UiO : Matematisk institutt

Det matematisk-naturvitenskapelige fakultet

STK-4051/9051 Computational Statistics Spring 2022
SGD

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Last time

- EM in mixture Gauss distribution
- EM in Exponential family
- Variance estimate in EM
- Bootstrap
- EM for hidden Markov model

- Stochastic gradient decent
  – What it is
  – Minibatch is one type of randomness

Info

- Many good videos on course topics online
  - Some gives a an overview
  - Some gives details
  - Be critical, is what you get what you need?
- Explanation and example of the EM algorithm for the for the mixture gaussian case:
  - https://www.youtube.com/watch?v=REypj2sy_5U
  - https://www.youtube.com/watch?v=iQoXFmbXRJA

Main Idea

- $F(\cdot)$ is nice and smooth, a necessary requirement is

$$\boldsymbol{g}(\boldsymbol{\theta}^*) = \frac{\partial}{\partial \boldsymbol{\theta}} F(\boldsymbol{\theta}) \mid_{\boldsymbol{\theta}=\boldsymbol{\theta}^*} = \mathbf{0} \tag{1}$$

- Ordinary gradient descent methods:

$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^t - \boldsymbol{M}_t^{-1}\boldsymbol{g}(\boldsymbol{\theta}^t), \quad \boldsymbol{M}_t \text{ is some positive definite matrix}$$

- Main problem: gradient might be difficult to compute.
- The stochastic gradient algorithm replaces the gradient by an estimate instead:

$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^t - \alpha_t \boldsymbol{M}_t^{-1}\boldsymbol{Z}(\boldsymbol{\theta}^t; \boldsymbol{\phi}^t), \quad \boldsymbol{Z}(\boldsymbol{\theta}^t; \boldsymbol{\phi}^t) \approx \boldsymbol{g}(\boldsymbol{\theta}^t) \tag{2}$$

«some stochastic element»

- A class of possibilities are given by

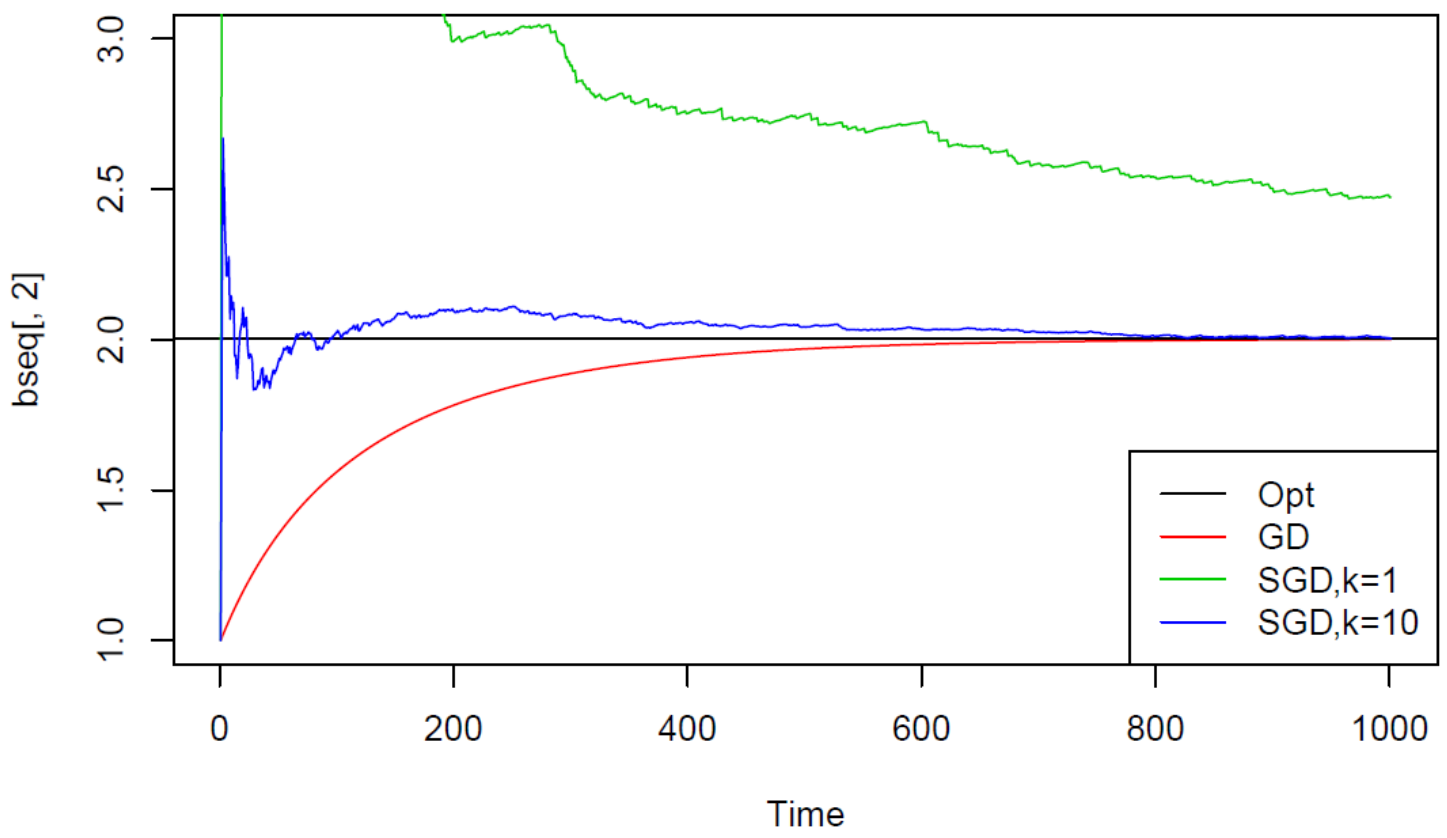
$$\boldsymbol{Z}(\boldsymbol{\theta}^t; \boldsymbol{\phi}^t) = \frac{1}{n_t}\sum_{i\in\mathcal{S}_t} \nabla f_i(\boldsymbol{\theta}^t), \quad \mathcal{S}_t \subset \{1, \ldots, n\}, n_t = |\mathcal{S}_t|$$

$$\text{"}\phi^t = \mathcal{S}_t\text{"}$$

- Algorithm:

1: **for** $t = 1, 2, \ldots$ **do**
2: Simulate the stochastic gradient $Z(\boldsymbol{\theta}^t; \boldsymbol{\phi}^t)$;
3: Choose a stepsize α^t;
4: Update the new value by $\boldsymbol{\theta}^{t+1} \leftarrow \boldsymbol{\theta}^t - \alpha_t \boldsymbol{M}_t^{-1} Z(\boldsymbol{\theta}^t; \boldsymbol{\phi}^t)$.
5: **end for**

Convergence in example



Convergence of SGD

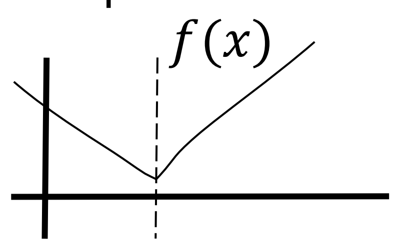
- Want to show that the SGD procedure is consistent

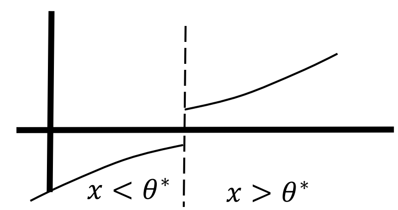
Definition 1.

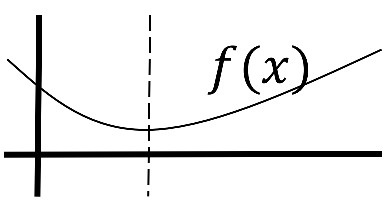
If $\lim_{t\to\infty} \theta^t = \theta^*$ in probability, irrespective of any arbitrary initial value θ^0, we call the procedure consistent. Here, convergence in probability means that for any $\varepsilon > 0$

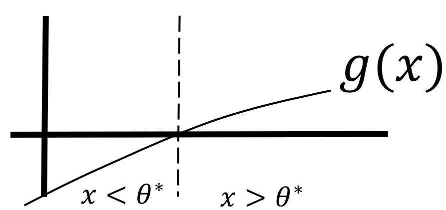
$$\lim_{t\to\infty} \Pr(|\theta^t - \theta^*| > \varepsilon) = 0.$$

- Do this in three steps (with some sub-steps on the way)
  1. Prove that L2 convergence gives consistency
  2. Prove that the sequence converge
  3. Prove that we converge to the true parameter
     1. Sharp transition at zero
     2. Smooth transition at zero









Step 1 L2 convergence gives consistency

Lemma 1.

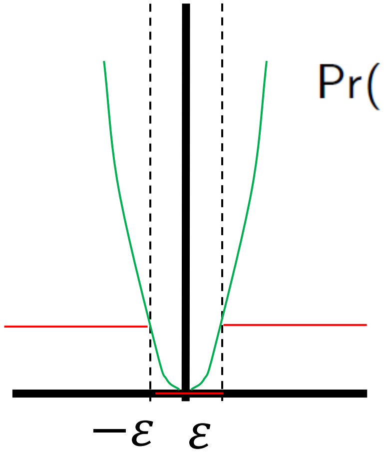
Define

$$b_t = E[||\theta^t - \theta^*||^2].$$

If $\lim_{t\to\infty} b_t = 0$, *then* $\{\theta^t\}$ *is consistent.*

- $\{\theta^t\}$ is stochastic and multidimensional
- $\{b_t\}$ is deterministic and one-dimensional
- Easier to prove convergence with respect to $\{b_t\}$

Defining $p_t(\cdot)$ to be the density of θ^t, we have that



$$\begin{aligned}\Pr(|\theta^t - \theta^*| > \varepsilon) &= \int_z I[(z-\theta^*)^2 > \varepsilon^2] p_t(z)dz \\ &\leq \int_z \frac{(z-\theta^*)^2}{\varepsilon^2} p_t(z)dz \\ &= \frac{1}{\varepsilon^2}\int_z (z-\theta^*)^2 p_t(z)dz = \frac{1}{\varepsilon^2} b_t \to 0\end{aligned}$$

Assumptions

- Requirements on the sequence $\{\alpha_t\}$:

$$\alpha_t > 0 \tag{A-1}$$

$$\sum_{t=2}^{\infty} \frac{\alpha_t}{\alpha_1 + \cdots + \alpha_{t-1}} = \infty \tag{A-2}$$

$$\sum_{t=1}^{\infty} \alpha_t^2 < \infty \tag{A-3}$$

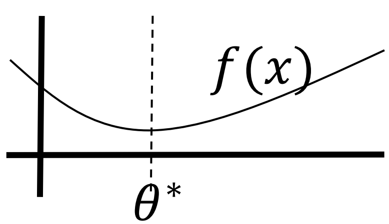
  Note that (A-2) implies $\sum_{t=1}^{\infty} \alpha_t = \infty$

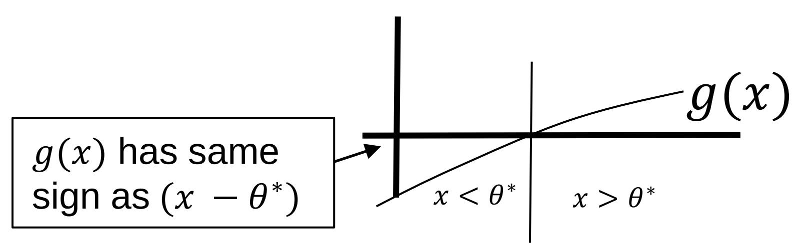
- Requirements on the function $g(x)$ combined with its estimate:

$$\exists \delta \geq 0 \text{ such that } g(x) \leq -\delta \text{ for } x < \theta^* \text{ and } g(x) \geq \delta \text{ for } x > \theta^*. \tag{A-4}$$

$$E[Z(\theta;\phi)] = g(\theta) \text{ and } \Pr(|Z(\theta;\phi)| < C) = 1 \tag{A-5}$$

  The constraint $|Z(\theta;\phi)| < C$ is included to simplify the proof. More general results are available.





Step 2 Prove that the sequence converge

Theorem 1.

Assume (A-1), (A-3), (A-4) *and* (A-5). *Then the sequence*

$$\theta^{t+1} = \theta^{t} - \alpha_t Z(\theta^t; \phi^t) \tag{3}$$

will converge in probability.

- This result only gives convergence to some value, not necessarily to the optimal value.
- Convergence to the optimal value will be proved later were also (A-2) will be assumed.
- Simplify the notation: Denoting $Z(\theta^t; \phi^t)$ by Z_t.

Recall: Z is the stochastic version of the gradient

$\boldsymbol{Z}(\boldsymbol{\theta}^t; \boldsymbol{\phi}^t) \approx \boldsymbol{g}(\boldsymbol{\theta}^t)$

Proof of Theorem 1

$$
\begin{aligned}
b_{t+1} &= E[(\theta^{t+1} - \theta^*)^2] = E[E[(\theta^{t+1} - \theta^*)^2|\theta^t]] = E[E[(\theta^t - \alpha_t Z_t - \theta^*)^2|\theta^t]] \\
&= E[(\theta^t - \theta^*)^2 + \alpha_t^2 E[Z_t^2|\theta^t] - 2\alpha_t(\theta^t - \theta^*)E[Z_t|\theta^t]] \\
&= b_t + \alpha_t^2 E[Z_t^2] - 2\alpha_t E[(\theta^t - \theta^*)g(\theta^t)]
\end{aligned}
$$

$$\boxed{e_t = E[Z_t^2] \quad d_t = E[(\theta^t - \theta^*)g(\theta^t)],}$$

we get

$$b_{t+1} - b_t = \alpha_t^2 e_t - 2\alpha_t d_t.$$

- By summing the equation above over t, we get

$$b_{t+1} = b_1 + \sum_{s=1}^{t} \alpha_s^2 e_s - 2\sum_{s=1}^{t} \alpha_s d_s. \qquad (4)$$

First series has only positive terms:
Since $e_t = E\{Z_t^2\} > 0$,

Second series has only positive terms:
Since by (A-4) : $g(x)$ has same sign as $(x - \theta^*)$, $d_t \geq 0$
Since by (A-1): $\alpha_t > 0$, we then have also $\alpha_t d_t \geq 0$

If we can show that both $\sum_{s=1}^{t} \alpha_s^2 e_s$ and $\sum_{s=1}^{t} \alpha_s d_s$ are bounded, then both series converge by monotone convergence. And thereby also b_t converge

Bounding the two series

$$b_{t+1} = b_1 + \sum_{s=1}^{t} \alpha_s^2 e_s - 2 \sum_{s=1}^{t} \alpha_s d_s.$$

From $|Z(\theta; \phi)| \leq C$ we have

$$\sum_{t=1}^{\infty} \alpha_t^2 e_t \leq C^2 \sum_{t=1}^{\infty} \alpha_t^2 < \infty$$

(A-5): Since $|Z_t| < C$, $\mathrm{e}_t = \mathrm{E}\{|Z_t|^2\} < C^2$

(A-3): $\sum {\alpha_t}^2 < \infty$

$$\sum_{s=t+1}^{\infty} \alpha_s^2 \, \mathrm{e}_s \geq 0$$

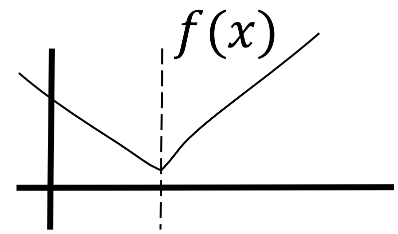
$$\sum_{s=1}^{t} \alpha_s d_s = \tfrac{1}{2}\left[b_1 + \sum_{s=1}^{t} \alpha_s^2 e_s - b_{t+1}\right] \leq \tfrac{1}{2}\left[b_1 + \sum_{s=1}^{\infty} \alpha_s^2 e_s\right]$$

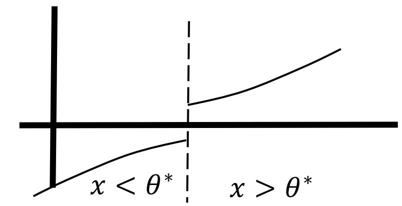
$$b_{t+1} = E[(\theta^{t+1} - \theta^*)^2] \geq 0$$

Thus if we remove it we reduce the sum

Add two Non-negative finite numbers

Both series are bounded and therefore converge





Two main results

Theorem 2.

Assume (A-1), (A-2), (A-3), (A-4) *and* (A-5). *Assume further* $\delta > 0$ *in* (A-4). *Then* $\lim_{t\to\infty} b_t = 0$.

$$\exists\delta \geq 0 \text{ such that } g(x) \leq -\delta \text{ for } x < \theta \text{ and } g(x) \geq \delta \text{ for } x > \theta. \qquad \text{(A-4)}$$

Theorem 3.

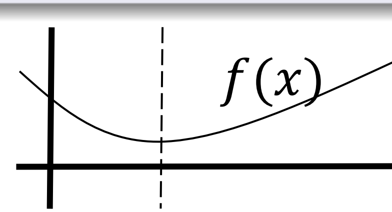
Assume (A-1), (A-2), (A-3) *and* (A-5). *Assume further*

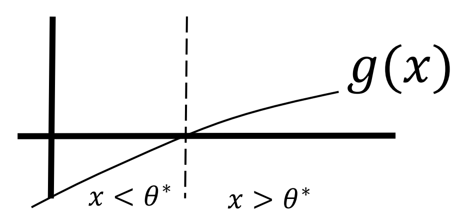
$$g(z) \text{ is nondecreasing;} \tag{9}$$

$$g(\theta^*) = 0; \tag{10}$$

$$g'(\theta^*) > 0. \tag{11}$$

Then $\lim_{t\to\infty} b_t = 0$.





Warm up to Theorems

Lemma 2.

Assume (A-1), (A-3), (A-4) *and* (A-5). *Assume* $\{k_t\}$ *is a sequence of nonnegative constants satisfying*

$$k_t b_t \leq d_t, \quad \sum_{t=1}^{\infty} \alpha_t k_t = \infty \tag{5}$$

Then $\lim_{t\to\infty} b_t = 0$.

So if we can find such a k_t-sequence we are done

Proof:

- We have that

$$\boxed{\sum_{s=1}^{t} \alpha_s d_s = \frac{1}{2}\left[b_1 + \sum_{s=1}^{t} \alpha_s^2 e_s - b_{t+1}\right] \leq \frac{1}{2}\left[b_1 + \sum_{s=1}^{\infty} \alpha_s^2 e_s\right]}$$

$$\sum_{t=1}^{\infty} \alpha_t k_t b_t \leq \sum_{t=1}^{\infty} \alpha_t d_t < \infty \tag{6}$$

  from the proof of the previous Theorem.
- From the second part of (5) there must be an infinite number of b_t's for which $b_t < \epsilon$ for any value of ϵ.
- Since we have already shown that $\lim_{t\to\infty} b_t$ exists, this shows that the limit has to be zero.

Warm up to Theorems cont…

Lemma 3.

Assume (A-1), (A-2), (A-3), (A-4) *and* (A-5). *Assume for some constant* $\delta > 0$ *that*

$$\inf_{z \in [\theta^* - A_t, \theta^* + A_t]} \left[\frac{g(z)}{z - \theta^*} \right] \geq \frac{\delta}{A_t} \text{ for } t > N \tag{7}$$

where

$$A_t = |\theta^1 - \theta^*| + C(\alpha_1 + \cdots + \alpha_{t-1}). \tag{8}$$

This δ need not be the one in (A-4)

Then $\lim_{t\to\infty} b_t = 0$.

- We have that $\theta^t = \theta^1 - \sum_{s=1}^{t-1} \alpha_s Z_s$ so that

$$\begin{aligned} |\theta^t - \theta^*| &= |\theta^1 - \theta^* - \sum_{s=1}^{t-1} \alpha_s Z_s| \\ &\leq |\theta^1 - \theta^*| + \sum_{s=1}^{t-1} \alpha_s |Z_s| \leq |\theta^1 - \theta^*| + \sum_{s=1}^{t-1} \alpha_s C = A_t \end{aligned}$$

  where the second inequality is with probability 1.
- Define

$$k_t = \inf_{x \in [\theta^* - A_n, \theta^* + A_n]} \left[\frac{g(x)}{x - \theta^*} \right] \geq 0 \quad \text{from (A-4)}$$

If we can show:
1. $k_t b_t \leq d_t$
2. $\sum_{t=1}^{\infty} \alpha_t k_t = \infty$

We can use lemma 2

Proof $k_t b_t \leq d_t$

$$k_t = \inf_{x \in [\theta^* - A_n, \theta^* + A_n]} \left[\frac{g(x)}{x - \theta^*} \right]$$

$$A_t = |\theta^1 - \theta^*| + C(\alpha_1 + \cdots + \alpha_{t-1})$$

- Define $p_t(\cdot)$ to be the density for θ^t:

$$k_t b_t = k_t E[(\theta^t - \theta^*)^2] = \int_z k_t (z - \theta^*)^2 p_t(z) dz$$

$$= \int_{|z-\theta^*| \leq A_t} k_t (z - \theta)^2 p_t(z) dz \leq \int_{|z-\theta^*| \leq A_t} \frac{g(z)}{z - \theta^*} (z - \theta^*)^2 p_t(z) dz$$

$$= \int_{|z-\theta^*| \leq A_t} g(z)(z - \theta^*) p_t(z) dz = E[g(\theta^t)(\theta^t - \theta^*)] = d_t$$

By the construction of A_t
The density p_t is
supported on this
interval

Proof $\sum_{t=1}^{\infty} \alpha_t k_t = \infty$

$$\boxed{A_t = |\theta^1 - \theta^*| + C(\alpha_1 + \cdots + \alpha_{t-1})}$$

- By (A-2), $\sum_{t=1}^{\infty} \alpha_t = \infty$ which implies that for t larger than some T

$$2C(\alpha_1 + \cdots + \alpha_{t-1}) = A_t + C(\alpha_1 + \cdots + \alpha_{t-1}) - |\theta^1 - \theta^*| \geq A_t.$$

This results in that

$$\sum_{t=1}^{\infty} \alpha_t k_t \geq \sum_{t=\min\{N,T\}}^{\infty} \alpha_t k_t \geq \sum_{t=\min\{N,T\}}^{\infty} \frac{\alpha_t \delta}{A_t}$$

$$\geq \sum_{t=\min\{N,T\}}^{\infty} \frac{\alpha_t \delta}{2C(\alpha_1 + \cdots + \alpha_{t-1})} = \infty$$

showing the second requirement in (5).

$$\boxed{k_t = \inf_{x \in [\theta^* - A_n, \theta^* + A_n]} \left[\frac{g(x)}{x - \theta^*}\right]}$$

$$\inf_{z \in [\theta^* - A_t, \theta^* + A_t]} \left[\frac{g(z)}{z - \theta^*}\right] \geq \frac{\delta}{A_t} \text{ for } t > N$$

Theorem 2

Theorem 2.

Assume (A-1), (A-2), (A-3), (A-4) *and* (A-5). *Assume further* $\delta > 0$ *in* (A-4). *Then* $\lim_{t\to\infty} b_t = 0$.

Proof:
We have for any $z \in [\theta - A_t, \theta + A_t]$

$$\frac{g(z)}{z-\theta} \geq \frac{\delta}{|z-\theta|} \geq \frac{\delta}{A_t}$$

Here
«δ» in (A-4)
can be used directly as
«δ» in Lemma 3

implying that (7) is fulfilled which by Lemma 3 imply the result.

$$\alpha_t > 0 \tag{A-1}$$

$$\sum_{t=1}^{\infty} \frac{\alpha_t}{\alpha_1 + \cdots + \alpha_{t-1}} = \infty \tag{A-2}$$

$$\sum_{t=1}^{\infty} \alpha_t^2 < \infty \tag{A-3}$$

$$\exists \delta \geq 0 \text{ such that } g(x) \leq -\delta \text{ for } x < \theta \text{ and } g(x) \geq \delta \text{ for } x > \theta. \tag{A-4}$$

$$E[Z(\theta;\phi)] = g(\theta) \text{ and } \Pr(|Z(\theta;\phi)| < C) = 1 \tag{A-5}$$

Theorem 3

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Assume (A-1), (A-2), (A-3) *and* (A-5). *Assume further*

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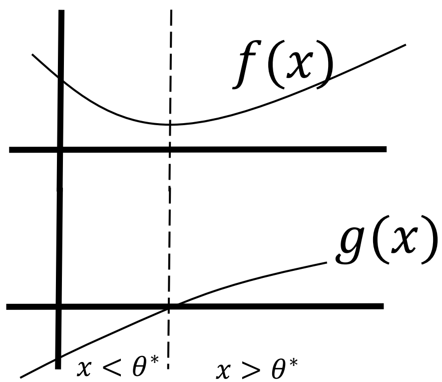
$$g(\theta^*) = 0; \tag{10}$$
$$g'(\theta^*) > 0. \tag{11}$$

Then $\lim_{t\to\infty} b_t = 0$.

$$\alpha_t > 0 \tag{A-1}$$
$$\sum_{t=1}^{\infty} \frac{\alpha_t}{\alpha_1 + \cdots + \alpha_{t-1}} = \infty \tag{A-2}$$
$$\sum_{t=1}^{\infty} \alpha_t^2 < \infty \tag{A-3}$$
$$\cancel{\exists\delta \geq 0 \text{ such that } g(x) \leq -\delta \text{ for } x < \theta \text{ and } g(x) \geq \delta \text{ for } x > \theta.} \tag{A-4}$$
$$E[Z(\theta;\phi)] = g(\theta) \text{ and } \Pr(|Z(\theta;\phi)| < C) = 1 \tag{A-5}$$

(A4) with a $\delta = 0$

$\exists\delta \geq 0$ such that $g(x) \leq -\delta$ for $x < \theta^*$ and $g(x) \geq \delta$ for $x > \theta^*$.



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Then $\lim_{t\to\infty} b_t = 0$.

Lemma 3.

Assume (A-1), (A-2), (A-3), (A-4) *and* (A-5). *Assume for some constant* $\delta > 0$ *that*

$$\inf_{z\in[\theta^*-A_t,\theta^*+A_t]} \left[\frac{g(z)}{z-\theta^*}\right] \geq \frac{\delta}{A_t} \text{ for } t > N \tag{7}$$

Need to be clever to come up with a “new δ” to this Lemma. We do not have a lover limit on g(z) directly.

where

$$A_t = |\theta^1 - \theta^*| + C(\alpha_1 + \cdots + \alpha_{t-1}). \tag{8}$$

Then $\lim_{t\to\infty} b_t = 0$.

Proof of Theorem 3

- $g'(\theta^*) = \lim_{x\to\theta^*} \frac{g(x)-g(\theta^*)}{x-\theta^*}$ imply

$$\frac{g(x)}{x-\theta^*} = g'(\theta^*) + \varepsilon(x-\theta^*), \quad \text{with } \lim_{t\to 0} \varepsilon(t) = 0$$

giving

$$\varepsilon(x-\theta^*) = \frac{g(x)}{(x-\theta^*)} - g'(\theta^*) \geq -\frac{1}{2} g'(\theta^*)$$

for $|x-\theta^*| < \delta$ and δ small enough. Thereby

$$\frac{g(x)}{x-\theta^*} \geq \frac{1}{2} g'(\theta^*), \quad \text{for } |x-\theta^*| \leq \delta$$

- For $\theta^* + \delta \leq x \leq \theta^* + A_t$, since $g(z)$ is nondecreasing

$$\frac{g(x)}{x-\theta^*} \geq \frac{g(x+\delta)}{A_t} \geq \frac{\delta g'(\theta^*)}{2A_t}$$

while for $\theta^* - A_t \leq x \leq \theta^* - \delta$

$$\frac{g(x)}{x-\theta^*} = \frac{-g(x)}{\theta^*-x} \geq \frac{-g(x-\delta)}{A_t} \geq \frac{\delta g'(\theta^*)}{2A_t}$$

- Assuming (without loss of generality) $\delta/A_t \leq 1$ gives

$$\frac{g(x)}{x-\theta^*} \geq \frac{\delta g'(\theta^*)}{2A_t} \quad \text{for } 0 < |x-\theta^*| \leq A_t \Rightarrow \ (7)$$

$g(z)$ is nondecreasing;
$g(\theta^*) = 0$;
$g'(\theta^*) > 0$.

Since $g'(\theta^*) > 0$
we can choose a δ so small that the inequality is fulfilled for all values closer to θ^*

$$A_t = |\theta^1 - \theta^*| + C(\alpha_1 + \cdots + \alpha_{t-1})$$

Here
«δ» in Lemma 3
Is: $\frac{\delta g'(\theta^*)}{2}$
where «δ» is selected above

Stochastic gradients and neural nets

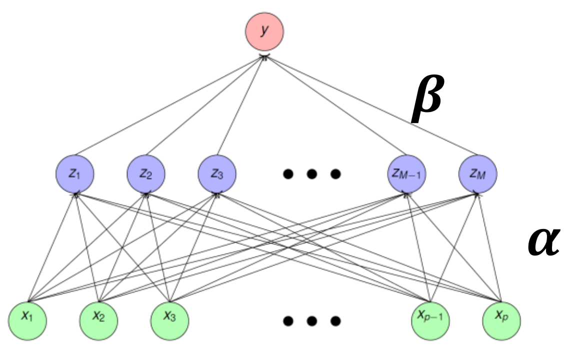
$$Q(\theta) = R(\theta) + \lambda J(\theta) \qquad R(\theta) = \sum_{i=1}^{n} (y_i - f(\mathbf{x}_i))^2$$

$$f(X) = \sum_{m=1}^{M_{NN}} \beta_m \sigma(\alpha_m^T X + \alpha_0)$$

- Q and their derivatives require a sum of n terms
- Can use a stochastic version by sampling randomly a subset of $\{1, \ldots, n\}$
- Called mini-batching
- Advantages (LeCun et al., 2012)
  - Much faster
  - Often give better solutions
  - Can be used to track changes
- Initial values (assuming $g(z) = z$):
  - Given $\boldsymbol{\alpha}$, the model is

    $$y_i = \beta_0 + \boldsymbol{\beta}^T \boldsymbol{z}_i$$

  - Can obtain reasonable values of $\boldsymbol{\beta}$ through least squares
  - Random guess on $\boldsymbol{\alpha}$.
- `Stoch_grad_NN.R`



One hidden layer

Stochastic gradients and neural nets

- Many versions implemented
  - In R: ANN2::neuralnetwork, RSNNS::mlp, nnet::nnet, ...
- Typically, different tricks applied
  - Slow convergence: Fixed learning rate
  - SG through
    - randomly dividing data into minibatches
    - Updating sequentially on each minibach
    - epoch: One go through all data
  - Normalizing imput!
  - Momentum:

$$v^{t+1} = \gamma v^t + \alpha \nabla F(\theta^t)$$
$$\theta^{t+1} = \theta^t - v^{t+1}$$

  - Adaptive learning rates

$$\theta^{t+1} = \theta^t - \frac{\alpha}{\sqrt{||\nabla F(\theta^t)||^2 + \varepsilon}} \nabla F(\theta^t)$$

- Reference: LeCun et al. (2012)
- Example: `ANN2_zip.R`

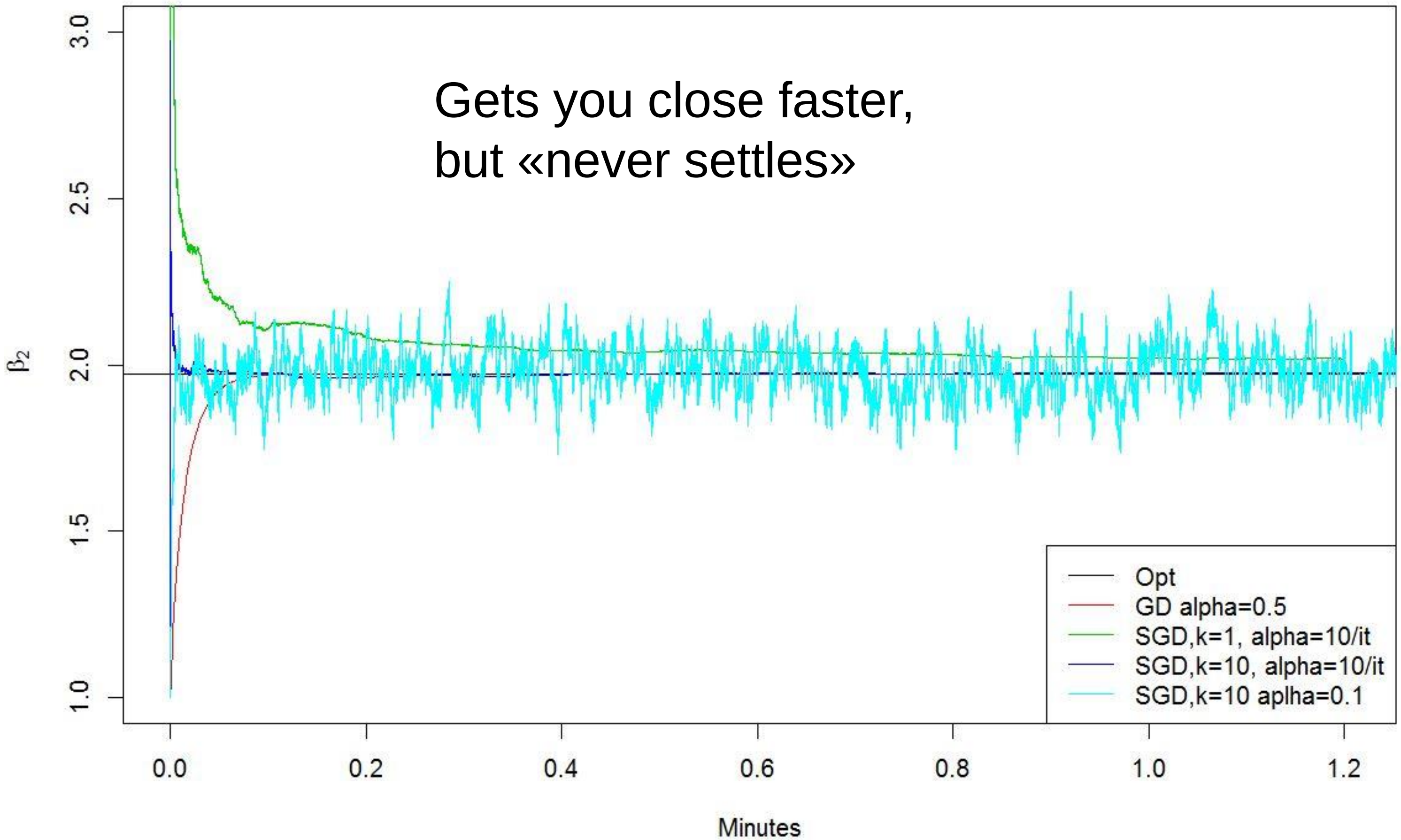
Questions?

- What is the convergence result for SGD?
  - If the function is sufficiently regular (A-4) & the stochastic gradient is unbiased and not too large and (A-5). SGD will converge to the optimum by choosing the learning rate according to (A-1), (A-2)& (A-3)

- Have we proven convergence of SGD for Neural Nets?
  - No, we haven't proven that the NN- function is well behaved

- It is common to use fixed step size when applying SGD for Neural Nets, what might be the reason for this?
  - It converges faster to something close to the optimum.
  - Do you need to get all the way to θ^* to have a good enough result?
  - Half the stepsize if the convergence stall…

Constant learning rate

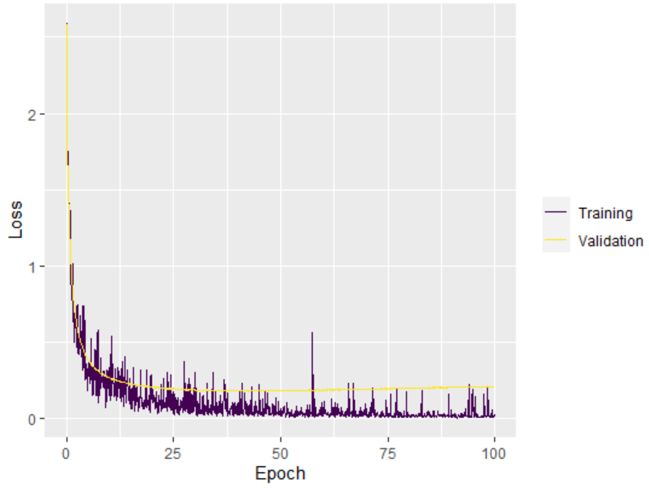


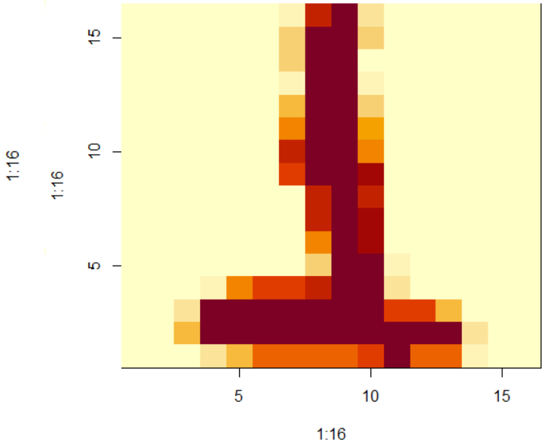
ANN2_zip.R

- Data: https://www.uio.no/studier/emner/matnat/math/STK4051/data/
- Code:

```
# Train neural network on classification task
NN <- neuralnetwork(X = X_train,
                    y = y_train,
                    hidden.layers = c(15,15,15),
                    activ.functions="tanh",
                    optim.type = 'sgd',
                    learn.rates = 0.001,
                    val.prop = 0.1,
                    loss.type='log')
plot(NN)
```

```
neuralnetwork(
  X,
  y,
  hidden.layers,
  regression = FALSE,
  standardize = TRUE,
  loss.type = "log",
  huber.delta = 1,
  activ.functions = "tanh",
  step.H = 5,
  step.k = 100,
  optim.type = "sgd",
  learn.rates = 1e-04,
  L1 = 0,
  L2 = 0,
  sgd.momentum = 0.9,
  rmsprop.decay = 0.9,
  adam.beta1 = 0.9,
  adam.beta2 = 0.999,
  n.epochs = 100,
  batch.size = 32,
  drop.last = TRUE,
  val.prop = 0.1,
  verbose = TRUE,
  random.seed = NULL
)
```





SGD for dependent data

- Consider spatial data:

$$\boldsymbol{Y} = \begin{pmatrix} Y(s_1) \\ Y(s_2) \\ \vdots \\ Y(s_n) \end{pmatrix} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

where $\boldsymbol{\mu} = \mu \boldsymbol{I}$ and $\boldsymbol{\Sigma} = \sigma^2 \boldsymbol{R} + \boldsymbol{\tau}^2 \boldsymbol{I}$, that is

$$\text{cov}[Y(s_i), Y(s_j)] = \begin{cases} \sigma^2 r(||s_i - s_j||; \boldsymbol{\phi}) & s_i \neq s_j \\ \sigma^2 + \tau^2 & s_i = s_j \end{cases}$$

- Realisation of a process defined continuously in a space $\mathcal{S}$
- Log-likelihood with $\boldsymbol{\theta} = (\boldsymbol{\mu}, \sigma^2, \tau^2, \boldsymbol{\phi})$

$$l(\boldsymbol{\theta}) = -\frac{n}{2} \log 2\pi - \frac{1}{2} \log(|\boldsymbol{\Sigma}|) - \frac{1}{2} (\boldsymbol{y} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{y} - \boldsymbol{\mu})$$

- In general, computational burden is $O(n^3)$, problematic for large n

ML and Kullback-Leibler divergence

- True distribution $g(y)$, assumed model $f_\theta(y)$
- Aim: Specify θ so that $f_\theta(y) \approx g(y)$
- Approach: Minimize Kullback-Leibler distance

$$KL(f_\theta, g) = \int \log\left(\frac{g(y)}{f_\theta(y)}\right) g(y)dy$$
$$= \int \log(g(y))g(y)dy - \int \log(f_\theta(y))g(y)dy \geq 0$$

- Equivalent to maximize $\int \log(f_\theta(y))g(y)dy$, problem $g(y)$ unknown
- IID data: Approximate $g(y)$ by $\hat{g}(y) : \Pr(Y = y_i) = \frac{1}{n}$
  - Maximize $\sum_{i=1}^{n} \frac{1}{n} \log(f_\theta(y_i)) = \frac{1}{n}\ell(\theta)$
- Spatial data:

$$KL(f_\theta, g) = \int\int \log\left(\frac{g(\mathbf{y}|\mathbf{s})}{f_\theta(\mathbf{y}|\mathbf{s})}\right) g(\mathbf{y}|\mathbf{s})g(\mathbf{s})d\mathbf{y}d\mathbf{s}$$
$$= \int\int \log(g(\mathbf{y}|\mathbf{s}))g(\mathbf{y}|\mathbf{s})g(\mathbf{s})d\mathbf{y}d\mathbf{s} -$$
$$\int\int \log(f_\theta(\mathbf{y}|\mathbf{s}))g(\mathbf{y}|\mathbf{s})g(\mathbf{s})d\mathbf{y}d\mathbf{s}$$

Not obvious how to approximate $g(\mathbf{y}, \mathbf{s}) = g(\mathbf{y}|\mathbf{s})g(\mathbf{s})$!

KL and Geostatistics

- We have one set of observations $\boldsymbol{y}$. Can approximate $g(\boldsymbol{y},\boldsymbol{s})$ giving probability 1 to this.
  - Leads to the maximum (log-)likelihood approach
  - Has the computational burden mentioned earlier
  - Also has a problem in a poor description of g, lead to that ML estimate may not behave well!
- Liang et al. (2013): Approximate KL by

$$\widehat{KL}(f_\theta,g) = C - \frac{1}{\binom{n}{m}}\sum_{k=1}^{\binom{n}{m}}\log(f_\theta(\boldsymbol{y}_k|\boldsymbol{s}_k))$$

  where $(\boldsymbol{y}_k,\boldsymbol{s}_k)$ is a subset of $(\boldsymbol{y},\boldsymbol{s})$ of size m.
- Find θ as the solution of

$$\frac{\partial}{\partial\theta}\widehat{KL}(f_\theta,g) = C - \frac{1}{\binom{n}{m}}\sum_{k=1}^{\binom{n}{m}}H(\theta,\boldsymbol{y}_k,\boldsymbol{s}_k)$$

$$H(\theta,\boldsymbol{y}_k,\boldsymbol{s}_k) = \frac{\partial}{\partial\theta}\log(f_\theta(\boldsymbol{y}_k|\boldsymbol{s}_k))$$

  by the stochastic gradient algorithm!

Example

$$\log f(\boldsymbol{y}_k|\boldsymbol{s}_k) = -\frac{m}{2}\log 2\pi - \frac{1}{2}\log|\Sigma_k| - \frac{1}{2}(y_k - \mu\mathbf{1}_{\boldsymbol{m}})^T\Sigma_k^{-1}(y_k - \mu\mathbf{1}_{\boldsymbol{m}})$$

$$(\boldsymbol{\Sigma}_k)_{i,j} = \mathrm{cov}(Y(\boldsymbol{s}_{k,i}) - Y(\boldsymbol{s}_{k,j}) = \tau^2 I(j=j) + \sigma^2 \exp(-(||\boldsymbol{s}_{k,i} - \boldsymbol{s}_{k,j}||/\phi)$$

$$(\boldsymbol{R}_k)_{i,j} = \exp(-(||\boldsymbol{s}_{k,i} - \boldsymbol{s}_{k,j}||/\phi)$$

$$H_\mu(\boldsymbol{\theta}, \boldsymbol{y}_k, \boldsymbol{s}_k) = \mathbf{1}_m^T\boldsymbol{\Sigma}_k^{-1}(\boldsymbol{y}_k - \mu\mathbf{1}_m)$$

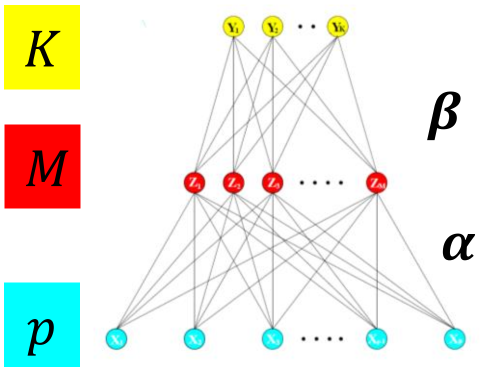
$$H_{\sigma^2}(\boldsymbol{\theta}, \boldsymbol{y}_k, \boldsymbol{s}_k) = -\frac{1}{2}\mathrm{tr}(\boldsymbol{\Sigma}_k^{-1}\boldsymbol{R}_k) + \frac{1}{2}(\boldsymbol{y}_k - \mu\mathbf{1}_m)^T\boldsymbol{\Sigma}_k^{-1}\boldsymbol{R}_k\boldsymbol{\Sigma}_k^{-1}(\boldsymbol{y}_k - \mu\mathbf{1}_m)$$

$$H_{\tau^2}(\boldsymbol{\theta}, \boldsymbol{y}_k, \boldsymbol{s}_k) = -\frac{1}{2}\mathrm{tr}(\boldsymbol{\Sigma}_k^{-1}) + \frac{1}{2}(\boldsymbol{y}_k - \mu\mathbf{1}_m)^T\boldsymbol{\Sigma}_k^{-2}(\boldsymbol{y}_k - \mu\mathbf{1}_m)$$

$$H_\phi(\boldsymbol{\theta}, \boldsymbol{y}_k, \boldsymbol{s}_k) = -\frac{1}{2}\mathrm{tr}(\boldsymbol{\Sigma}_k^{-1}\frac{d\boldsymbol{R}_k}{d\phi}) + \frac{1}{2}(\boldsymbol{y}_k - \mu\mathbf{1}_m)^T\boldsymbol{\Sigma}_k^{-1}\frac{d\boldsymbol{R}_k}{d\phi}\boldsymbol{\Sigma}_k^{-1}(\boldsymbol{y}_k - \mu\mathbf{1}_m)$$

$$\frac{d(\boldsymbol{R}_k)_{i,j}}{d\phi} = ||\boldsymbol{s}_{k,i} - \boldsymbol{s}_{k,j}||/\phi^2 \cdot \exp(-(||\boldsymbol{s}_{k,i} - \boldsymbol{s}_{k,j}||/\phi)$$

Fitting neural networks



θ: Statistical slang for all parameters

Here:

$\{\alpha_{0,m}, \alpha_m\}$, # parameters: $(p+1)M$

$\{\beta_{0,m}, \beta_m\}$, # parameters: $(M+1)K$

$$f(X) = \sum_{m=1}^{M_{NN}} \beta_m \sigma(\alpha_m^T X + \alpha_0)$$

$$R(\theta) = L\left(Y, \hat{f}(X)\right)$$

Quadratic loss
K output variables

$$= \sum_{i=1}^{N} \sum_{k=1}^{K} \left(y_{ik} - \hat{f}_k(x_i)\right)^2$$

$$= \sum_{i=1}^{N} R_i(\theta)$$

Contribution of
the i'th data record $R_i(\theta) = \sum_{k=1}^{K} \left(y_{ik} - \hat{f}_k(x_i)\right)^2$

The "standard" approach:

- Minimize the loss
- Use steepest decent to solve this minimization problem

- The key to success is the efficient way of computing the gradient

Steepest decent

$$R(\theta) = \sum_{i=1}^{N} R_i(\theta)$$

- Minimize $R(\theta)$ wrt θ,
  - Initialize: $\theta^{(0)}$
  - Iterate:

$$\theta_j^{(r+1)} = \theta_j^{(r)} - \underbrace{\gamma_r}_{\text{Learning rate}} \left.\frac{\partial R(\theta)}{\partial \theta_j}\right|_{\theta=\theta^{(r)}}$$

$$\frac{\partial R(\theta)}{\partial \theta_j} = \sum_{i=1}^{N} \frac{\partial R_i(\theta)}{\partial \theta_j}$$

we compute term per data record (easily aggregated from parallel computation) $\frac{\partial R_i(\theta)}{\partial \theta_j}$

$$f(X) = \sum_{m=1}^{M_{NN}} \beta_m \sigma(\alpha_m^T X + \alpha_0)$$

$$R_i(\theta) = \sum_{k=1}^{K} \left(y_{ik} - \hat{f}_k(x_i)\right)^2$$

Squared error loss

Here: $g_k(T) = T = \beta^T z$,=> g_k'=1

Output layer:

$$\frac{\partial R_i(\theta)}{\partial \beta_{k,m}} = \underbrace{-2\left(y_{i,k} - f_k(x_i)\right) g_k'\left(\beta_k^T z_i\right)}_{\delta_{k,i}} z_{m,i}$$
$$= \delta_{k,i} \cdot z_{m,i}$$

Hidden layer:

$$\frac{\partial R_i(\theta)}{\partial \alpha_{m,l}} = \underbrace{-\sum_{k=1}^{K} 2\left(y_{ik} - f_k(x_i)\right) g_k'\left(\beta_k^T z_i\right) \beta_{km}\, \sigma'(\alpha_m^T x_i)}_{s_{m,i}} x_{i,l}$$
$$= s_{m,i} \cdot x_{i,l}$$

Back propagation equation

$$s_{m,i} = \sigma'(\alpha_m^T x_i) \sum_{k=1}^{K} \beta_{km} \delta_{k,i}$$

Back propagation (delta rule)

- At top level. compute:

$$\delta_{k,i} = -2\left(y_{i,k} - f_k(x_i)\right) g_k'\left(\beta_k^T z_i\right), \qquad \forall(i,k)$$

- At hidden level, compute:

$$s_{m,i} = \sigma'(\alpha_m^T x_i) \sum_{k=1}^{K} \beta_{k,m}\delta_{k,i}\,, \qquad \forall(i,m)$$

- Evaluate:

$$\frac{\partial R_i(\theta)}{\partial \beta_{k,m}} = \delta_{k,i} z_{m,i} \;\;\&\;\; \frac{\partial R_i(\theta)}{\partial \alpha_{m,l}} = s_{m,i} x_{i,l}$$

- Update : γ_r is fixed

$$\beta_{k,m}^{(r+1)} = \beta_{k,m}^{(r)} - \gamma_r \sum_{i=1}^{N} \left.\frac{\partial R_i}{\partial \beta_{k,m}}\right|_{\theta=\theta^{(r)}}$$

$$\alpha_{m,l}^{(r+1)} = \alpha_{m,l}^{(r)} - \gamma_r \sum_{i=1}^{N} \left.\frac{\partial R_i}{\partial \alpha_{m,l}}\right|_{\theta=\theta^{(r)}}$$

Stochastic gradient decent using minibatch

$$\beta_{k,m}^{(r+1)} = \beta_{k,m}^{(r)} - \gamma_r \sum_{i=1}^{N} \frac{\partial R_i}{\partial \beta_{k,m}}\bigg|_{\theta=\theta^{(r)}} \quad \alpha_{m,l}^{(r+1)} = \alpha_{m,l}^{(r)} - \gamma_r \sum_{i=1}^{N} \frac{\partial R_i}{\partial \alpha_{\ m,l}}\bigg|_{\theta=\theta^{(r)}}$$

- Equations above updates with all data at the same time
- The form invites to update estimate using fractions of data
  - Perform a random partition of training data in to batches:$\{B_j\}_{j=1}^{\#\text{Batches}}$
  - For all batches cycle over the data in this batch to update data

$$\beta_{k,m}^{(r+1)} = \beta_{k,m}^{(r)} - \gamma_r \sum_{i \in \mathrm{B}_j} \frac{\partial R_i}{\partial \beta_{k,m}}\bigg|_{\theta=\theta^{(r)}} \quad \alpha_{m,l}^{(r+1)} = \alpha_{m,l}^{(r)} - \gamma_r \sum_{i \in B_j} \frac{\partial R_i}{\partial \alpha_{\ m,l}}\bigg|_{\theta=\theta^{(r)}}$$

  - Repeat

- One **iteration** is one update of the parameter (using one batch)
- One **Epoch** is one scan through all data (using all batches in the partition)

Online learning (Batch size =1)

- Learning based on one data point at the time

$$\beta_{k,m}^{(r)} = \beta_{k,m}^{(r-1)} - \gamma_r \frac{\partial R_i}{\partial \beta_{k,m}}\bigg|_{\theta=\theta^{(r-1)}}$$

$$\alpha_{m,l}^{(r)} = \alpha_{m,l}^{(r-1)} - \gamma_r \frac{\partial R_i}{\partial \alpha_{m,l}}\bigg|_{\theta=\theta^{(r-1)}}$$

- You might re-iterate (for several epochs) when completed or if you have an abundance of data just take on new data as they come along (hence the name)

- For convergence: $\gamma_r \to 0$, as $\sum \gamma_r \to \infty$ and $\sum \gamma_r^2 < \infty$, e.g. $\gamma_r = \frac{1}{r}$ (as shown earlier)