Machine Learning and Data Mining

Meta-algorithms

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September 20, 2017

In the last episode

```
def data_science(problem_description,
                 domain_expertise=None,
                 *args, **kwargs):
  if problem_description is None:
    raise Exception('Learning is impossible!')

  prior_on_algorithms = \
    data_scientist.world_knowledge.infer(
      problem_description,
      domain_expertise,
      *args, **kwargs
    )

  return prior_on_algorithms
```

Making algorithms

Constructing learning algorithms from scratch is hard:

- it is the reason people use machine learning instead of classical statistical approach.

- producing tons of simple, rude algorithms is quite easy;
- fitting all-powerful zero-bias classifier is easy.

Can an good algorithm be assembled from a set of simple ones?

Bootstrap

Settings

Suppose we have a quite good learning algorithm $f(x, D)$ where:

- D is a dataset,
- x is a point of interest,

with **high variance** and **low bias**.

What is the most common way of decreasing variance of mean estimate of a random variable?

Bootstrap

Let's consider average over multiple datasets:

$$F(x) = \frac{1}{n}\sum_i f(x, D_i) \approx \mathop{\mathbb{E}}_{D\sim P^n(X,Y)} f(x, D) = \hat{F}(x)$$

If D_i are i.i.d:

- $F(x)$ would reduce variance.

If D_i are correlated (via $f(x, D_i)$):

$$\mathbb{D}\left[\frac{1}{n}\sum_i Z_i\right] = \frac{\sigma^2}{n}\left(1 + (n-1)\rho\right) \to_{n\to\infty} \rho$$

where:

- $\mathbb{D}\left[Z_i\right] = \sigma^2$, $\rho = \mathrm{corr}(Z_i, Z_j)$ $(i \neq j)$.

Non-parametric bootstrap

Let's approximate $P(X, Y)$ by $\mathbb{U}\{D\}$:

- consider $D_i = \{(x_j^i, y_j^i)\}_{j=1}^m$ drawn i.i.d from D with replacement:

$$F(x) = \sum_{D_i \sim \mathbb{U}^m\{D\}} f(x, D_i)$$

- it will reduce variance.

Seems like model's variance was reduced for 'free', where is the catch?

Parametric bootstrap

If we have a sacred knowledge then we can:

- **using D produce more accurate $\hat{P}(X, Y)$ than $\mathbb{U}^n \{D\}$**

E.g. for regression:

$$D_i = \{(x_i, y_i + \varepsilon)\}_{i=1}^{N}$$

where:

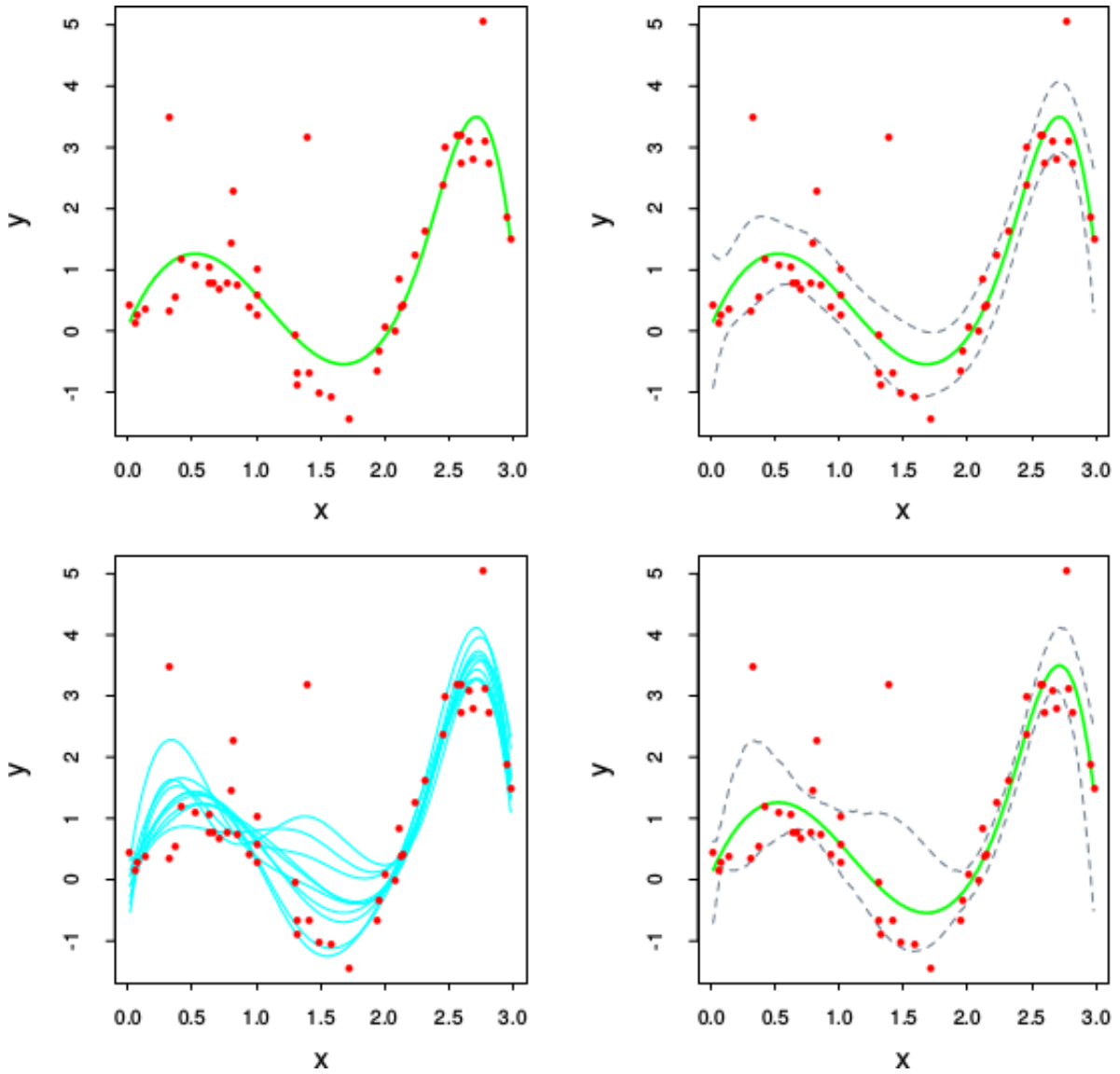
- $\varepsilon \sim \mathcal{N}(0, \sigma_\varepsilon)$

Parametric bootstrap

...the bootstrap mean is approximately a posterior average ...

For details:
Hastie, T., Tibshirani, R. and Friedman, J., 2001. The elements of statistical learning, ser., chapter 8

Bootstrap



Bootstrap: a note

Sometimes we can produce more diverse $\{f(x, D_i)\}_i$ by training on feature subsets.

Stacking: settings

Bayesian averaging:

- ζ - variable of our interest (e.g. f(x));
- $\mathcal{M}_m, m = 1, \ldots, M$ - a candidate models;
- D - training dataset.

$$\mathbb{E}(\zeta \mid D) = \sum_m \mathbb{E}(\zeta \mid \mathcal{M}_m, D) P(\mathcal{M}_m \mid D) = \sum_m w_m \, \mathbb{E}(\zeta \mid \mathcal{M}_m, D)$$

$$w_m = P(\mathcal{M}_m \mid D)$$

Stacking: BIC

$$P(\mathcal{M}_m \mid D) \sim P(\mathcal{M}_m) P(D \mid \mathcal{M}_m)$$

$P(D \mid \mathcal{M}_m)$ can be:

- computed directly;
- estimated by Bayesian Information Coefficient:

$$-\log P(D \mid \mathcal{M}_m) \underbrace{\approx}_{\text{uniform prior}} \frac{1}{2}\mathrm{BIC} = -\mathrm{LogLik} \frac{d}{2} N + O(1)$$

Stacking

Frequentist view:

$$\hat{w} = \arg\min_{w} \sum_{i} \left[y_i - \sum_{m} w_m f_m^{-i}(x_i) \right]^2$$

where:

- f_m^{-i} - m-th model trained without i-th sample.

Stacking in general

Often the following procedure is referred as stacking:

- base dataset, stacking dataset: $D_b \cap D_s = \varnothing$;
- let $\{f_m\}_m$ be different models trained on D_s;
- train stacking model:

$$\mathcal{L}_g = \sum_{i \in D_s} l\left(g(f_1(x_i), f_2(x_i), \ldots, f_m(x_i)), y_i\right) \to_g \min$$

Random forest

$$\mathrm{RandomForest} = \left\{ \begin{array}{c} \text{sample bagging} \\ + \\ \text{feature bagging} \end{array} \right\} \text{(Decision Tree)}$$

Stacking: discussion

- usually stacking model is simple:
  - linear models (e.g. LASSO, Ridge);
  - logistic regression;
- stacking is great:
  - when base model has high variance:
  - i.e. the model is over parametrized;
- can be easily trained in parallel;
- can't make model more complex;
- in practice, often, though as one of the last resorts.

Calibration

- if base model does not provide proper probability estimates (e.g. SVM, Trees)
- logistic regression (or simple network) over its scores
- trained with proper loss (e.g. cross-entropy)
- can **calibrate** base model.

Stacking: discussion

Why not just use one tree with fewer terminal nodes instead of random forest?

Boosting

Boosting: settings

Settings:

- a number of simple, **weak** (high bias, low variance) models;
- for simplicity, we consider one big set of models $\mathcal{H} = \{h^i\}_i$:
  - (the most common case) one training procedure.

Boosting: general idea

Like in stacking we wish to build an ensemble:

$$F(x) = \sum_i \alpha_i h^i(x)$$

Matching pursuit strategy:

- sequentially add models one by one into ensemble:

$$\begin{aligned} F^0 &= \text{const}; \\ h^{t+1} &= \arg\min_{\alpha; h \in \mathcal{H}} \mathcal{L}(F^t + \alpha_{t+1} h); \\ F^{t+1} &= F^t + \alpha h^{t+1}. \end{aligned}$$

AdaBoost

AdaBoost is a classifier, that utilizes exponential loss:

$$\mathcal{L}(f) = \sum_i \exp\left[-y_i f(x_i)\right]$$

$$\mathcal{L}(F^{t+1}) = \sum_i \exp\left[-y_i(F^t(x) + \alpha h(x))\right] =$$

$$\sum_i \exp\left[-y_i F^t(x)\right] \cdot \exp\left[-y_i \alpha h(x)\right] =$$

$$\sum_i w_i^t \exp\left[-y_i \alpha h(x)\right] \to \min$$

AdaBoost

An interesting properties of AdaBoost:

- training of the sequential classifier is a classification problem;
- if weak classifier return values $\{-1, 1\}$:

$$\alpha^{t+1} = \frac{1}{2}\left(\frac{\sum_{i \in \text{correct}} w_i^t}{\sum_{i \in \text{incorrect}} w_i^t}\right)$$

- due to exponential loss AdaBoost tends to everfit quickly;
- proper multiclass formulation can be found in:

  Zhu, J., Zou, H., Rosset, S. and Hastie, T., 2009. Multi-class adaboost. Statistics and its Interface, 2(3), pp.349-360.

Gradient boosting machine

In general solving:

$$\mathcal{L}(F^{t+1}) = \mathcal{L}(F^t + \alpha h) \rightarrow_{\alpha,h} min$$

might not be tractable.

Gradient boosting machine

Strategy:

$$\mathcal{L}(F^{t+1}) = \sum_i l\left[y_i, F^t(x) + \alpha h(x)\right] \to \min \tag{1}$$

for small $\alpha h(x)$:

$$\alpha h(x) \approx -\nabla_{F^t} l\left[y_i, F^t(x)\right]$$

Gradient boosting machine

- $F^0 = \text{const}$;
- repeat for $t \in 0, \ldots, (T-1)$:
  - compute pseudo-residuals $r_i^{t+1} = -\nabla_{F^t} l\left[y_i, F^t(x)\right]$;
  - fit h^{t+1} to r_i^t;
  - compute α^{t+1}.
  - $F^{t+1} \leftarrow F^t + \alpha^{t+1} h^{t+1}$

GBM: discussion

- $\nabla_{F_t} l\left[y_i, F_t(x)\right]$ almost always can be computed analytically;
- solving for

$$\alpha^{t+1} = \arg\min_{\alpha} \mathcal{L}(F^t + \alpha h^{t+1})$$

  is a one-dimensional problem;
- typically, a shrinkage factor ρ is also introduced:

$$F^{t+1} \leftarrow F^t + \rho\alpha^{t+1} h^{t+1}$$

- sometimes α is just omitted (if ρ is small enough).

Boosted Decision Trees

BDT: settings

Boosted Decision Trees is a gradient boosting on decision trees:

- loss:

$$\mathcal{L}(F) = \sum_i l(y_i, F(x)) + \Omega(F)$$

$$\Omega(f_t) = \gamma N^t + \frac{\lambda}{2} \sum_{k=1}^{N} w_k^t$$

where:

- l - cross-entropy loss is commonly used;
- $\Omega(F) = \sum_t \Omega(f^t)$;
- N^t - number of leafs in tree h^t;
- w_k^t - prediction of k-th leaf of f^t.

BDT

Performing one step of Newton-Raphson:

$$\mathcal{L}(F^t + f) \approx$$

$$\mathcal{L}(F^t) + \underbrace{\nabla\mathcal{L}(F^t)}_{=\sum_i g_i^t} f + \frac{1}{2}\underbrace{\mathbb{H}\mathcal{L}(F^t)}_{=\sum_i h_i^t} f^2 + \Omega(F^t + h) =$$

$$\mathcal{L}(F^t) + \sum_i g_i^t h + \frac{1}{2}\sum h_i^t f^2 + \Omega(F^t) + \Omega(f)$$

where:

- $\nabla\mathcal{L}(FTt) = \sum_i \nabla_{F^t(x_i)} l(y_i, F^t(x_i))$ - gradient;
- $\mathbb{H}$ - hessian, second derivative;

BDT

Let's consider each individual leaf k:

$$\Delta\mathcal{L}(f) = \sum_i g_i^t f_i + \frac{1}{2}\sum h_i^t f_i^2 + \Omega(f) =$$

$$\sum_{k=1}^{N}\left[G_k w_k + \frac{1}{2}(H_k + \lambda)w_k^2\right] + \gamma N$$

Solution for w_k:

$$w_k^* = -\frac{G_k}{H_k + \lambda}$$

Loss:

$$\mathcal{L}^* = -\frac{1}{2}\sum_k \frac{G_k^2}{H_k + \lambda} + \gamma N$$

BDT

$$\mathcal{L}^* = -\frac{1}{2}\sum_k \frac{G_k^2}{H_k + \lambda} + \gamma N$$

Splitting criteria:

$$\text{gain} = \frac{1}{2}\left[\frac{G_L^2}{H_L + \lambda} + \frac{G_R^2}{H_R + \lambda} - \frac{G_L^2 + G_R^2}{H_L + H_R + \lambda}\right] - \gamma$$

BDT

$$\text{gain} = \frac{1}{2}\left[\frac{G_L^2}{H_L+\lambda} + \frac{G_R^2}{H_R+\lambda} - \frac{G_L^2+G_R^2}{H_L+H_R+\lambda}\right] - \gamma$$

Tree growing algorithm:

- for each feature compute gain of optimal split;
- select best feature with $\text{gain} > 0$, perform split;
- repeat until no features with $\text{gain} > 0$.

Discussion

- BDT replaces gradient-step with Newton-Raphson step;
- usage of Decision Trees allows for a good training procedure;
- search for split by each feature is a one dimensional problem:
  - H_L, H_R, G_L, G_R can be recomputed efficiently;
- can be parallelized by features;
- BDT uses **regression** trees for classification (just a little bit odd);

Discussion

- boosting can actually create fundamentally new algorithm:
  - consider Decision Trees as kind of boosting;
- a tons of implementations and modifications:
  - classic: XGBoost;
  - oblivious trees: CatBoost (MatrixNet);
- achieves state-of-the-art results ...sometimes, blah-blah-blah... No-Free-Lunch.

Discussion

Why so greedy?

References

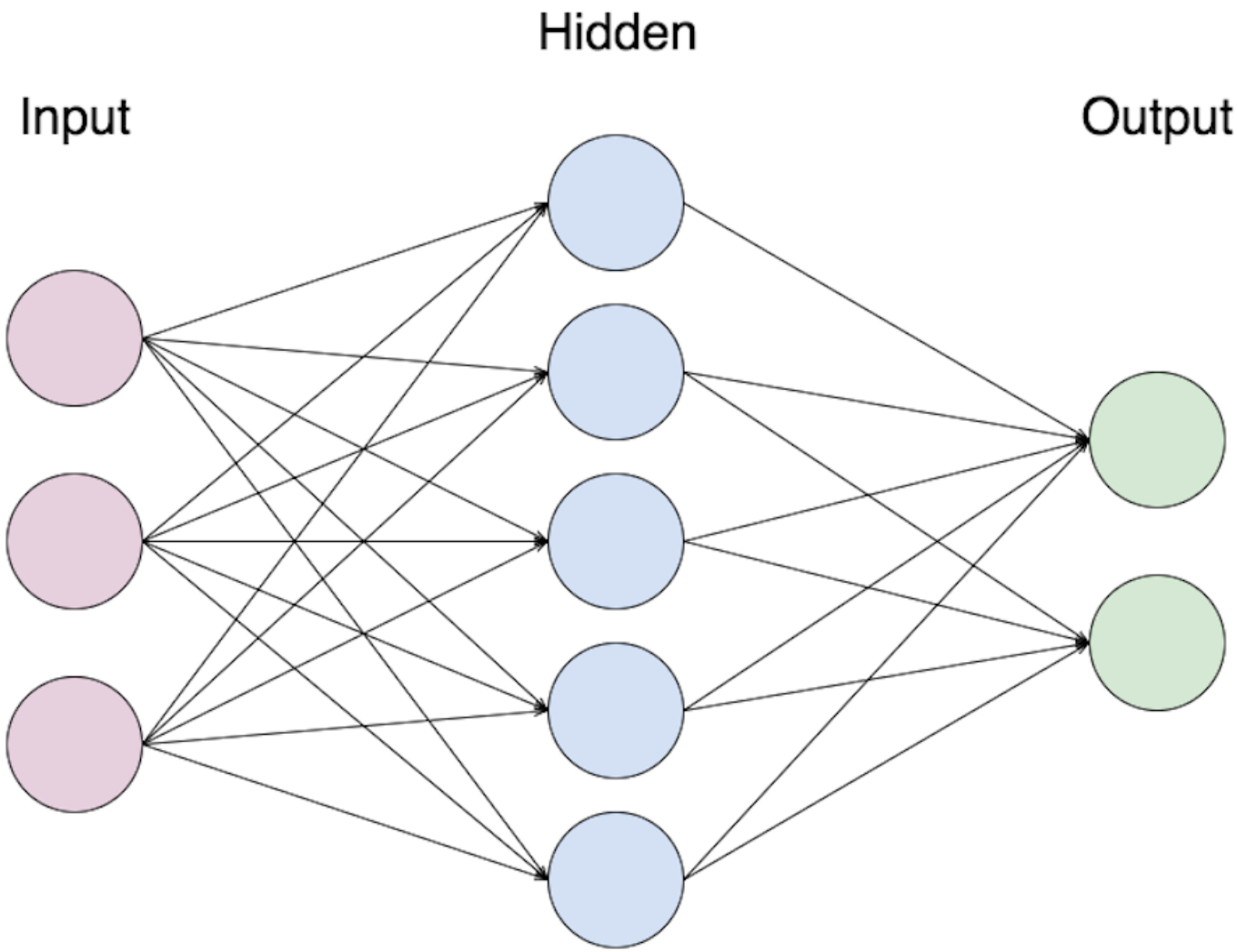
- Bishop, C.M., 2006. Pattern recognition and machine learning. springer.
- Friedman, J., Hastie, T. and Tibshirani, R., 2001. The elements of statistical learning (Vol. 1, pp. 241-249). New York: Springer series in statistics.
- Freund, Y., Schapire, R. and Abe, N., 1999. A short introduction to boosting. Journal-Japanese Society For Artificial Intelligence, 14(771-780), p.1612.
- Zhu, J., Zou, H., Rosset, S. and Hastie, T., 2009. Multi-class adaboost. Statistics and its Interface, 2(3), pp.349-360.
- Friedman, J.H., 2001. Greedy function approximation: a gradient boosting machine. Annals of statistics, pp.1189-1232.
- https://xgboost.readthedocs.io/en/latest/model.html

Bonus

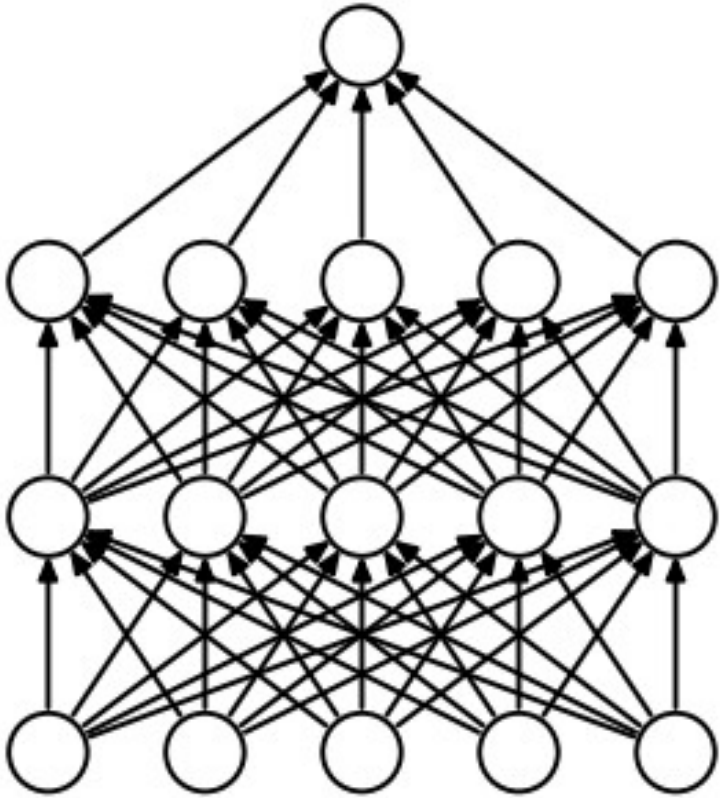
Bonus 1

Is it a good idea to boost logistic regression?

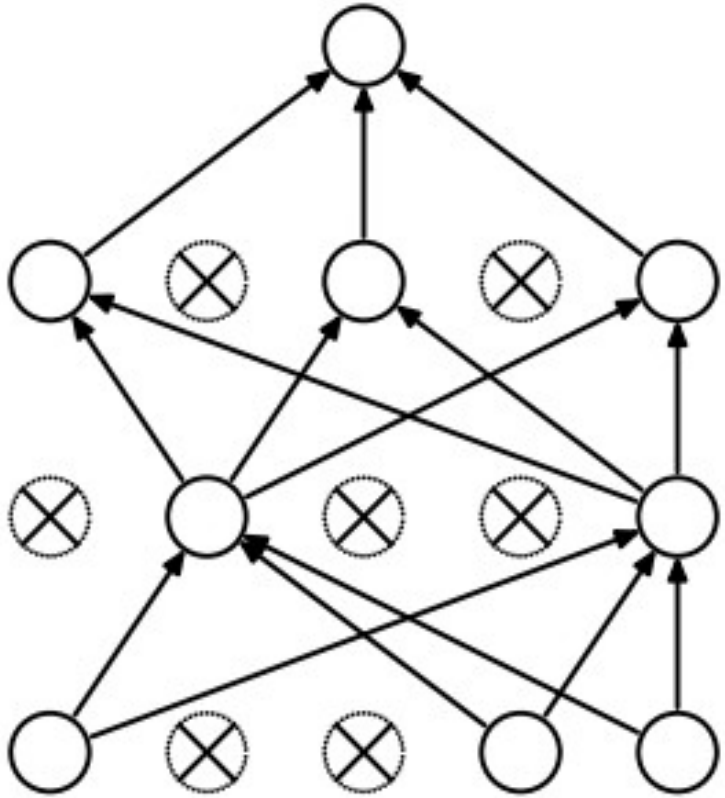
A one-layer neural network



Almost bagging in Deep Learning

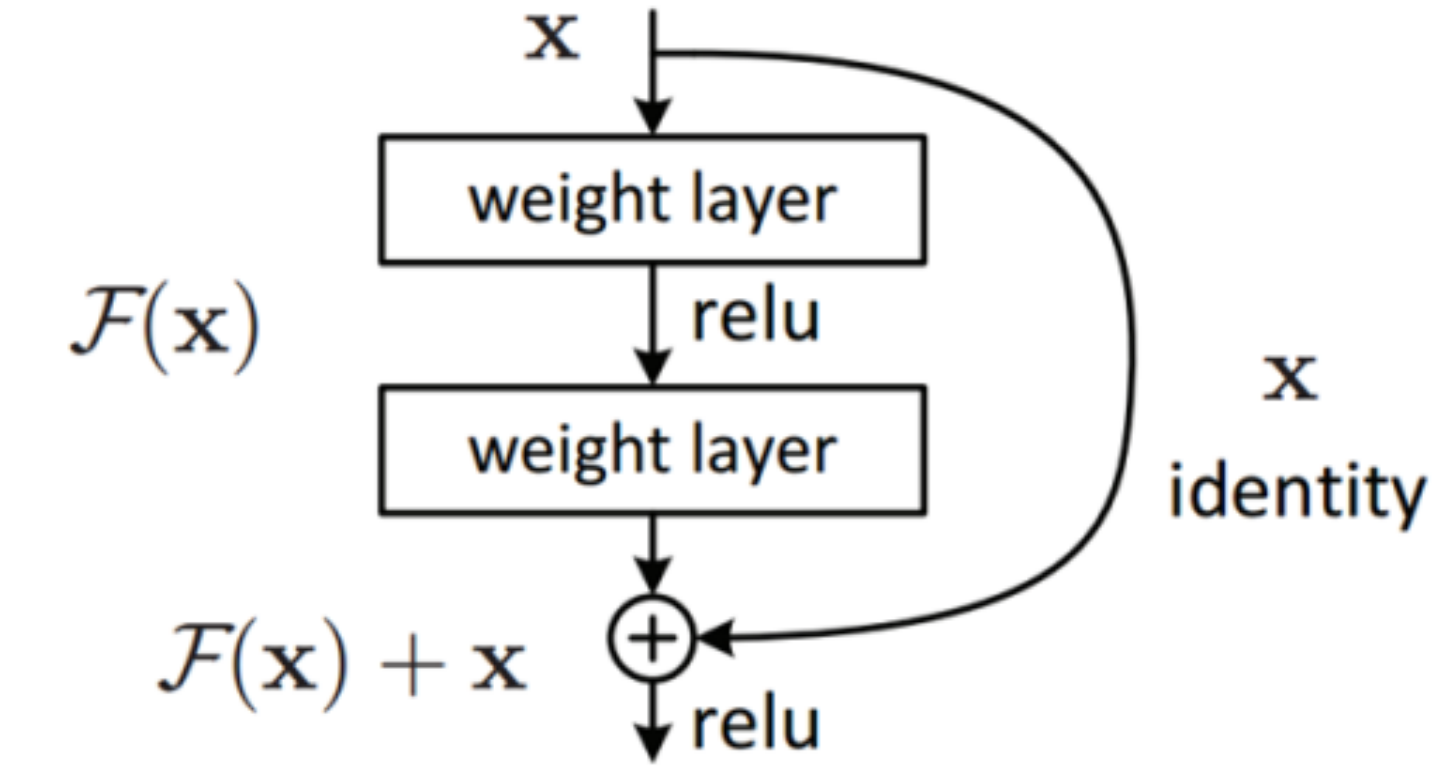


(a) Standard Neural Net



(b) After applying dropout.

Boosting (?)



A residual block

Boosting and neural networks

If Decision Tree can be viewed as equal to a 2-layer network boosting add third layer.