Can a biological neuron do linear regression?

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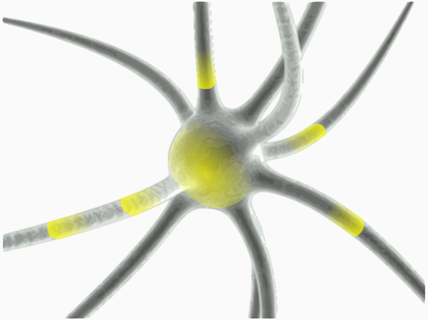


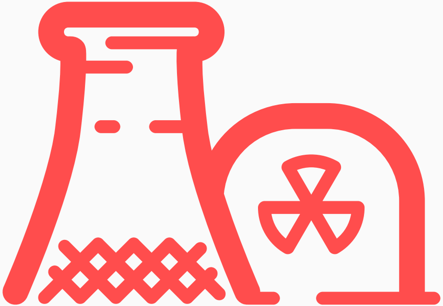
Warm Thanks

Johannes Schmidt-Hieber

Menu

1. Neuroscience in one slide
2. Benchmark Task: Zeroth order Linear Regression
3. BNN meets Linear Regression
4. Reflections

The Main Riddle



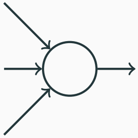
Artificial NN

VS

Biological NN

Neuroscience in one slide

Simplified/concrete/tractable form



Model for single **biological** neuron (Schmidt-Hieber, 2023): with $\mathbf{U}, \mathbf{U}'$ uniform

$$\boldsymbol{\theta}_k \;=\; \boldsymbol{\theta}_{k-1} + \alpha_k \Big(L(\boldsymbol{\theta}_{k-1} + \mathbf{U}_k, \mathbf{X}_k, Y_k) - L(\boldsymbol{\theta}_{k-1} + \mathbf{U}'_k, \mathbf{X}_k, Y_k) \Big) \big(e^{-\mathbf{U}_k} - e^{\mathbf{U}_k} \big).$$

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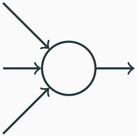

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- Zeroth order: evaluates loss $L(\boldsymbol{\theta}_{k-1} + \mathbf{U}_k, \mathbf{X}_k, Y_k)$, **no derivatives**
- Two-point scheme: for each data item $\mathbf{X}_k, Y_k$ evaluate loss of *two* parameters $\boldsymbol{\theta}_{k-1} + \mathbf{U}_k$ and $\boldsymbol{\theta}_{k-1} + \mathbf{U}'_k$

Benchmark Task: Zeroth order Linear Regression

Linear Regression

Model $(\boldsymbol{\theta}^\star, \mathbb{P}, \sigma^2)$: well-specified linear regression with random design.

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- Risk (expected loss) of parameter $\boldsymbol{\theta}$ is

$$\mathbb{E}\big[L(\boldsymbol{\theta}, \mathbf{X}, Y)\big] \; = \; \mathbb{E}\left[(\mathbf{X}^\intercal(\boldsymbol{\theta} - \boldsymbol{\theta}^\star) - \epsilon)^2\right] \; = \; \|\boldsymbol{\theta} - \boldsymbol{\theta}^\star\|_Q^2 + \sigma^2$$

  where we write $Q := \mathbb{E}[\mathbf{X}\mathbf{X}^\intercal] \succ 0$ for the (uncentred) covariance matrix of the covariates.

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- Excess risk of $\boldsymbol{\theta}$ over risk minimiser $\boldsymbol{\theta}^\star$ is

$$\|\boldsymbol{\theta} - \boldsymbol{\theta}^\star\|_Q^2$$

Interaction Protocol: Two-Point Zeroth-order Stochastic Optimization

For $k = 1, 2, \ldots$

1. Learner picks *two* query points $\boldsymbol{\theta}_{k-1}^{(1)}$ and $\boldsymbol{\theta}_{k-1}^{(2)}$
2. Data item $\mathbf{X}_k, Y_k$ is drawn from linear regression model behind the scenes
3. Learner observes losses $L(\boldsymbol{\theta}_{k-1}^{(1)}, \mathbf{X}_k, Y_k)$ and $L(\boldsymbol{\theta}_{k-1}^{(2)}, \mathbf{X}_k, Y_k)$ of the two query points
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NB: Learner has **no access** to data $\mathbf{X}_k, Y_k$ or gradient $\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}_{k-1}^{(1)}, \mathbf{X}_k, Y_k), \dots$

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The evaluation point $\boldsymbol{\theta}_k$ is random due to random data $\mathbf{X}_1, Y_1, \ldots$ (and randomised queries)
So we evaluate a strategy for Learner by its expected excess risk after k rounds

$$\mathbb{E}_{(\boldsymbol{\theta}^{(1)}_0, \boldsymbol{\theta}^{(2)}_0, \mathbf{X}_1, Y_1) \ldots (\boldsymbol{\theta}^{(1)}_{k-1}, \boldsymbol{\theta}^{(2)}_{k-1}, \mathbf{X}_k, Y_k)} \left[\|\boldsymbol{\theta}_k - \boldsymbol{\theta}^\star\|^2_Q \right]$$

Impact of the Query model for Linear Regression

If we query at $\boldsymbol{\theta}$, we see the scalar loss

$$L = (\mathbf{X}^\intercal \boldsymbol{\theta} - Y)^2 = (\mathbf{X}^\intercal (\boldsymbol{\theta} - \boldsymbol{\theta}^\star) - \epsilon)^2$$

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If further $\mathbf{X} \sim \mathbb{P} = \mathcal{N}(0, I)$ for simplicity, we have

$$\mathbf{X}^\intercal(\boldsymbol{\theta} - \boldsymbol{\theta}^\star) - \epsilon \quad \sim \; \mathcal{N}\left(0, \|\boldsymbol{\theta} - \boldsymbol{\theta}^\star\|^2 + \sigma^2\right)$$

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Multiplicative noise. Very different from additive noise $L \sim \left(\|\boldsymbol{\theta} - \boldsymbol{\theta}^\star\|^2 + \sigma^2\right) + \mathcal{N}(0, \text{const})$.

How hard is this task?

Minimax lower bound for any two-point scheme $\mathcal{V}_k, \widehat{\boldsymbol{\theta}}$.

Theorem

If $d \geq 3$ and $k \geq d^2$, then,

$$\inf_{\mathcal{V}_k, \widehat{\boldsymbol{\theta}}} \sup_{\boldsymbol{\theta}^\star \in B_R(0)} \mathbb{E}_{\boldsymbol{\theta}^\star, \mathcal{V}_k} \left[\|\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}^\star\|^2 \right] \geq \frac{1}{162}\left(1 - \frac{1}{\sqrt{2}}\right)\left(R^2 \wedge \frac{d^2}{k}\sigma^2\right).$$

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Minimax excess risk lower bound for non-adaptive two-point schemes

Theorem

If $d \geq 6$, then for any $k = 1, 2, \ldots$

$$\inf_{\mathcal{V}_k \in \mathcal{M}_k, \widehat{\boldsymbol{\theta}}} \sup_{\boldsymbol{\theta}^\star \in B_R(0)} \mathbb{E}_{\boldsymbol{\theta}^\star, \mathcal{V}_k} \left[\|\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}^\star\|^2 \right] \geq 2^{-18}\left(R^2 \wedge \frac{d^2}{k}(R^2 \vee \sigma^2)\right).$$

BNN meets Linear Regression

Slogan

For our combination of loss and update, (almost) everything is fully explicit **linear/quadratic**.

Connecting BNN to 2P-0O-StochOpt

We query at

$$\boldsymbol{\theta}_{k-1}^{(1)} = \boldsymbol{\theta}_{k-1} + \mathbf{U}_k \qquad \boldsymbol{\theta}_{k-1}^{(2)} = \boldsymbol{\theta}_{k-1} + \mathbf{U}'_k$$

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and update using

$$\begin{aligned}\theta_k &= \theta_{k-1} + \alpha_k \Big((\mathbf{X}_k^\intercal(\theta_{k-1} + \mathbf{U}_k) - Y_k)^2 - (\mathbf{X}_k^\intercal(\theta_{k-1} + \mathbf{U}'_k) - Y_k)^2 \Big) \big(e^{-\mathbf{U}_k} - e^{\mathbf{U}_k} \big) \\ &= \theta_{k-1} + \alpha_k \Big((\mathbf{X}_k^\intercal(\theta_{k-1} - \theta^\star + \mathbf{U}_k) - \epsilon_k)^2 - (\mathbf{X}_k^\intercal(\theta_{k-1} - \theta^\star + \mathbf{U}'_k) - \epsilon_k)^2 \Big) \big(e^{-\mathbf{U}_k} - e^{\mathbf{U}_k} \big).\end{aligned}$$

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So with $\delta_k := \theta_k - \theta^\star$, we get the recurrence

$$\begin{aligned}\delta_k &= \delta_{k-1} + \alpha_k\Big((\mathbf{X}_k^\intercal(\delta_{k-1} + \mathbf{U}_k) - \epsilon_k)^2 - (\mathbf{X}_k^\intercal(\delta_{k-1} + \mathbf{U}'_k) - \epsilon_k)^2\Big)\big(e^{-\mathbf{U}_k} - e^{\mathbf{U}_k}\big).\\ &= \delta_{k-1} + \alpha_k\Big(2(\mathbf{X}_k^\intercal\delta_{k-1} - \epsilon_k)\mathbf{X}_k^\intercal(\mathbf{U}'_k - \mathbf{U}_k) + (\mathbf{X}_k^\intercal\mathbf{U}_k)^2 - (\mathbf{X}_k^\intercal\mathbf{U}'_k)^2\Big)\big(e^{-\mathbf{U}_k} - e^{\mathbf{U}_k}\big).\\ &= \Big(I + 2\alpha_k\big(e^{-\mathbf{U}_k} - e^{\mathbf{U}_k}\big)(\mathbf{U}'_k - \mathbf{U}_k)^\intercal\mathbf{X}_k\mathbf{X}_k^\intercal\Big)\delta_{k-1}\\ &\quad + \alpha_k\Big(-2\epsilon_k\mathbf{X}_k^\intercal(\mathbf{U}'_k - \mathbf{U}_k) + (\mathbf{X}_k^\intercal\mathbf{U}_k)^2 - (\mathbf{X}_k^\intercal\mathbf{U}'_k)^2\Big)\big(e^{-\mathbf{U}_k} - e^{\mathbf{U}_k}\big)\end{aligned}$$

Does it even make sense on average?

We expressed our update rule in Stochastic Approximation form

$$\boldsymbol{\delta}_k = (I - \alpha_k \mathbf{A}_k)\boldsymbol{\delta}_{k-1} + \alpha_k \mathbf{b}_k$$

for i.i.d. random matrix $\mathbf{A}_k$ and vector $\mathbf{b}_k$ given by

$$\begin{aligned}
\mathbf{A}_k &:= -2\left(e^{-\mathbf{U}_k} - e^{\mathbf{U}_k}\right)(\mathbf{U}_k' - \mathbf{U}_k)^\intercal \mathbf{X}_k \mathbf{X}_k^\intercal, \\
\mathbf{b}_k &:= \left(-2\epsilon_k \mathbf{X}_k^\intercal (\mathbf{U}_k' - \mathbf{U}_k) + (\mathbf{X}_k^\intercal \mathbf{U}_k)^2 - (\mathbf{X}_k^\intercal \mathbf{U}_k')^2\right)\left(e^{-\mathbf{U}_k} - e^{\mathbf{U}_k}\right).
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We have $\mathbb{E}[\mathbf{b}] = 0$ and $\mathbb{E}[\mathbf{A}] = \eta Q$ with constant $\eta \coloneqq 2\,\mathbb{E}[\left(e^{-U} - e^{U}\right)U]$ depending on the scale A of noise $\mathbf{U}$.

In expectation, our update gives

$$\mathbb{E}_k[\boldsymbol{\delta}_k] \;=\; \left(I - \alpha_k \eta Q\right)\boldsymbol{\delta}_{k-1}$$

That is **exactly** gradient descent on the **risk** $\|\boldsymbol{\delta}\|_Q^2 + \sigma^2$, with learning rate $\frac{1}{2}\alpha_k\eta$.

Case closed?

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So let's work on the expected excess risk after k rounds (whp bounds also interesting):

$$\Xi_k \;:=\; \mathbb{E}\left[\|\boldsymbol{\delta}_k\|_Q^2\right] \qquad \text{where} \qquad Q \;=\; \mathbb{E}[\mathbf{X}\mathbf{X}^\intercal]$$

Can we get a recurrence for Ξ_k? Yes!

Recurrence for excess risk

Recall our update rule is of the form

$$\boldsymbol{\delta}_k \;=\; (I - \alpha_k \mathbf{A}_k)\boldsymbol{\delta}_{k-1} + \alpha_k \mathbf{b}_k$$

for i.i.d. random matrix $\mathbf{A}_k$ and vector $\mathbf{b}_k$, with $\mathbb{E}[\mathbf{A}] = \eta Q$, and $\mathbb{E}[\mathbf{b}] = \mathbb{E}[\mathbf{A}^\intercal Q \mathbf{b}] = 0$.

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So the excess risk satisfies

$$\begin{aligned}
\Xi_k \;&=\; \mathbb{E}_k\left[\boldsymbol{\delta}_k^\intercal Q \boldsymbol{\delta}_k\right] \\
&=\; \mathbb{E}_k\left[((I - \alpha_k \mathbf{A}_k)\boldsymbol{\delta}_{k-1} + \alpha_k \mathbf{b}_k)^\intercal Q((I - \alpha_k \mathbf{A}_k)\boldsymbol{\delta}_{k-1} + \alpha_k \mathbf{b}_k)\right] \\
&=\; \boldsymbol{\delta}_{k-1}^\intercal\, \mathbb{E}_k\left[(I - \alpha_k \mathbf{A}_k)^\intercal Q (I - \alpha_k \mathbf{A}_k)\right] \boldsymbol{\delta}_{k-1} + \alpha_k^2\, \mathbb{E}_k\left[\mathbf{b}_k^\intercal Q \mathbf{b}_k\right] \\
&=\; \boldsymbol{\delta}_{k-1}^\intercal \left\{(I - \alpha_k \eta Q)^\intercal Q (I - \alpha_k \eta Q) + \alpha_k^2\, \mathbb{E}_k\left[(\mathbf{A}_k - \eta Q)^\intercal Q (\mathbf{A}_k - \eta Q)\right]\right\} \boldsymbol{\delta}_{k-1} + \alpha_k^2\, \mathbb{E}_k\left[\mathbf{b}_k^\intercal Q \mathbf{b}_k\right] \\
&\le\; \left((1 - \alpha_k \eta \lambda_{\min}(Q))^2 + \alpha_k^2 \beta\right) \Xi_{k-1} + \alpha_k^2 \gamma
\end{aligned}$$

abbreviating $\beta := \lambda_{\max}\left(\mathbb{E}_k\left[Q^{-1/2}(\mathbf{A}_k - \eta Q)^\intercal Q (\mathbf{A}_k - \eta Q) Q^{-1/2}\right]\right)$ and $\gamma := \mathbb{E}_k\left[\mathbf{b}_k^\intercal Q \mathbf{b}_k\right]$.

Inspecting where we are

Our state of progress so far is

$$\Xi_k \ \leq \ \Big((1 - \alpha_k \eta \lambda_{\mathsf{min}}(Q))^2 + \alpha_k^2 \beta\Big) \Xi_{k-1} + \alpha_k^2 \gamma$$

for fixed η, $\lambda_{\mathsf{min}}(Q)$, β and γ. The question is how to tune α_k. This is now a scalar problem.

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for fixed η, $\lambda_{\min}(Q)$, β and γ. The question is how to tune α_k. This is now a scalar problem.

Cancelling derivative reveals this bound is optimised in α_k at

$$\alpha_k^* \;=\; \frac{\eta\lambda_{\min}(Q)}{\eta^2\lambda_{\min}(Q)^2+\beta+\frac{\gamma}{\Xi_{k-1}}}$$

and at that point we obtain

$$\Xi_k \;\le\; \left(\frac{\beta+\frac{\gamma}{\Xi_{k-1}}}{\eta^2\lambda_{\min}(Q)^2+\beta+\frac{\gamma}{\Xi_{k-1}}}\right)\Xi_{k-1}$$

Cute ODE upper bound

We can write our recurrence so far as a difference equation

$$\frac{\Xi_k - \Xi_{k-1}}{\Xi_{k-1}} \leq -\frac{\eta^2 \lambda_{\min}(Q)^2}{\eta^2 \lambda_{\min}(Q)^2 + \beta + \frac{\gamma}{\Xi_{k-1}}}$$

and solve the corresponding **differential equation** with equality to find

$$\frac{\Xi_k}{\Xi_1} \leq \frac{y}{W\left(y e^{y+xk}\right)} \quad \text{with} \quad x := \frac{\eta^2 \lambda_{\min}(Q)^2}{\eta^2 \lambda_{\min}(Q)^2 + \beta} \quad \text{and} \quad y := \frac{\gamma/\Xi_1}{\eta^2 \lambda_{\min}(Q)^2 + \beta}$$

so that all in all the excess risk decays as $\Xi_k \cong \Xi_1/k$ and the **learning rate** as $\alpha_k^* \cong 1/k$.

More precisely in terms of relevant problem-dependent constants

We arrive at excess risk bound

Theorem

$$\Xi_k \;\leq\; \frac{121\kappa d^2}{2\lambda_{\min}(Q)} \frac{48\sigma^2 M_2 + 107 A^2 d M_4}{k + C}$$

where $\kappa = \frac{\lambda_{\max}(Q)}{\lambda_{\min}(Q)}$ *is the condition number of* Q*, and* M_p *bounds the* i^{th} *moment of each entry of the covariate vector* $\mathbf{X} \sim \mathbb{P}$*.*

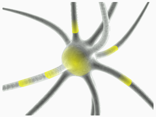
If $A^2 d$ is at most of order σ^2, this is d^2/k. Matching lower bounds.

Reflections

To think about

- Is the optimal tuning $\alpha_k \cong 1/k$ biologically realistic?
- Learning rate α_k needs to decay. What decides a *new task* in the brain?
- Optimal tuning for α_k depends on zoo of unknowns. How are these estimated?
- Brutal tuning $\alpha_k = \frac{c}{C+k}$ may result in risk rising to e^{const} before $1/k$ decay kicks in.
- Is the noise rate A biologically small compared to $\sigma/\sqrt{d}$?
- Realism in the model
  - More than one neuron
  - Depth, architecture
  - Other tasks and losses

Conclusion



We saw a simple model for spiking neurons inspired by biology.

We saw a concrete rendering of resulting update rule.

We interpreted it as a zeroth-order two-point iterative scheme.

We evaluated this scheme on a linear regression task.

We derived a rate for the excess risk, and proved that it matches lower bounds.

Let's talk!

References i

Schmidt-Hieber, J. (2023). **“Interpreting learning in biological neural networks as zero-order optimization method”.** In: *arXiv preprint*, arXiv:2301.11777.