Deep Learning and Mixed Integer Optimization

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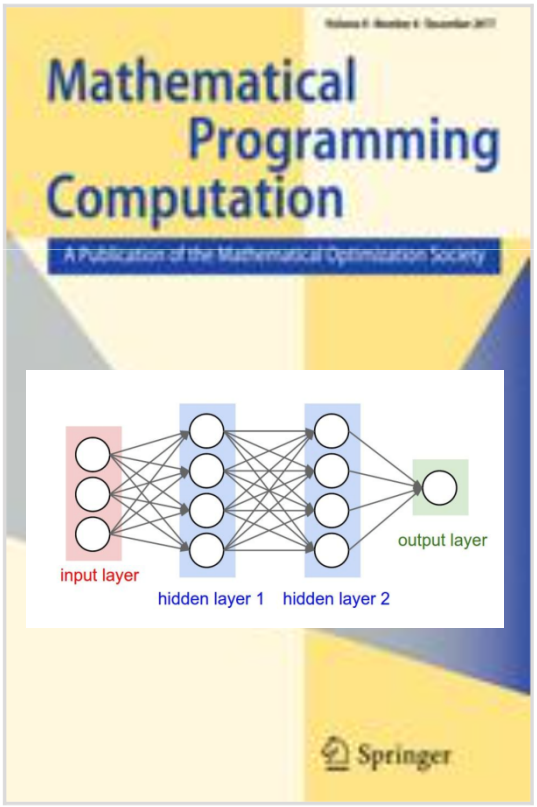
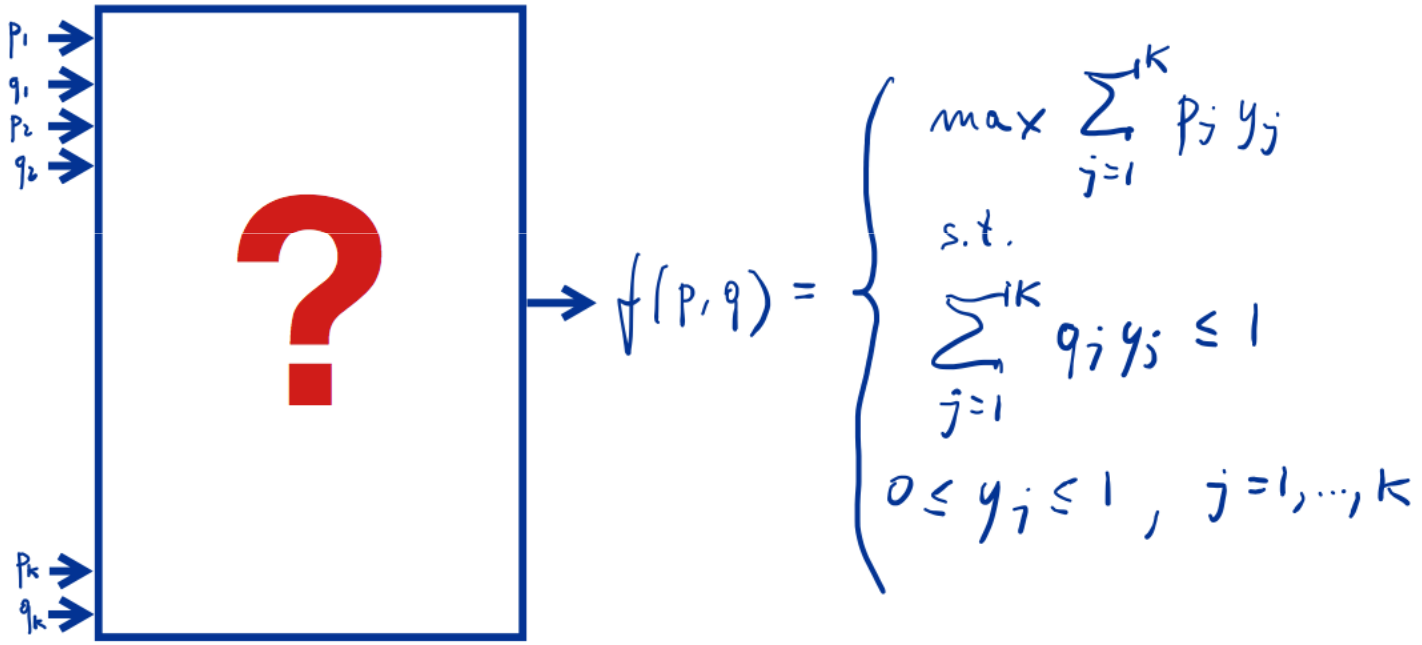
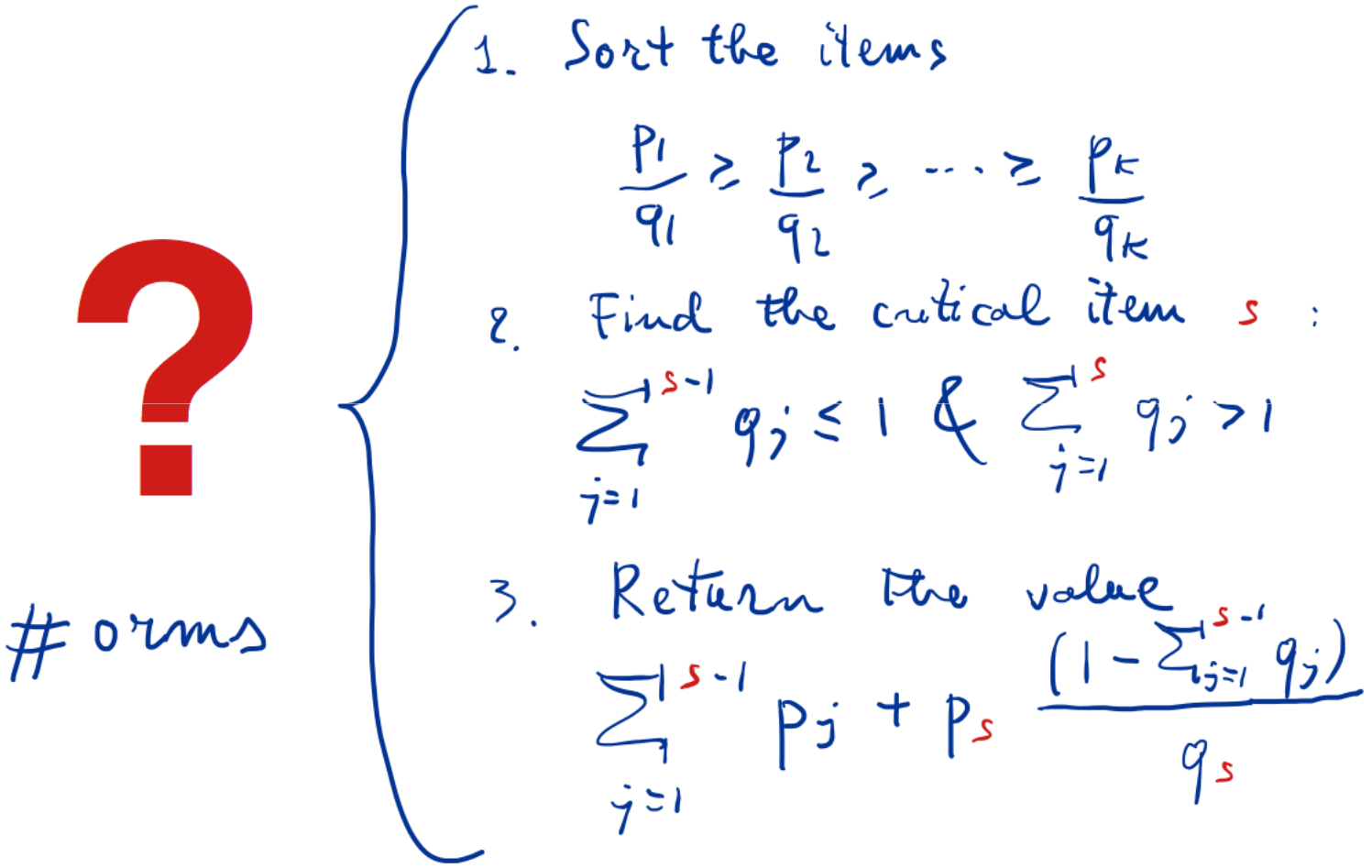


Machine Learning

- **Example** (MIPpers only!): Continuous 0-1 Knapack Problem with a fixed n. of items



Implementing the ? in the box



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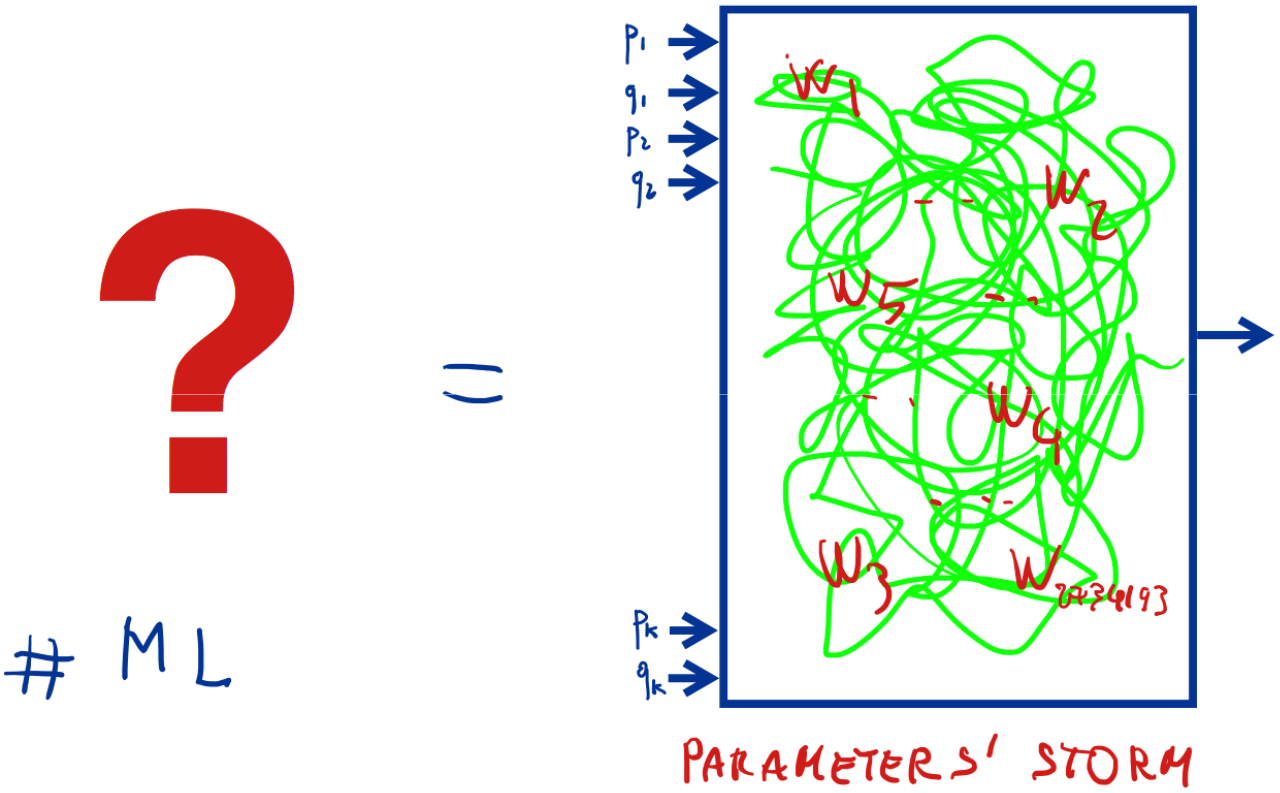
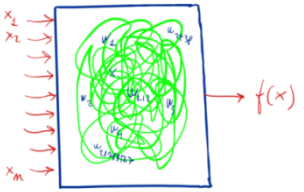
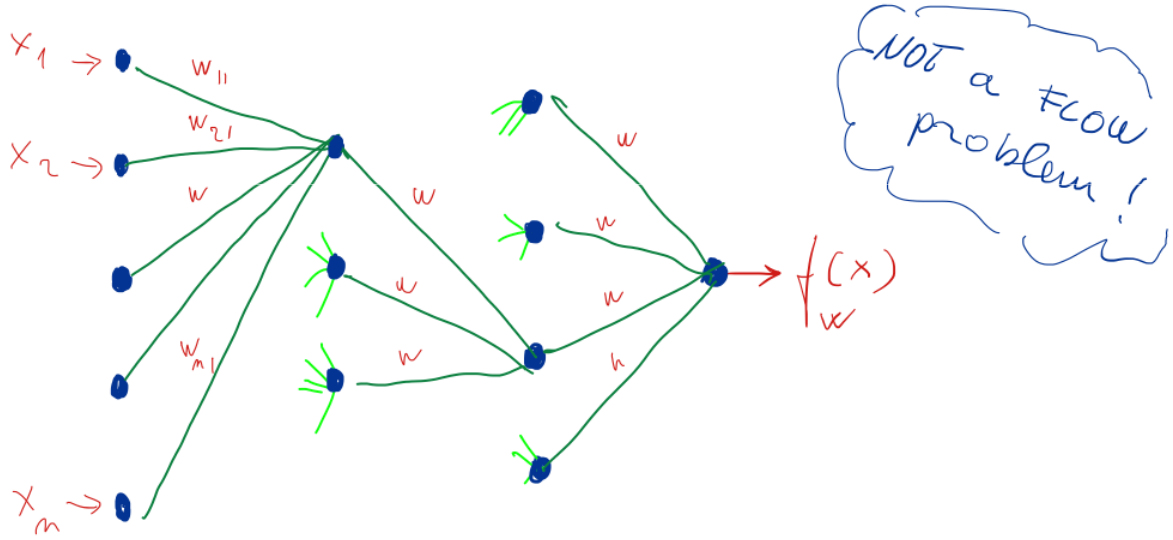


Deep Neural Networks (DNNs)



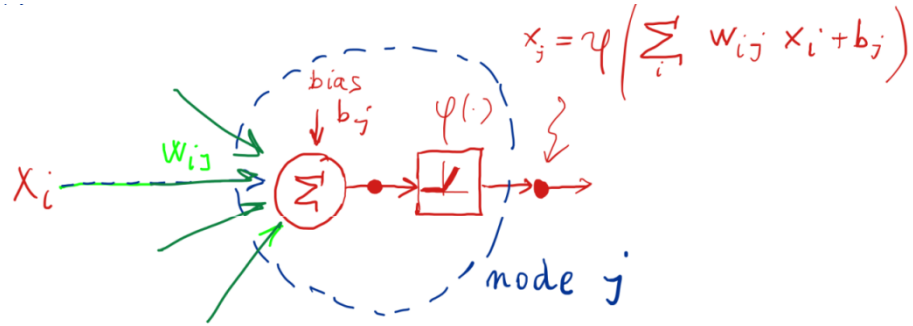
- Parameters *w*'s are organized in a layered feed-forward **network** (DAG = Directed Acyclic Graph)



- Each node (or "**neuron**") makes a **weighted sum** of the outputs of the previous layer → no "flow splitting/conservation" here!

The need of nonlinearities

- We want to be able to play with a huge n. of parameters, but if everything stays **linear** we actually have ***n+1*** parameters only → we need **nonlinearities** somewhere!
- Zooming into neurons we see the nonlinear "**activation functions**"



- Each neuron acts as a **linear SVM**, however …

  … its output is not interpreted immediately …

  … but it becomes a new feature …

  … to be forwarded to the next layer for further analysis **#SVMcascade**

Training

- For a given DNN, we need to give appropriate values to the *(w,b)* parameters to approximate the output function *f* well

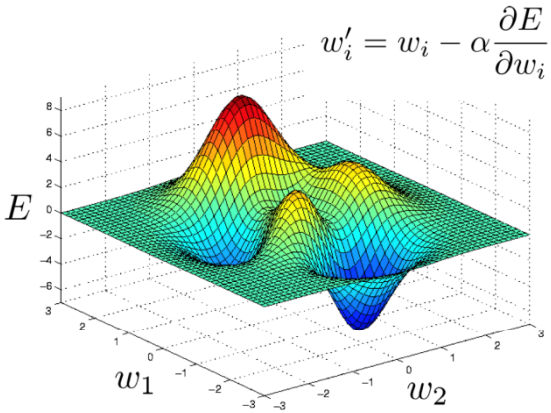
- Warning: DNNs are usually highly over-parametrized!

Table 1 showing different architectures statistics

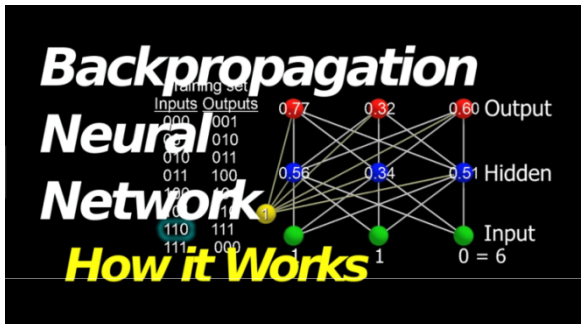
Model	AlexNet	GoogleNet	ResNet152	VGGNet16	NIN
#Param	60M	7M	60M	138M	7.6M
#OP	1140M	1600M	11300M	15740M	1100M
Storage (MB)	217	51	230	512.24	29

- **Supervised learning**:
  - define an **optimization problem** where the parameters are the unknowns
  - (huge) **training set** of points *x* for which we know the "true" value *f*(x)*
  - **objective function**: average loss/error over the training set (+ regularization terms) → to be minimized on the training set **(but … not too much!)**
  - **validation set**: can be used to select "hyperparameters" not directly handled by the optimizer (it plays a crucial role indeed…)
  - **test set:** points not seen during training, used to evaluate the actual accuracy of the DNN on (future) unseen data.

The three pillars of (practical) Deep Learning



1) Stochastic Gradient Descent



2) Backpropagation

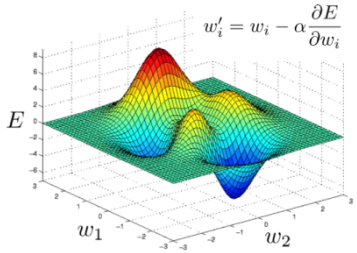
3) GPUs (and open-source Python libraries like Keras, pyTorch, TensorFlow etc.)

Stochastic Gradient Descent (SGD)

- Objective function to minimize:

  average error over a huge training set

  (hundreds of millions of param.s and training points)

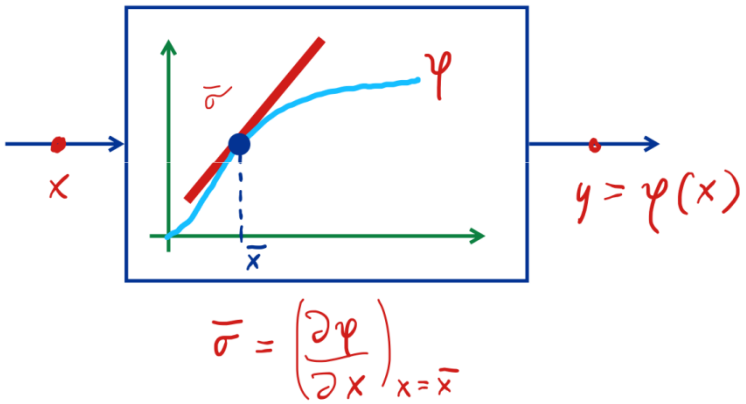


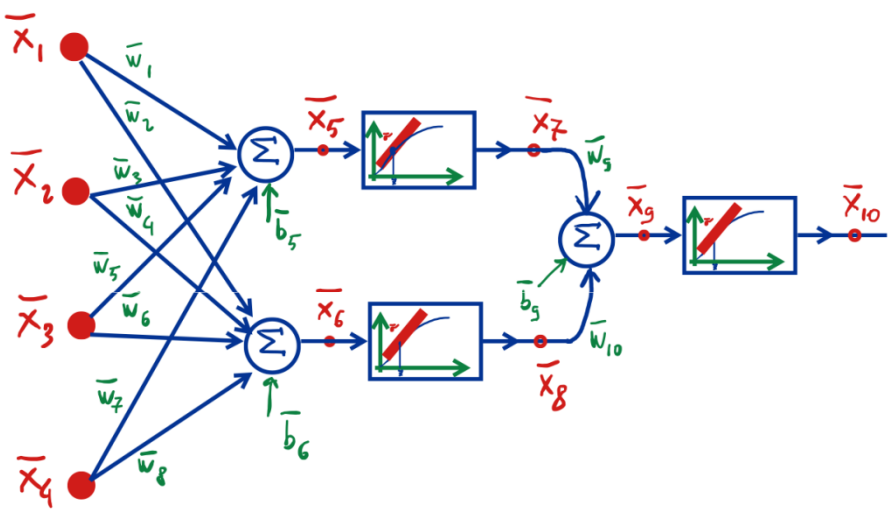
- **SGD is not at all a naïve approach**!
  - Very well suited here as the objective is an **average** over the training set, so one can approximate it by selecting a **random training point** (or a small "**mini-batch**" of such points) at each iteration
  - Practical experience shows that it often leads to a very good local minimum that "**generalizes well**" over unseen points
  - Further regularization by **dropout** (just an easy way to hurt optimization!)
- **Question**: does it make sense to look for global optimal solutions using much more sophisticated methods, that are more time consuming and are unlike to generalize equally well?

Efficient gradient computation

- We are given a **single** training point $\overline{x}$ and the **current param.s** $(\overline{w}, \overline{b})$ and we want to compute the **gradient** of the error function *E* in $(\overline{x}, \overline{w}, \overline{b})$

- **Linearize** the DNN w.r.t. $(\overline{x}, \overline{w}, \overline{b})$



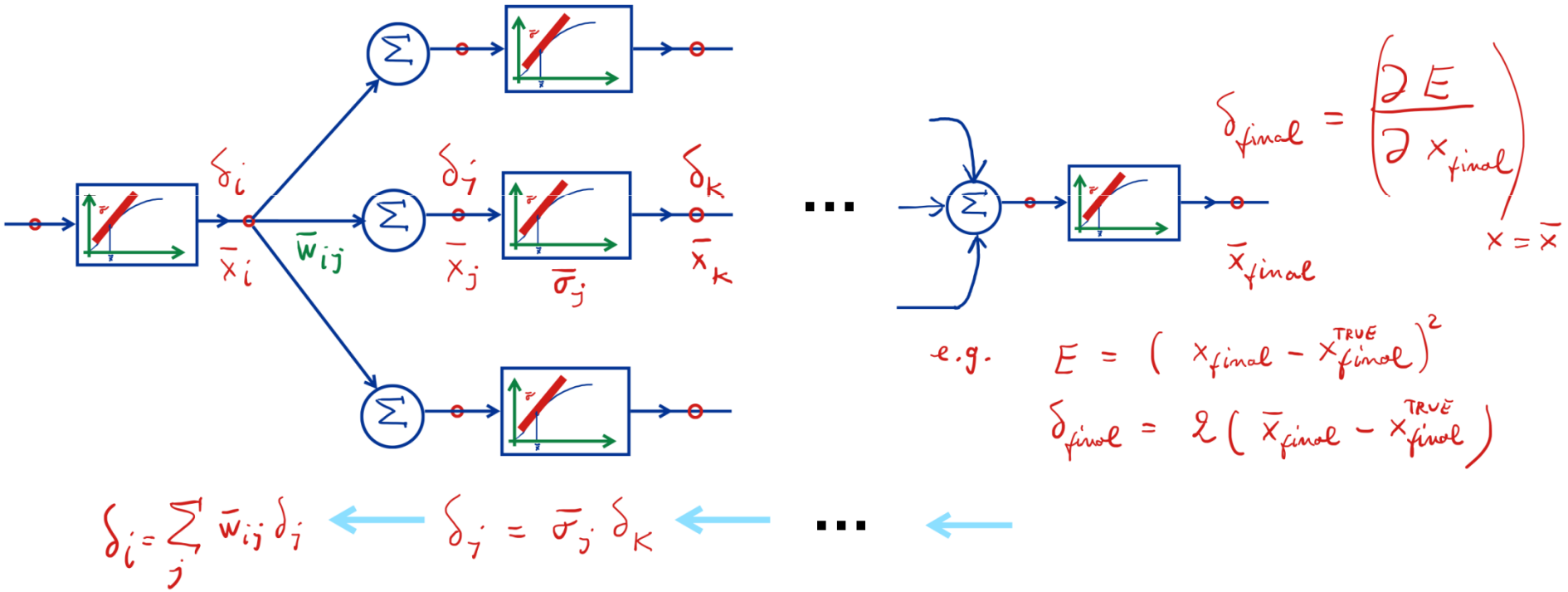


Notation: we have a "measure point" X_j before and after each activation

→ in the linearization, the **slope** $\overline{\sigma}$ gives the output change when the input *x* is increased by 1 w.r.t. $\overline{x}$

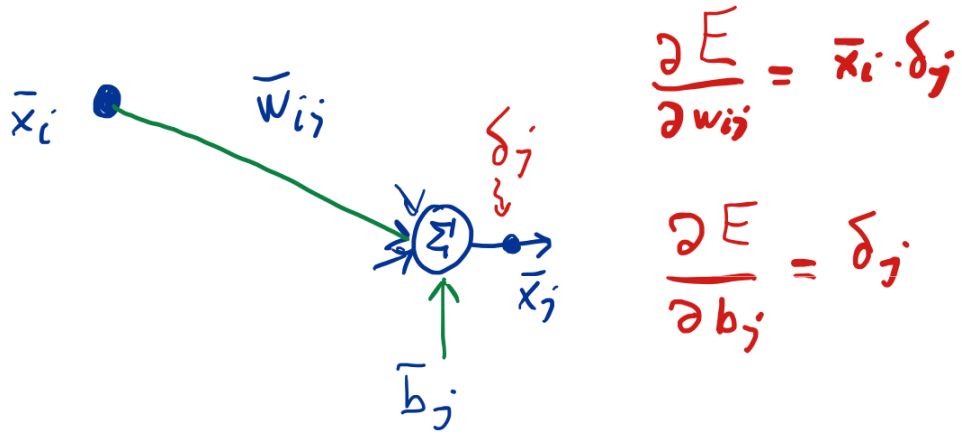
Backpropagation

- Let $\delta_j = \left(\frac{\partial E}{\partial x_j}\right)_{\substack{x=\bar{x} \\ w=\bar{w}}}$ be the increase of E when x_j is increased by 1
- Iteratively compute the δ_j's **backwards** (starting from the final x_j)



Backpropagation

- Once all δ_j's have been computed (after/before each activation) one can easily read each gradient component (in the linearized network, this is just the increase of *E* when a parameter is increased by 1)

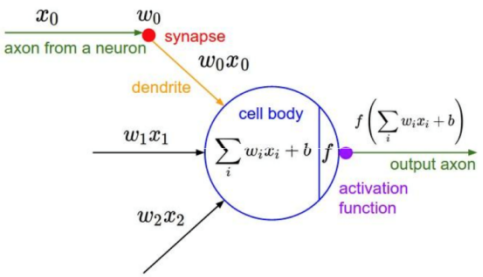


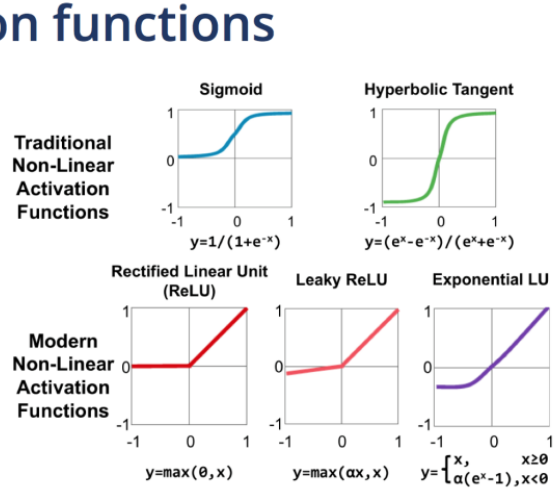
increasing w_{ij} by 1 increases x_j by $\overline{x}_i$, and hence E by $\overline{x}_i\delta_j$

increasing b_j by 1 increases x_j by 1, and hence E by δ_j

Modeling a DNN with fixed param.s

- Assume all the parameters (weights/biases) of the DNN are **fixed**
- We want to model the computation that produces the output value(s) as a function of the inputs, using a MINLP #MIPpersToTheBone
- Each hidden node corresponds to a summation followed by a nonlinear activation function

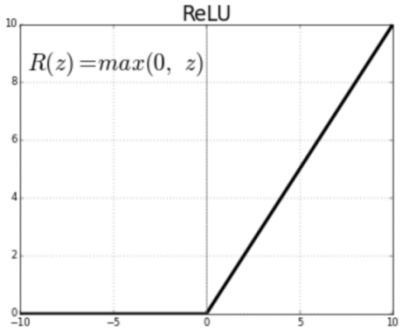




Sze et. al., "Efficient Processing of Deep Neural Networks: A Tutorial and Survey." *arXiv (2017)*

Modeling ReLU activations

- Recent work on DNNs almost invariably only use ReLU activations



$$x = ReLU(w^T y + b)$$

- Easily modeled as $w^T y + b = x - s, \quad x \geq 0, \quad s \geq 0$
  - plus the bilinear condition $x\, s \leq 0$
  - or, alternatively, the indicator constraints

$$\left.\begin{aligned} z = 1 \rightarrow x \leq 0 \\ z = 0 \rightarrow s \leq 0 \\ z \in \{0, 1\} \end{aligned}\right\}$$

A complete 0-1 MILP

$$\min \sum_{k=0}^{K} \sum_{j=1}^{n_k} c_j^k x_j^k + \sum_{k=1}^{K} \sum_{j=1}^{n_k} \gamma_j^k z_j^k$$

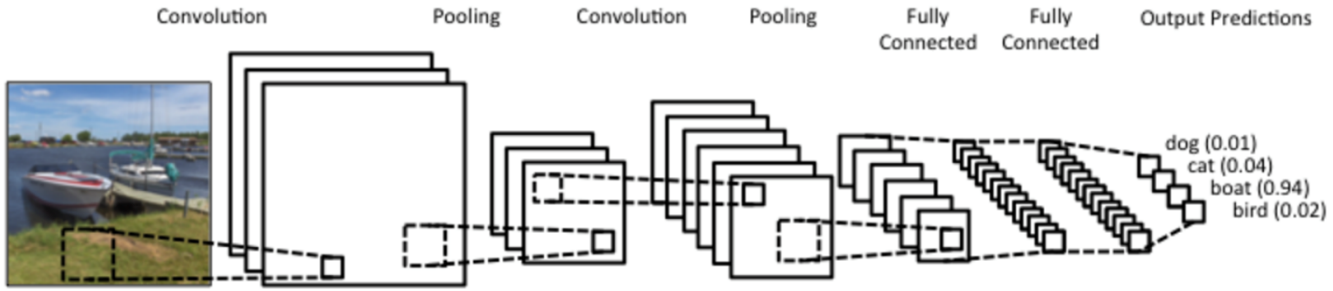
$$\left.\begin{aligned} \sum_{i=1}^{n_{k-1}} w_{ij}^{k-1} x_i^{k-1} + b_j^{k-1} &= x_j^k - s_j^k \\ x_j^k, s_j^k &\geq 0 \\ z_j^k &\in \{0,1\} \\ z_j^k = 1 &\rightarrow x_j^k \leq 0 \\ z_j^k = 0 &\rightarrow s_j^k \leq 0 \end{aligned}\right\} k = 1, \ldots, K, \ j = 1, \ldots, n_k$$

$$lb_j^0 \leq x_j^0 \leq ub_j^0, \qquad j = 1, \ldots, n_0$$

$$\left.\begin{aligned} lb_j^k \leq x_j^k \leq ub_j^k \\ \overline{lb}_j^k \leq s_j^k \leq \overline{ub}_j^k \end{aligned}\right\} k = 1, \ldots, K, \ j = 1, \ldots, n_k.$$

Convolutional Neural Networks (CNNs)

- CNNs play a key role, e.g., in image recognition



- Besides ReLUs, CNNs use **pooling** operations of the type

$$x = AvgPool(y_1, \ldots, y_t) = \frac{1}{t} \sum_{i=1}^{t} y_i$$

$$x = MaxPool(y_1, \ldots, y_t) = \max\{y_1, \ldots, y_t\}$$

- *AvgPool* is just **linear** and can be modeled as a linear constraint

- *MaxPool* can easily be modeled within a 0-1 MILP as

$$\sum_{i=1}^{t} z_i = 1$$

$$\left.\begin{array}{r} x \geq y_i, \\ z_i = 1 \rightarrow x \leq y_i \\ z_i \in \{0,1\} \end{array}\right\} i = 1, \cdots, t$$

Adversarial problem: trick the DNN …

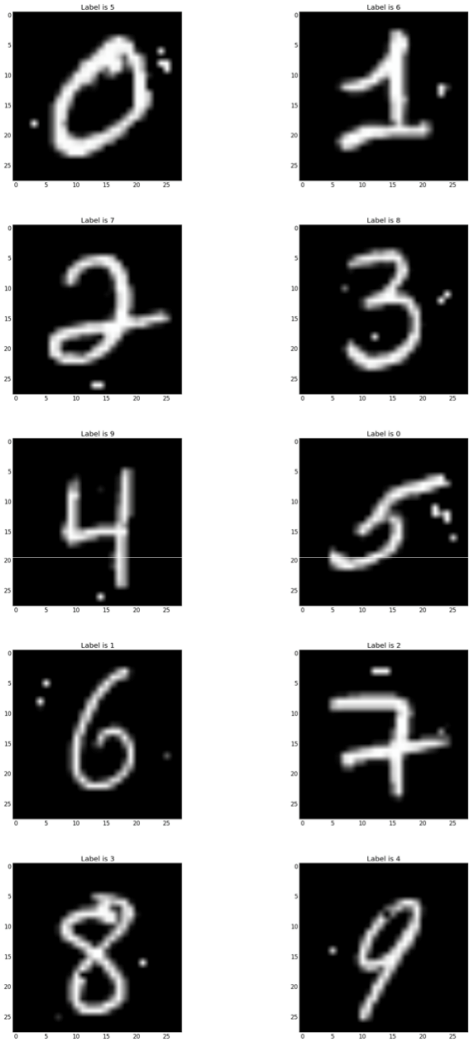


Fig. 2 Adversarial examples computed through our 0-1 MILP model; the reported label is the one having maximum activation according to the DNN (that we imposed to be the true label plus 5, modulo 10). Note that the change of just few well-chosen pixels often suffices to fool the DNN and to produce a wrong classification.

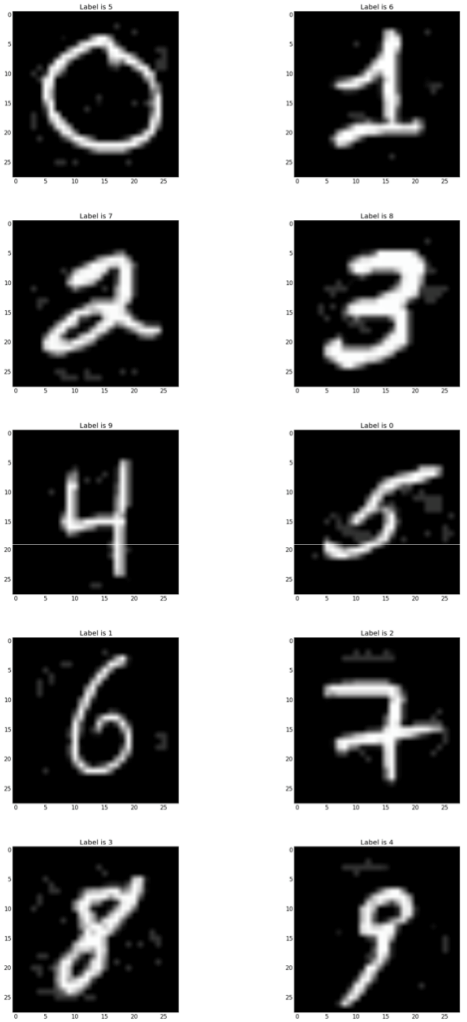


Fig. 3 Adversarial examples computed through our 0-1 MILP model as in Figure 2, but imposing that the no pixel can be changed by more than 0.2 (through the additional conditions $d_j \leq 0.2$ for all j).

… by changing few well-chosen pixels

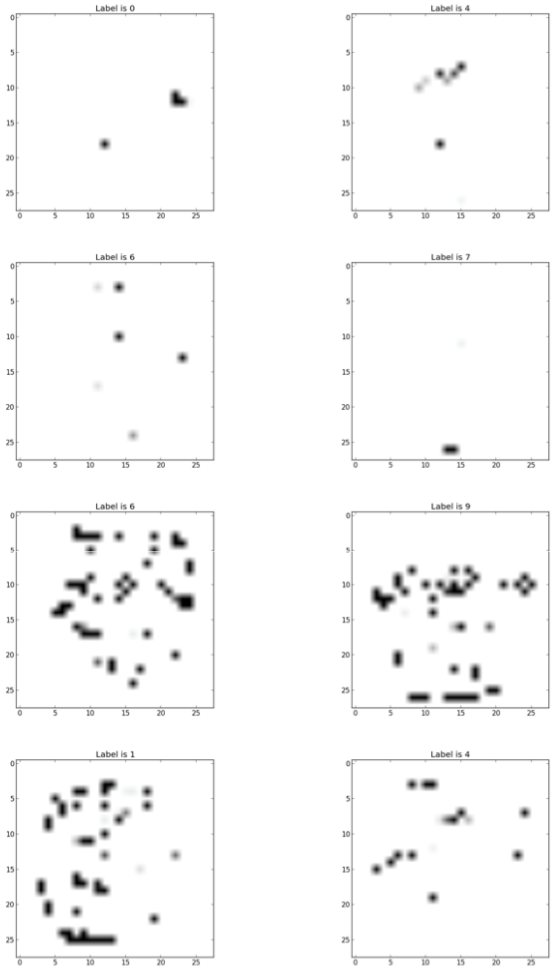
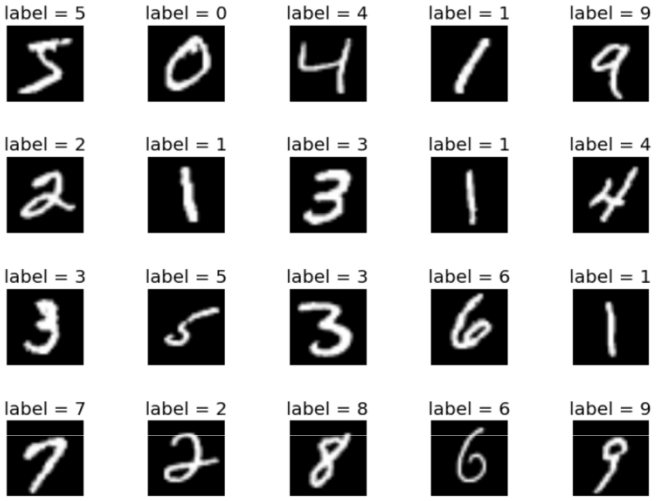


Fig. 4 Pixel changes (absolute value) that suffice to trick the DNN: the four top subfigures correspond to the model where pixels can change arbitrarily, while those on the bottom refer to the case where each pixel cannot change by more than 0.2 (hence more pixels need be changed). To improve readability, the black/white map has been reverted and scaled, i.e., white corresponds to unchanged pixels ($d_j = 0$) while black corresponds to the maximum allowed change ($d_j = 1$ for the four top figures, $d_j = 0.2$ for the four bottom ones).

Experiments on small DNNs

- The MNIST database (Modified National Institute of Standards and Technology database) is a large database of handwritten digits that is commonly used for training various image processing systems



- We considered the following (small) DNNs and trained each of them to get a fair accuracy (93-96%) on the test-set
  - `DNN1`: 8+8+8 internal units in 3 hidden layers, as in [13];
  - `DNN2`: 8+8+8+8+8+8 internal units in 6 hidden layers;
  - `DNN3`: 20+10+8+8 internal units in 4 hidden layers;
  - `DNN4`: 20+10+8+8+8 internal units in 5 hidden layers;
  - `DNN5`: 20+20+10+10+10 internal units in 5 hidden layers.

Computational experiments

- **Instances:** 100 MNIST training figures (each with its “true” label 0..9)
- **Goal:** Change some of the 28x28 input pixels (real values in 0-1) to convert the true label *d* into (*d + 5) mod 10* (e.g., “0” → “5”, “6” → “1”)
- **Metric:** L1 norm (sum of the abs. differences original-modified pixels)
- **MILP solver**: IBM ILOG CPLEX 12.7 (as black box)
  - **Basic model:** only obvious bounds on the continuous var.s
  - **Improved model:** apply a MILP-based preprocessing to compute tight lower/upper bounds on all the continuous variables, as in

    P. Belotti, P. Bonami, M. Fischetti, A. Lodi, M. Monaci, A. Nogales-Gomez, and D. Salvagnin. On handling indicator constraints in mixed integer programming. Computational Optimization and Applications, (65):545–566, 2016.

Differences between the two models

	basic model				improved model			
	%solved	%gap	nodes	time (s)	%solved	%gap	nodes	time (s)
DNN1	100	0.0	1,903	1.0	100	0.0	552	0.6
DNN2	97	0.2	77,878	48.2	100	0.0	11,851	7.5
DNN3	64	11.6	228,632	158.5	100	0.0	20,309	12.1
DNN4	24	38.1	282,694	263.0	98	0.7	68,563	43.9
DNN5	7	71.8	193,725	290.9	67	11.4	76,714	171.1

Table 1 Comparison of the basic and improved models with a time limit of 300 sec.s, clearly showing the importance of bound tightening in the improved model. In this experiment, the preprocessing time needed to optimally compute the tightened bounds is not taken into account.

- `DNN1`: 8+8+8 internal units in 3 hidden layers, as in [13];
- `DNN2`: 8+8+8+8+8+8 internal units in 6 hidden layers;
- `DNN3`: 20+10+8+8 internal units in 4 hidden layers;
- `DNN4`: 20+10+8+8+8 internal units in 5 hidden layers;
- `DNN5`: 20+20+10+10+10 internal units in 5 hidden layers.

Effect of bound-tightening preproc.

	Improved model									
	Exact bounds					Weaker bounds				
	t.pre.	%sol.	%gap	nodes	time (s)	t.pre.	%sol.	%gap	nodes	time (s)
DNN4	1,112.1	98	0.7	68,563	43.9	69.4	98	0.4	80,180	45.5
DNN5	4,913.1	67	11.4	76,714	171.1	72.6	57	16.9	84,328	185.0

Table 2 Performance of the improved model with a time limit of 300 sec.s, with exact vs weaker bounds (the latter being computed with a time limit of 1 sec. for each bound computation). The overall preprocessing time (t.pre.) is greatly reduced in case of weaker bounds, without deteriorating too much the performance of the model. The difference w.r.t. the basic model in Table 1 is still striking.

- `DNN1`: 8+8+8 internal units in 3 hidden layers, as in [13];
- `DNN2`: 8+8+8+8+8+8 internal units in 6 hidden layers;
- `DNN3`: 20+10+8+8 internal units in 4 hidden layers;
- `DNN4`: 20+10+8+8+8 internal units in 5 hidden layers;
- `DNN5`: 20+20+10+10+10 internal units in 5 hidden layers.

Reaching 1% optimality

	Basic model				Improved model (weaker bounds)			
	#timlim	time (s)	nodes	%gap	#timlim	time (s)	nodes	%gap
DNN1	0	1.0	1,920	0.5	0	0.6	531	0.3
DNN2	0	47.0	76,286	0.9	0	7.5	12,110	0.8
DNN3	8	632.8	568,579	2.2	0	11.3	19,663	0.9
DNN4	36	1806.8	1,253,415	10.2	0	50.0	89,380	1.0
DNN5	81	3224.0	1,587,892	43.5	11	851.0	163,135	3.8

Table 3 Performance of the basic and improved model (the latter with the 1-sec. weaker bounds as in Table 2) to get solutions with guaranteed error of 1% or less; each run had a time limit of 3,600 sec.s; the number of time limits, out of 100, is reported in column #timlim.

- `DNN1`: 8+8+8 internal units in 3 hidden layers, as in [13];
- `DNN2`: 8+8+8+8+8+8 internal units in 6 hidden layers;
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- `DNN4`: 20+10+8+8+8 internal units in 5 hidden layers;
- `DNN5`: 20+20+10+10+10 internal units in 5 hidden layers.

Thanks for your attention!

Slides available at http://www.dei.unipd.it/~fisch/papers/slides/

Paper:

M. Fischetti, J. Jo, "Deep Neural Networks as 0-1 Mixed Integer Linear Programs: A Feasibility Study", 2017, arXiv preprint arXiv:1712.06174 (accepted in CPAIOR 2018)