Statistical Learning VIII

0. Exam
1. Stochastic Optimization
2. Deep Learning / Neural Networks
   a) Neural Networks
   b) Size
   c) Overfitting and Generalization
   d) Stochastic Gradient Descent and Backpropagation
   e) Hardware and Software

0. Exam

- Open book (bring a paper copy!)
- Bring anything on paper you like (notes, prints, etc.)
- Long calculations in lectures: I care about conclusions/interpretation, not about the calculations

1. Stochastic Optimization

a) Non-stochastic Optimization

$$\beta^* = \underset{\beta}{\operatorname{argmin}}\, F(\beta)$$

~~$\beta = (\beta_1, \ldots, \beta_p)$~~

$\beta = (b_1, \ldots, b_p)$

Examples:

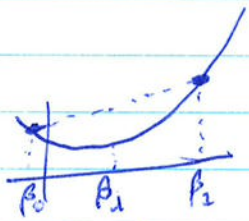
$$F(\beta) = \frac{1}{N}\sum_{i=1}^{N}(y_i - x_i^T\beta)^2 \quad \text{(least squares)}$$

$$F(\beta) = \frac{1}{N}\sum_{i=1}^{N}(y_i - x_i^T\beta)^2 + \lambda\sum_{j=2}^{p}\beta_j^2 \quad \text{(ridge regression)}$$

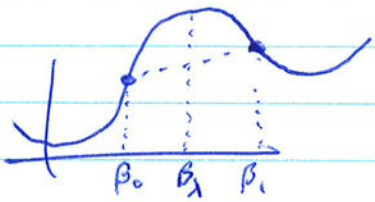
$$F(\beta) = \frac{1}{N}\sum_{i=1}^{N}(y_i - x_i^T\beta)^2 + \lambda\sum_{j=2}^{p}|\beta_j| \quad \text{(lasso)}$$

$$F(\beta) = \frac{1}{N}\sum_{i=1}^{N}\log(1+e^{-y_i x_i^T\beta}) \quad \text{(logistic regression)}$$

All these examples convex functions $F(\beta)$:



convex



not convex

$\beta_\lambda = (1-\lambda)\beta_0 + \lambda\beta_1$

see Fig1 handout

$$F(\beta_\lambda) \leq (1-\lambda)F(\beta_0) + \lambda F(\beta_1) \quad \text{for all } \lambda \in [0,1]$$

Convexity ⇒ Can find minimum by making small improvements to the parameters:

$$\beta_{t+1} = \beta_t - \eta_t \nabla F(\beta_t) \quad \text{(gradient descent)}$$

η_t: step size

β_{t+1}: new parameters

β_t: previous parameters

$\nabla F(\beta_t)$: gradient

$$\nabla F(\beta) = \begin{pmatrix} \frac{\partial}{\partial b_1} F(\beta) \\ \vdots \\ \frac{\partial}{\partial b_p} F(\beta) \end{pmatrix}$$

- vector pointing in direction that is the most up from β
- so move in direction of negative gradient to go the most down

Best choice of η_t depends on type of function.

For instance:

~~If F is differentiable and two times and~~

If F is γ-smooth, then for $\eta_t = \frac{1}{\gamma}$:

$$F(\beta_t) - F(\beta^*) \leq \frac{2\gamma \|\beta_1 - \beta^*\|^2}{t-1}$$

($\|\beta_1 - \beta^*\|^2$ ← starting distance from optimum)

more steps ⇒ closer to optimum

(γ-Smooth means that second derivative in any direction is at most γ.)

b) Stochastic Optimization

Suppose $F(\beta) = \frac{1}{N} \sum_{i=1}^{N} f_i(\beta)$ for some (convex) functions $f_1, \dots, f_N$.

Then computing

$$\nabla F(\beta) = \frac{1}{N} \sum_{i=1}^{N} \nabla f_i(\beta)$$

takes a lot of computation when N is large

All examples are of this form!

(For ridge and lasso take

$$f_i(\beta) = (y_i - X_i^T \beta)^2 + \lambda \text{pen}(\beta).$$)

Stochastic Gradient Descent:

Pick one data point at random and do gradient descent step based on only that data point instead of the whole data:

choose i_t randomly from $\{1, \ldots, N\}$

$$\beta_{t+1} = \beta_t - \eta_t \nabla f_{i_t}(\beta_t)$$

* Can do N steps in same time as one update of regular gradient descent.

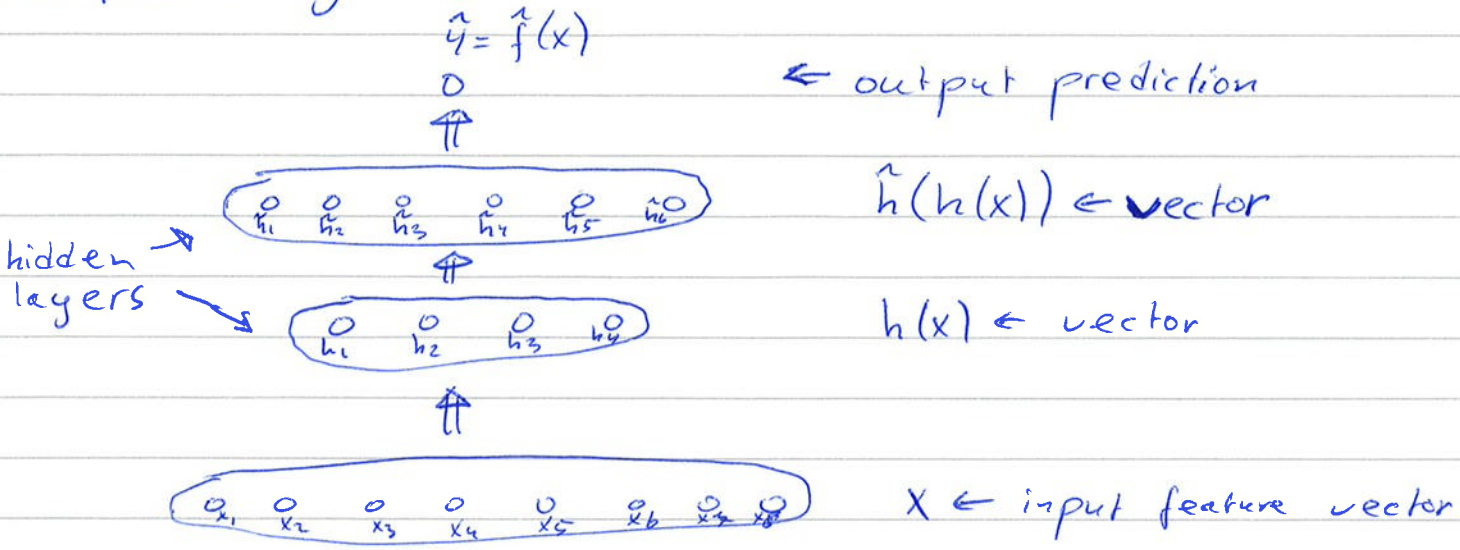
* $\nabla f_{i_t}(\beta_t)$ is an <u>unbiased</u> estimator of $\nabla F(\beta_t)$:

$$\mathop{\mathbb{E}}_{i_t}[\nabla f_{i_t}(\beta_t)] = \frac{1}{N}\sum_{i=1}^{N} \nabla f_{i_t}(\beta_t) = \nabla F(\beta_t)$$

uniform probabilities when choosing i_t.

* So we can go in right direction on average with much less computation.

Deep learning = Big neural networks



CASI: Fig 18.8

Learn feature transformations from the data!

└ completely replaced manually designed SWIFT features in computer vision ← took 10 years to design these

Important applications: images (best), speech recognition (best), natural language processing (often best)

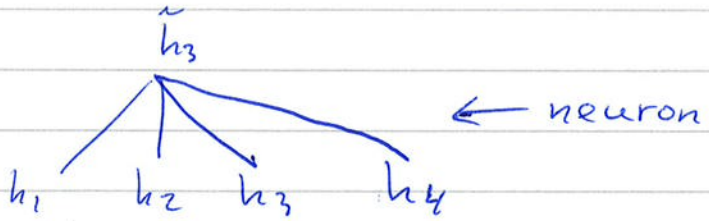
* Can have >3 layers
* Intermediate vectors often very large

} "deep" learning

* Loss $L(y, \hat{y})$ can be ~~anything~~ anything. E.g. quadratic for regression, logistic for classification, etc

How do we learn transformations between layers?

Zoom in.



$$\tilde{a}_3 = \sum_{i=1}^{4} w_{h_i \to \tilde{h}_3} \cdot h_i + \text{intercept}_{\tilde{h}_3}$$

linear "activation"

parameters

$$\tilde{h}_3 = \sigma(\tilde{a}_3)$$

activation function (nonlinear)

- sigmoid: $\sigma(a) = \frac{1}{1+e^{-a}}$

- tanh: $\sigma(a) = \frac{1-e^{-2a}}{1+e^{-2a}} = 2 \cdot \text{sigmoid}(2a) - 1$

- rectified linear unit: $\sigma(a) = \max\{a, 0\}$ ← (piece-wise linear; helped a lot in performance)
  (ReLu) ← recently popular

- ...

Size: At least 2 or 3 hidden layers

- every neuron has its own parameters
- modern network may have
  - inputs: 65536 = 256 x 256 color pixels
  - layers: 500
    500
    2000

rough estimate nr of parameters:

$65536 \times 2000 + 2000 \times 500 + 500 \times 500 + 500 \times 1$

$\approx$ 130 million parameters

So will overfit like crazy...

c) Overfitting and Generalization

- nr. of parameters much bigger than N, so typically get training error for classification to (approximately) 0.
- Which solution with 0 training error is chosen? $L(y, \hat{f}(x))$ is non-convex function of network parameters, so optimization gets stuck before reaching the global minimum.
  ↳ solution depends on which optimization method we use.
- Solutions tend to have large margin empirically. (like SVM)
- Because optimizer explores restricted part of parameter space, it acts like a regularizer! (Compare Lasso, Ridge, which minimize squared error over a ball of allowed parameter value.)
- How does this regularizer behave?
  Active research topic!

How to further reduce overfitting

1. Very large data sets (15 million examples in ImageNet data set)
2. Exploit domain knowledge to reduce nr. of parameters: images have locally similar structures, so tie parameters together in first layers ⇐ convolutional layers (optional reading)
3. Regularize (L_1, L_2, ...)
4. Early stopping: monitor generalization error on validation set during optimization, and stop when it starts to increase.

d) Stochastic Gradient Descent and Backpropagation

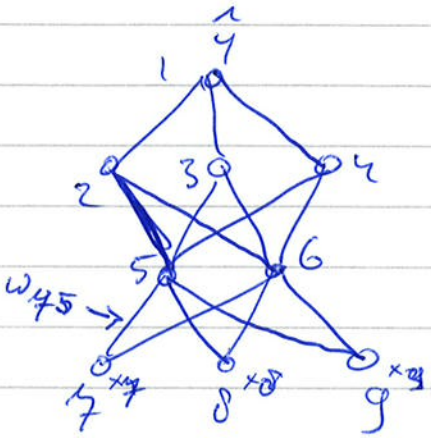
- θ is a vector with all weights (e.g. 130 million parameters)
- minimize $F(\theta) = \frac{1}{N} \sum_{i=1}^{N} L(y_i, f_\theta(x_i))$ using stochastic gradient descent
- $L(y_i, f_\theta(x_i))$ is <u>not convex</u> in θ, but we accept to find a local minimum
- Big open question: why does it find good local minima in practise? ← appears to work better when number of parameters is much larger than N

How to compute gradients $\nabla_\theta L(y_t, \hat{f}_\theta(x_t))$?

130 million parameters: only have time for fixed nr. of computations per parameter

Solution: Backpropagation ← use chain rule for derivatives many times:

$$\frac{\delta a}{\delta b} = \frac{\delta a}{\delta c} \cdot \frac{\delta c}{\delta b}$$



For each neuron in o:

$o_m = \sigma(a_m)$ (o: output, a: activation) $\quad m = 2, \dots, 9$

$o_1 = \hat{y}$

1. $\frac{\delta L(y_t, \hat{f}_\theta(x_t))}{\delta o_1}$ is $\frac{\delta L(y_t, \hat{y})}{\delta \hat{y}}$ is derivative of the loss

2. chain rule:

Suppose we have $\frac{\delta L(y_t, \hat{f}_\theta(x_t))}{\delta o_5}$, then

$$\frac{\delta L(y_t, \hat{f}_\theta(x_t))}{\delta w_{45}} = \frac{\delta L(y_t, \hat{f}_\theta(x_t))}{\delta o_5} \cdot \frac{\delta o_5}{\delta w_{45}}$$

$\uparrow$ 9

$$\frac{\delta o_5}{\delta w_{45}} = \frac{\delta o_5}{\delta a_5} \cdot \frac{\delta a_5}{\delta w_{45}}$$

$$\frac{\delta o_5}{\delta a_5} = \frac{\delta \sigma(a_5)}{\delta a_5} = \sigma'(a_5)$$

$$\frac{\delta a_5}{\delta w_{45}} = \frac{\delta \sum_{i=4}^{9} w_{i5} \cdot x_i}{\delta w_{45}} = x_4$$

3. Work backwards from output to inputs to compute partial derivatives w.r.t. each o_m if we already have these partial derivatives higher up in the network.

already computed

vector chain rule:

$$\frac{\delta L(y, f_\theta(x))}{\delta o_5} = \frac{\delta L(y, f_\theta(x))}{\delta o_2} \cdot \frac{\delta o_2}{\delta o_5} + \frac{\delta L(y, f_\theta(x))}{\delta o_3} \cdot \frac{\delta o_3}{\delta o_5} + \frac{\delta L(y, f_\theta(x))}{\delta o_4} \cdot \frac{\delta o_4}{\delta o_5}$$

$$\frac{\delta o_2}{\delta o_5} = \frac{\delta o_2}{\delta a_2} \cdot \frac{\delta a_2}{\delta o_5}$$

$\sigma'(a_2)$

$a_2 = w_{52} \cdot o_5 + w_{62} \cdot o_6$

$$\frac{\delta(a_2)}{\delta o_5} = w_{52}$$

Conclusion: only need to do fixed (nr of) operations for each element of the network.

↳ compute gradient vector quickly