Common Data Analysis Tasks

- Given a large data, find some statistics
- Given a page view log, find the number of users
- Given a page view log, find the number of users group by browser
- Given a page view log, find the number of users from NY state group by browser

Map and Reduce

- PageRank
- PR(x) = \sum_{y links to (x)} (PR(y) / out_degree(y))

- Iterative disk I/O

Spark

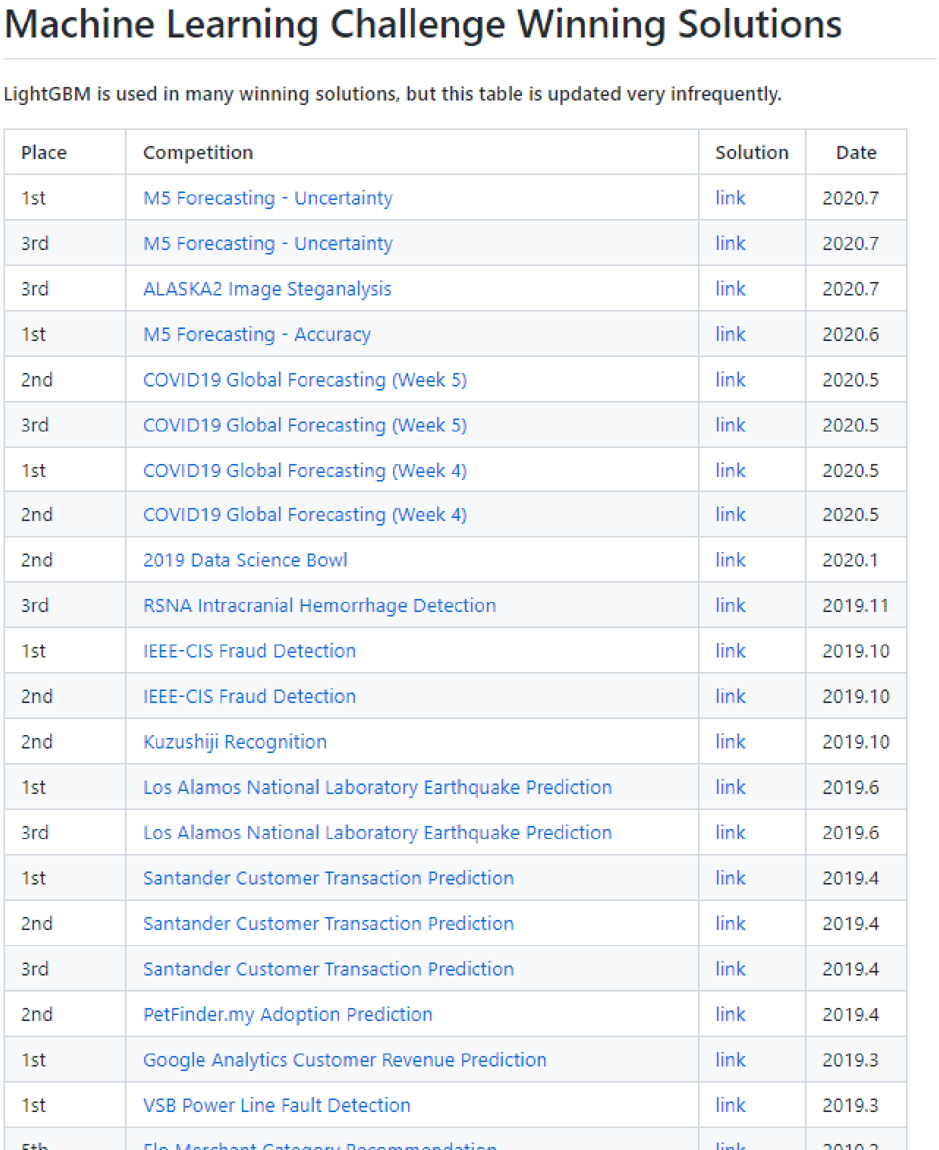
- Spark
- Resilient Distributed Dataset (RDD)
    - Immutable
    - Transformations
        - map
        - filter
        - reduceByKey
        - join
        - …
    - Actions
        - count
        - collect
        - …

Gradient Boosting

Weijie Zhao

09/20/2022

Why Gradient Boosting?



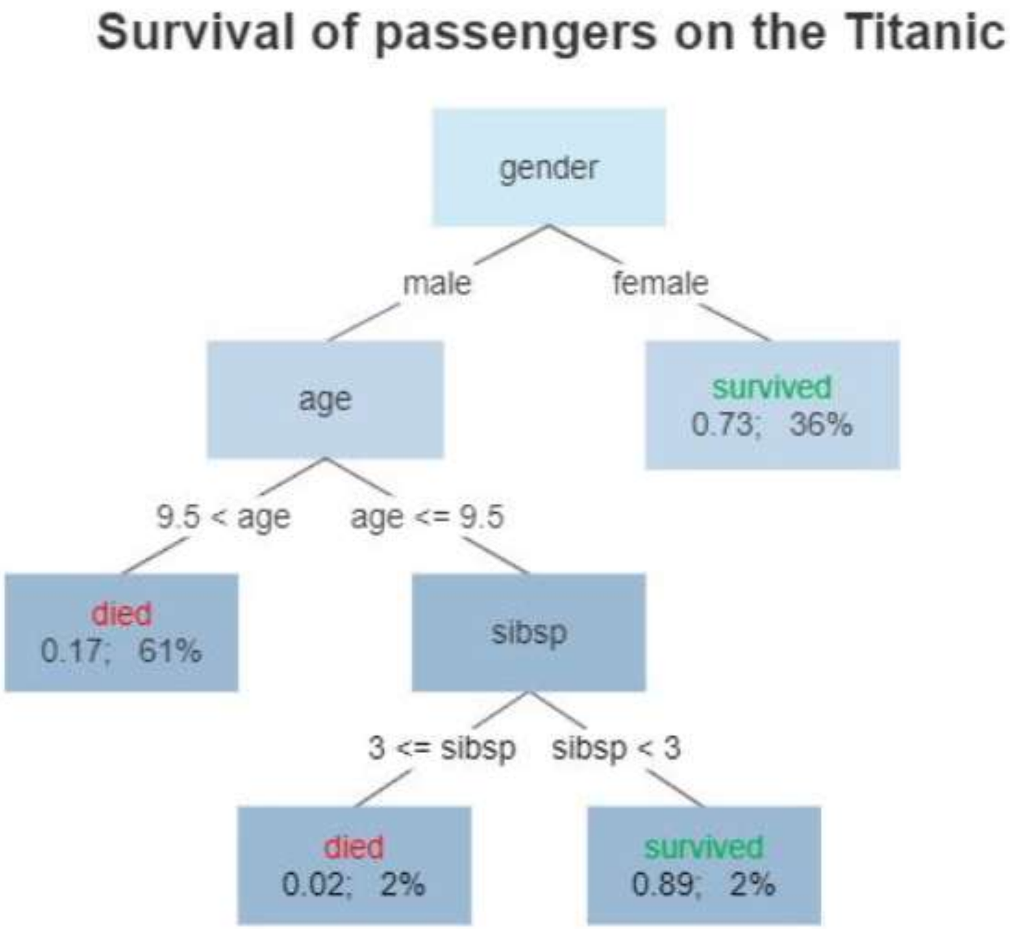
Machine Learning Challenge Winning Solutions

LightGBM is used in many winning solutions, but this table is updated very infrequently.

Place	Competition	Solution	Date
1st	M5 Forecasting - Uncertainty	link	2020.7
3rd	M5 Forecasting - Uncertainty	link	2020.7
3rd	ALASKA2 Image Steganalysis	link	2020.7
1st	M5 Forecasting - Accuracy	link	2020.6
2nd	COVID19 Global Forecasting (Week 5)	link	2020.5
3rd	COVID19 Global Forecasting (Week 5)	link	2020.5
1st	COVID19 Global Forecasting (Week 4)	link	2020.5
2nd	COVID19 Global Forecasting (Week 4)	link	2020.5
2nd	2019 Data Science Bowl	link	2020.1
3rd	RSNA Intracranial Hemorrhage Detection	link	2019.11
1st	IEEE-CIS Fraud Detection	link	2019.10
2nd	IEEE-CIS Fraud Detection	link	2019.10
2nd	Kuzushiji Recognition	link	2019.10
1st	Los Alamos National Laboratory Earthquake Prediction	link	2019.6
3rd	Los Alamos National Laboratory Earthquake Prediction	link	2019.6
1st	Santander Customer Transaction Prediction	link	2019.4
2nd	Santander Customer Transaction Prediction	link	2019.4
3rd	Santander Customer Transaction Prediction	link	2019.4
2nd	PetFinder.my Adoption Prediction	link	2019.4
1st	Google Analytics Customer Revenue Prediction	link	2019.3
1st	VSB Power Line Fault Detection	link	2019.3
5th	Elo Merchant Category Recommendation	link	2019.2

https://github.com/microsoft/LightGBM/blob/master/examples/README.md#machine-learning-challenge-winning-solutions

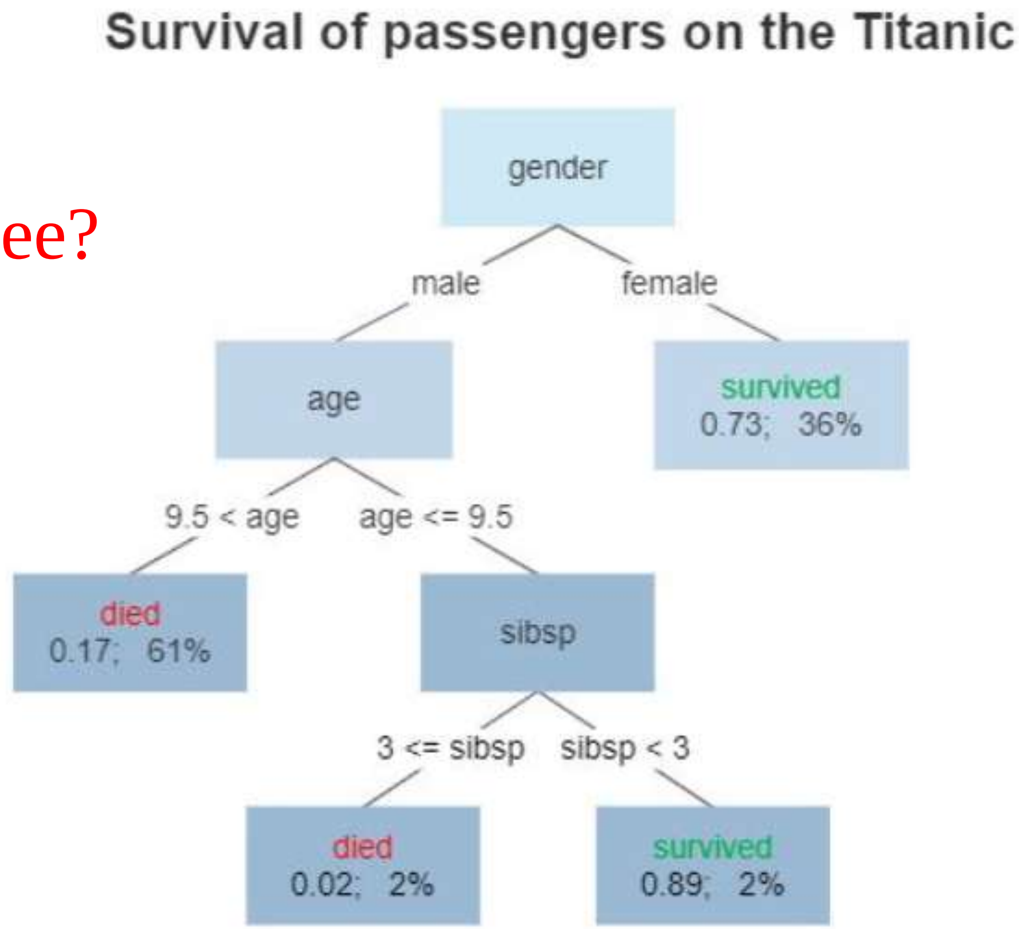
Decision Trees



https://en.wikipedia.org/wiki/Decision_tree_learning#/media/File:Decision_Tree.jpg

Decision Trees

Given a dataset, how to find the best decision tree?



https://en.wikipedia.org/wiki/Decision_tree_learning#/media/File:Decision_Tree.jpg

Tree Split Criteria

- Estimate of Positive Correctness

$$E_P = TP - FP$$

- Gini impurity

$$\mathrm{I}_G(p) = \sum_{i=1}^{J}\left(p_i \sum_{k\neq i} p_k\right) = \sum_{i=1}^{J} p_i(1-p_i) = \sum_{i=1}^{J}(p_i - p_i^2) = \sum_{i=1}^{J} p_i - \sum_{i=1}^{J} p_i^2 = 1 - \sum_{i=1}^{J} p_i^2$$

- MART gain

$$\frac{1}{s}\left[\sum_{i=1}^{s}(r_{i,k} - p_{i,k})\right]^2 + \frac{1}{N-s}\left[\sum_{i=s+1}^{N}(r_{i,k} - p_{i,k})\right]^2 - \frac{1}{N}\left[\sum_{i=1}^{N}(r_{i,k} - p_{i,k})\right]^2$$

$$r_{i,k} = 1 \text{ if } y_i = k \text{ and } r_{i,k} = 0 \text{ otherwise}$$

$$p_{i,k} = \mathbf{Pr}\left(y_i = k | \mathbf{x}_i\right)$$

Decision Trees

- Bagging
- Random Forest
- Gradient Boosting

Gradient Boosting

$$p_{i,k} = \mathbf{Pr}\left(y_i = k|\mathbf{x}_i\right) = \frac{e^{F_{i,k}(\mathbf{x_i})}}{\sum_{s=1}^{K} e^{F_{i,s}(\mathbf{x_i})}}, \qquad i = 1, 2, ..., N,$$

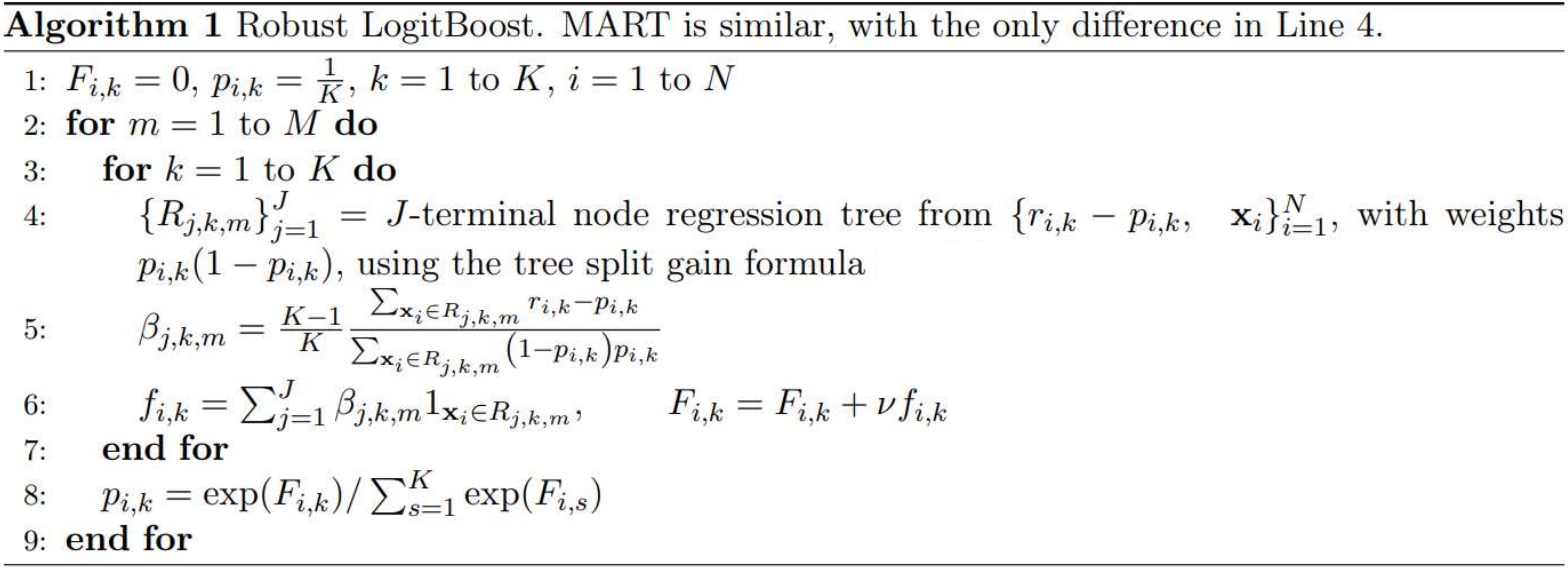
where $F_{i,k}(\mathbf{x}_i)$ is an additive model of M terms: $F^{(M)}(\mathbf{x}) = \sum_{m=1}^{M} \rho_m h(\mathbf{x}; \mathbf{a}_m),$

$$L = \sum_{i=1}^{N} L_i, \qquad L_i = -\sum_{k=1}^{K} r_{i,k} \log p_{i,k}$$

where $r_{i.k} = 1$ if $y_i = k$ and $r_{i.k} = 0$ otherwise.

$$\frac{\partial L_i}{\partial F_{i,k}} = -\left(r_{i,k} - p_{i,k}\right), \qquad \frac{\partial^2 L_i}{\partial F_{i,k}^2} = p_{i,k}\left(1 - p_{i,k}\right).$$

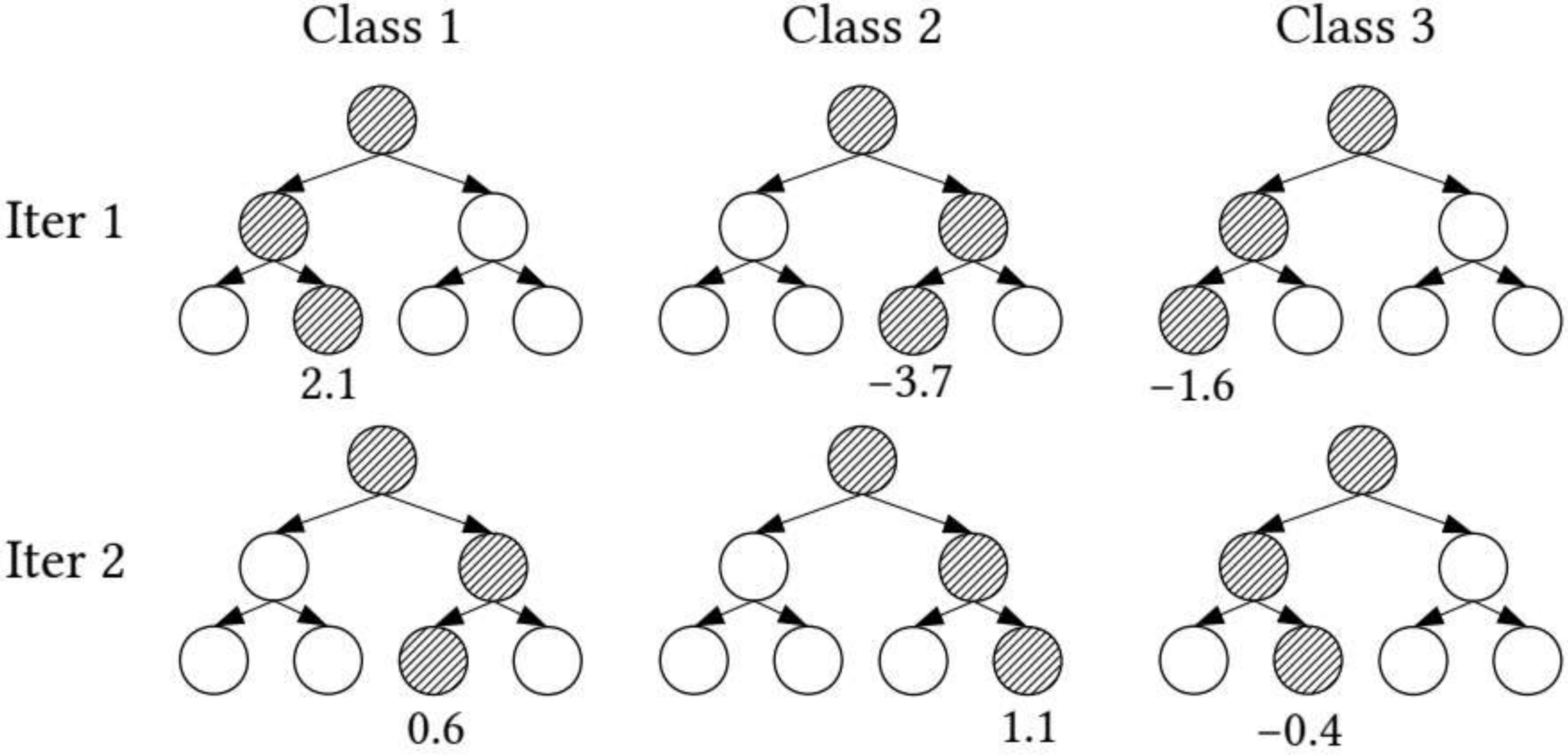
Gradient Boosting



Algorithm 1 Robust LogitBoost. MART is similar, with the only difference in Line 4.

```
1: $F_{i,k} = 0$, $p_{i,k} = \frac{1}{K}$, $k = 1$ to $K$, $i = 1$ to $N$
2: for $m = 1$ to $M$ do
3:     for $k = 1$ to $K$ do
4:         $\{R_{j,k,m}\}_{j=1}^{J}$ = $J$-terminal node regression tree from $\{r_{i,k} - p_{i,k}, \quad \mathbf{x}_i\}_{i=1}^{N}$, with weights $p_{i,k}(1 - p_{i,k})$, using the tree split gain formula
5:         $\beta_{j,k,m} = \frac{K-1}{K} \frac{\sum_{\mathbf{x}_i \in R_{j,k,m}} r_{i,k} - p_{i,k}}{\sum_{\mathbf{x}_i \in R_{j,k,m}} (1 - p_{i,k}) p_{i,k}}$
6:         $f_{i,k} = \sum_{j=1}^{J} \beta_{j,k,m} 1_{\mathbf{x}_i \in R_{j,k,m}}, \qquad F_{i,k} = F_{i,k} + \nu f_{i,k}$
7:     end for
8:     $p_{i,k} = \exp(F_{i,k}) / \sum_{s=1}^{K} \exp(F_{i,s})$
9: end for
```

Gradient Boosting



$F_{2,1} = 2.1 + 0.6 = 2.7$ $F_{2,2} = -3.7 + 1.1 = -2.6$ $F_{2,3} = -1.6 - 0.4 = -2.0$

$p_{2,1} = 0.986$ $p_{2,2} = 0.005$ $p_{2,3} = 0.009$

Data Reading

- Matrix Format
- CSV
- LIBSVM

Data Reading

- Matrix Format
- CSV
- LIBSVM

- How should we store the parsed data?

Serialization/Deserialization

- Handwritten
  - Endian problem

Endianness

- Danny Cohen introduced the terms big-endian and little-endian into computer science for data ordering in an Internet Experiment Note published in 1980.
- In the 1726 novel Gulliver's Travels, he portrays the conflict between sects of Lilliputians divided into those breaking the shell of a boiled egg from the big end or from the little end. He called them the Big-Endians and the Little-Endians.
- Cohen makes the connection to Gulliver's Travels explicit in the appendix to his 1980 note.

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

Serialization/Deserialization

- Handwritten
  - Endian problem

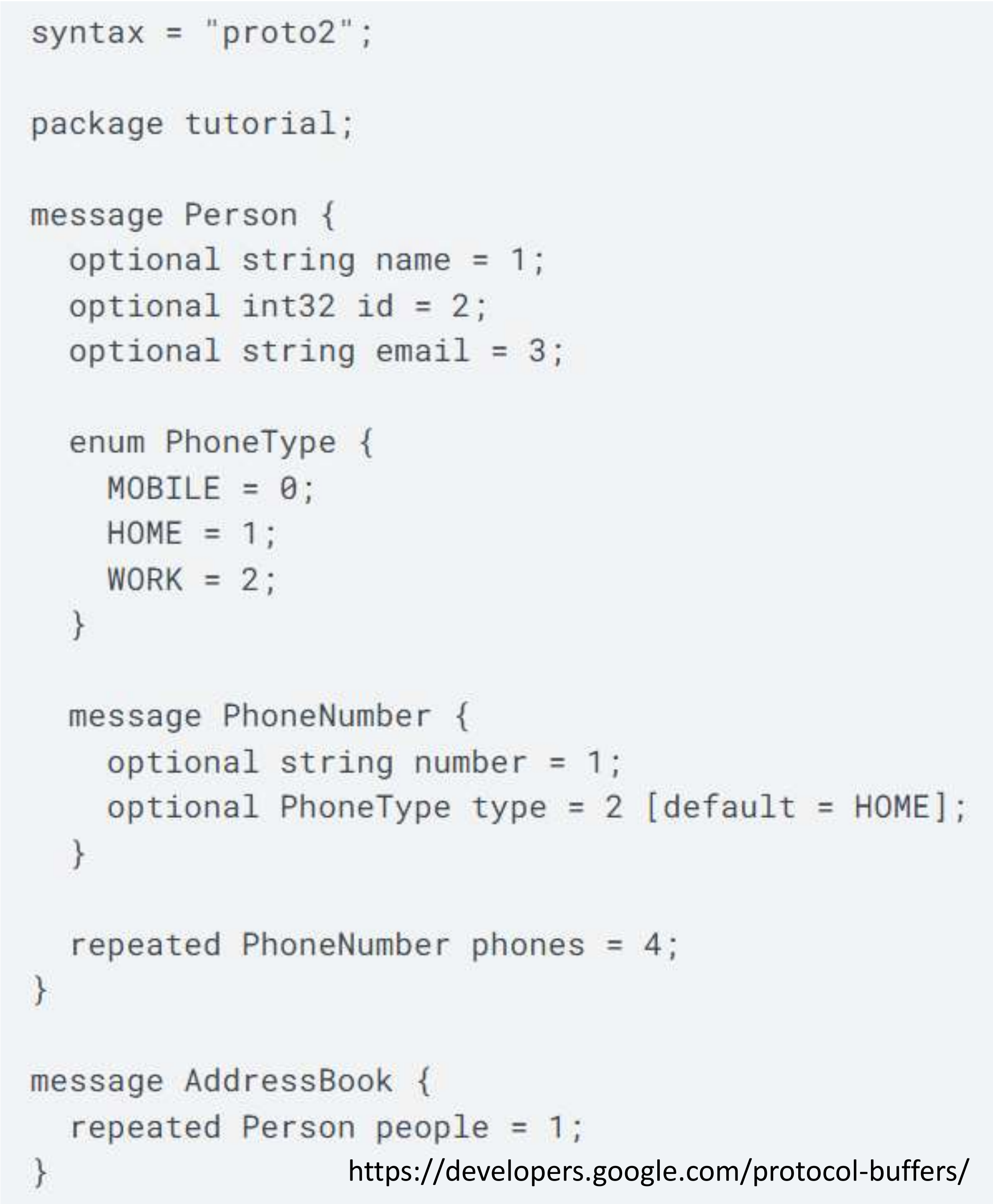
```
bool is_big_endian(void){
    union {
        uint32_t i;
        char c[4];
    } bint = {0x01020304};

    return bint.c[0] == 1;
}
```

Serialization/Deserialization

- Handwritten
  - Endian problem
- Protocol Buffer

conda install -c anaconda protobuf

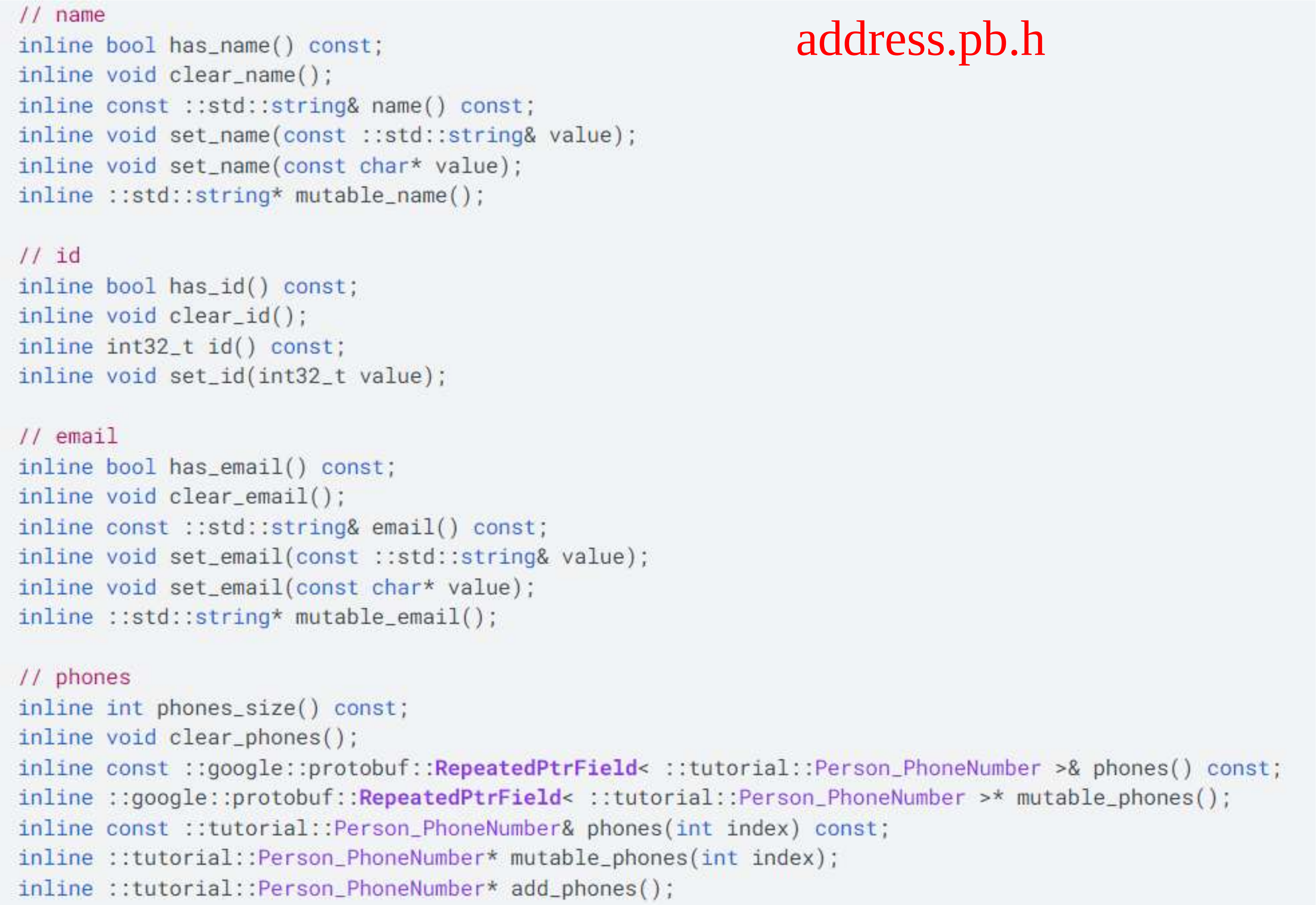
protoc --cpp_out=DST_DIR --
python_out=DST_DIR
path/to/file.proto



```
syntax = "proto2";

package tutorial;

message Person {
  optional string name = 1;
  optional int32 id = 2;
  optional string email = 3;

  enum PhoneType {
    MOBILE = 0;
    HOME = 1;
    WORK = 2;
  }

  message PhoneNumber {
    optional string number = 1;
    optional PhoneType type = 2 [default = HOME];
  }

  repeated PhoneNumber phones = 4;
}

message AddressBook {
  repeated Person people = 1;
}
```

https://developers.google.com/protocol-buffers/

address.pb.h



```
// name
inline bool has_name() const;
inline void clear_name();
inline const ::std::string& name() const;
inline void set_name(const ::std::string& value);
inline void set_name(const char* value);
inline ::std::string* mutable_name();

// id
inline bool has_id() const;
inline void clear_id();
inline int32_t id() const;
inline void set_id(int32_t value);

// email
inline bool has_email() const;
inline void clear_email();
inline const ::std::string& email() const;
inline void set_email(const ::std::string& value);
inline void set_email(const char* value);
inline ::std::string* mutable_email();

// phones
inline int phones_size() const;
inline void clear_phones();
inline const ::google::protobuf::RepeatedPtrField< ::tutorial::Person_PhoneNumber >& phones() const;
inline ::google::protobuf::RepeatedPtrField< ::tutorial::Person_PhoneNumber >* mutable_phones();
inline const ::tutorial::Person_PhoneNumber& phones(int index) const;
inline ::tutorial::Person_PhoneNumber* mutable_phones(int index);
inline ::tutorial::Person_PhoneNumber* add_phones();
```

Protocol Buffer

- bool SerializeToString(string* output) const
- bool ParseFromString(const string& data)
- bool SerializeToOstream(ostream* output) const
- bool ParseFromIstream(istream* input)

- #include “…pb.h”
- g++ ……. -lprotobuf