Introduction to Machine Learning (67577)

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Deep Learning

Outline

Gradient-Based Learning

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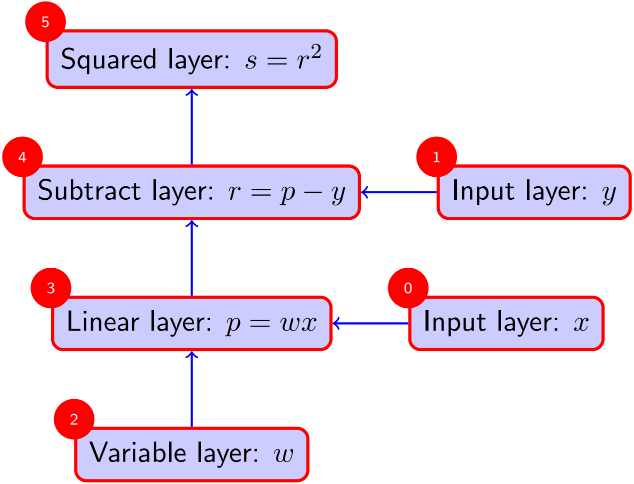
- SGD converges for convex problems. It may work for non-convex problems if we initialize “close enough” to a “good minimum”

Outline

A computation graph for a one dimensional Least Squares

(numbering of nodes corresponds to topological sort):



Gradient Calculation using the Chain Rule

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$$\begin{aligned}
\ell'(w) &= (s \circ r_y \circ p_x)'(w) \\
&= s'(r_y(p_x(w))) \cdot (r_y \circ p_x)'(w) \\
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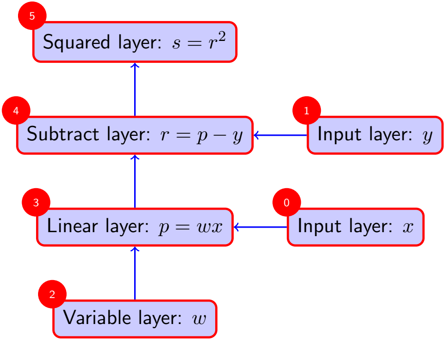
- Backpropagation: Calculate by a Forward-Backward pass over the graph

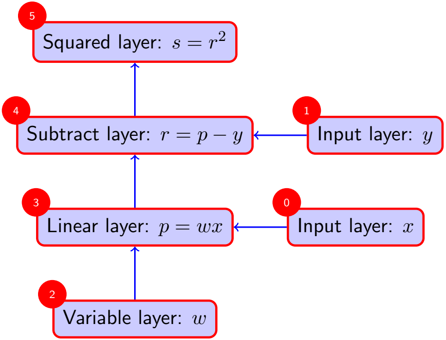
Computation Graph — Forward

- For $t = 0, 1, \ldots, T-1$
  - `Layer[t]->output = Layer[t]->function(Layer[t]->inputs)`



Computation Graph — Backward

- Recall: $\ell'(w) = s'(r_y(p_x(w))) \cdot r'_y(p_x(w)) \cdot p'_x(w)$
- `Layer[T-1]->delta = 1`
- For $t = T-1, T-2, \ldots, 0$
  - For `i in Layer[t]->inputs`:
    - `i->delta = Layer[t]->delta * Layer[t]->derivative(i,Layer[t]->inputs)`



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Main message

Computation graph enables us to construct very complicated functions from simple building blocks

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- The multiplication is matrix multiplication
- The correctness of the algorithm follows from the multivariate chain rule

$$J_{\mathbf{w}}(\mathbf{f} \circ \mathbf{g}) = J_{g(\mathbf{w})}(\mathbf{f}) J_{\mathbf{w}}(\mathbf{g})$$

Jacobian — Examples

- If $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^n$ is element-wise application of $\sigma : \mathbb{R} \to \mathbb{R}$ then $J_{\mathbf{x}}(\mathbf{f}) = \mathrm{diag}((\sigma'(x_1), \ldots, \sigma'(x_n)))$.

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- Let $\mathbf{f}(\mathbf{x}, \mathbf{w}, b) = \mathbf{w}^\top \mathbf{x} + b$ for $\mathbf{w}, \mathbf{x} \in \mathbb{R}^n, b \in \mathbb{R}^1$. Then:

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- Let $\mathbf{f}(W, \mathbf{x}) = W\mathbf{x}$. Then:

$$J_{\mathbf{x}}(\mathbf{f}) = W \quad , \quad J_W(\mathbf{f}) = \begin{pmatrix} \mathbf{x}^\top & 0 & \cdots & 0 \\ 0 & \mathbf{x}^\top & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{x}^\top \end{pmatrix} \quad .$$

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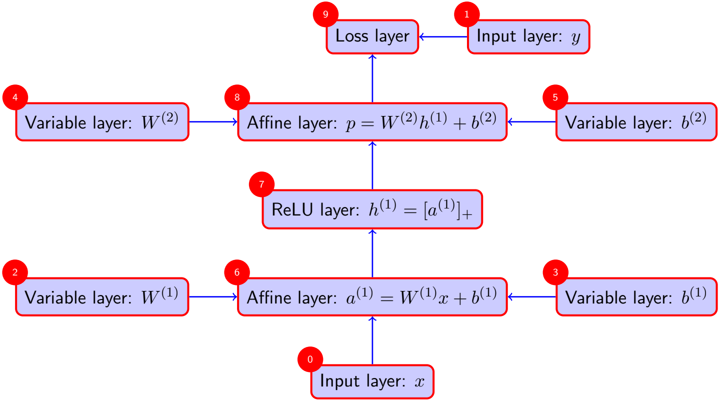
- Other ways to improve generalization is all sort of regularization

Expressiveness

- So far in the course we considered hypotheses of the form $x \mapsto w^\top x + b$
- Now, consider the following computation graph, known as "one hidden layer network":



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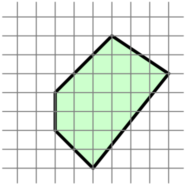
- Proof: Think on the VC dimension ...
- What type of functions can be implemented by small size networks?

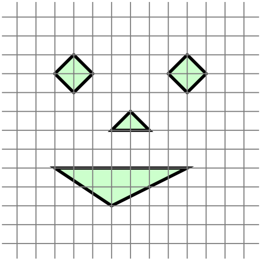
Geometric Intuition

- One hidden layer networks can express intersection of halfspaces



Geometric Intuition

- Two hidden layer networks can express unions of intersection of halfspaces



What can we express with T-depth networks ?

- Theorem: Let $T : \mathbb{N} \to \mathbb{N}$ and for every n, let $\mathcal{F}_n$ be the set of functions that can be implemented using a Turing machine using runtime of at most $T(n)$. Then, there exist constants $b, c \in \mathbb{R}_+$ such that for every n, there is a network of depth at most T and size at most $cT(n)^2 + b$ such that it implements all functions in $\mathcal{F}_n$.

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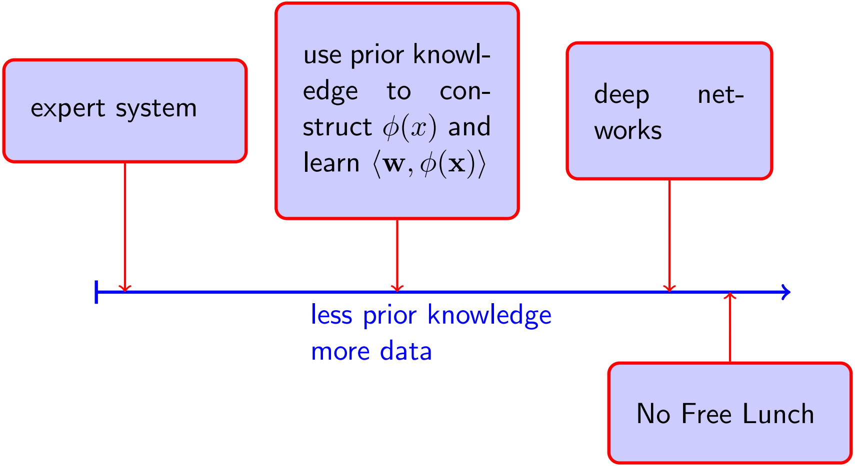
- Conclusion: A very weak notion of prior knowledge suffices — if we only care about functions that can be implemented in time $T(n)$, we can use neural networks of depth T and size $O(T(n)^2)$, and the sample complexity is also bounded by polynomial in $T(n)$!

The ultimate hypothesis class



Outline

Runtime of learning neural networks

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  - Need to apply some tricks (initialization, learning rate, mini-batching, architecture), and need some luck

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- Variants of SGD: There are plenty of variants that work better than vanilla SGD.

Failures of Deep Learning

- Parity of more than 30 bits
- Multiplication of large numbers
- Matrix inversion
- ...

Outline

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  - Calculation: Divide input image to $k \times k$ windows and for each such window output the maximal value (or average value)

Historical Remarks

- 1940s-70s:
  - Inspired by learning/modeling the brain (Pitts, Hebb, and others)
  - Perceptron Rule (Rosenblatt), Multilayer perceptron (Minksy and Papert)
  - Backpropagation (Werbos 1975)
- 1980s – early 1990s:
  - Practical Back-prop (Rumelhart, Hinton et al 1986) and SGD (Bottou)
  - Initial empirical success
- 1990s-2000s:
  - Lost favor to implicit linear methods: SVM, Boosting
- 2006 –:
  - Regain popularity because of unsupervised pre-training (Hinton, Bengio, LeCun, Ng, and others)
  - Computational advances and several new tricks allow training HUGE networks. Empirical success leads to renewed interest
  - 2012: Krizhevsky, Sustkever, Hinton: significant improvement of state-of-the-art on imagenet dataset (object recognition of 1000 classes), without unsupervised pre-training

Summary

- Deep Learning can be used to construct the ultimate hypothesis class
- Worst-case complexity is exponential
- . . . but, empirically, it works reasonably well and leads to state-of-the-art on many real world problems