A case where a spindly two-layer linear network ~~whips~~ decisively outperforms any neural network with a fully connected input layer

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Paradigmic sparse linear problem

$$\begin{pmatrix} -1 & -1 & 1 & -1 & -1 \\ 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} -1 \\ -1 \\ -1 \\ 1 \\ 1 \end{pmatrix}$$

$\pm$ matrix random or Hadamard

After receiving example $(\boldsymbol{x}_t, y_t)$
and incurring loss $1/2\,(\boldsymbol{x}_t^\top \boldsymbol{w}_t - y_t)^2$, update:

additive, GD: $$w_{t+1,i} = w_{t,i} - \eta \underbrace{\boldsymbol{x}_{t,i}(\boldsymbol{x}_t^\top \boldsymbol{w}_t - y_t)}_{\text{gradient}}$$

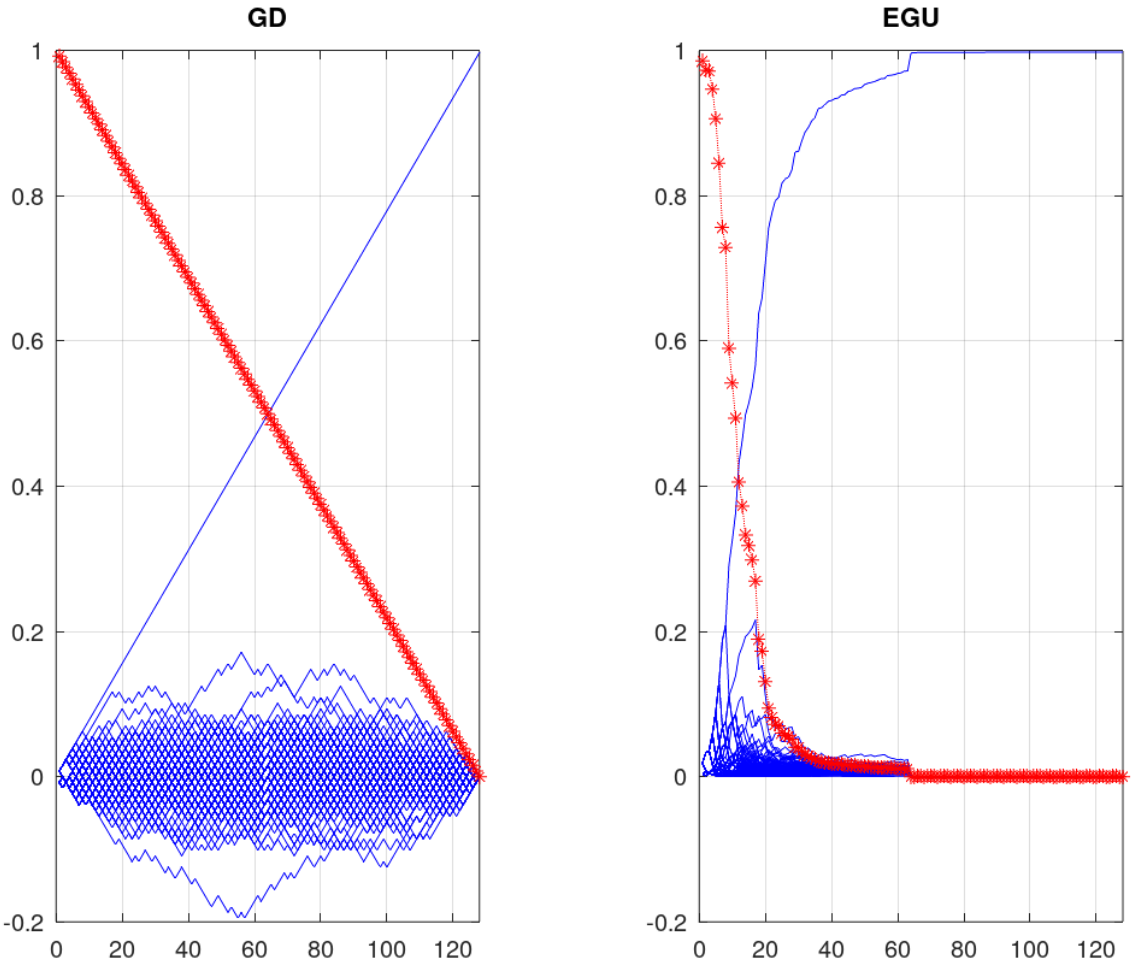
multiplicative, EGU: $$w_{t+1,i} = w_{t,i} \exp(-\eta \boldsymbol{x}_{t,i}(\boldsymbol{x}_t^\top \boldsymbol{w}_t - y_t))$$

Linear regression

Major differences in following paradigmatic setup:

128x128 Hadamard matrix

Permuted rows are instances, labels are any fixed column



x-axis: $k = 1..128$

Recent surprise and goal of this talk

Hadamard Problem: Instances are rows of the Hadamard matrix, labels are one of the features (e.g. $\boldsymbol{w} = \boldsymbol{e}_1$)

$$\begin{pmatrix} + & + & + & + \\ + & - & + & - \\ + & + & - & - \\ + & - & - & + \end{pmatrix}$$

Conjecture [DW14]: For the Hadamard problem all neural nets trained w. GD incur loss at least $1 - k/d$ after seeing k examples

Surprise: Spindly GD trained linear net cracks shifted Hadamard with loss $\leq \frac{\log d}{k}$

Simulates EGU [AW20]

Square reparameterization trick reintroduced in [GWBNS17]

Here: Lower bound of $\geq 1 - k/d$ for any GD trained net with a **fully connected input layer**

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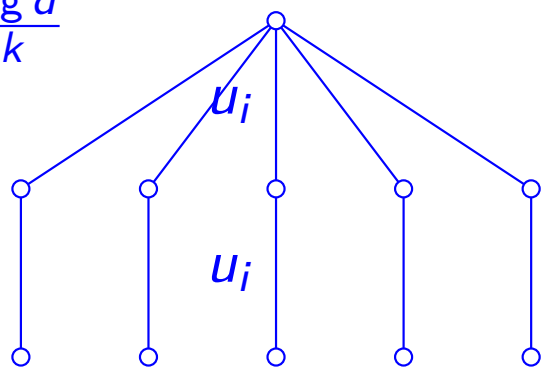

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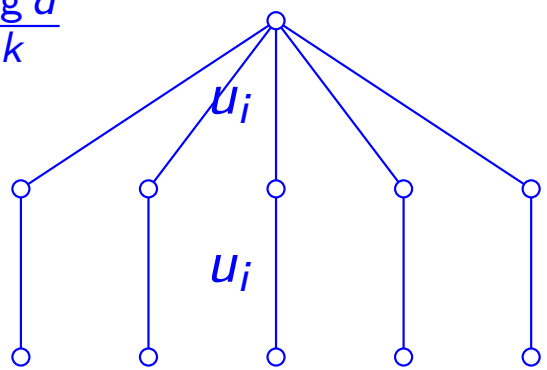

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Old versus new lower bounds

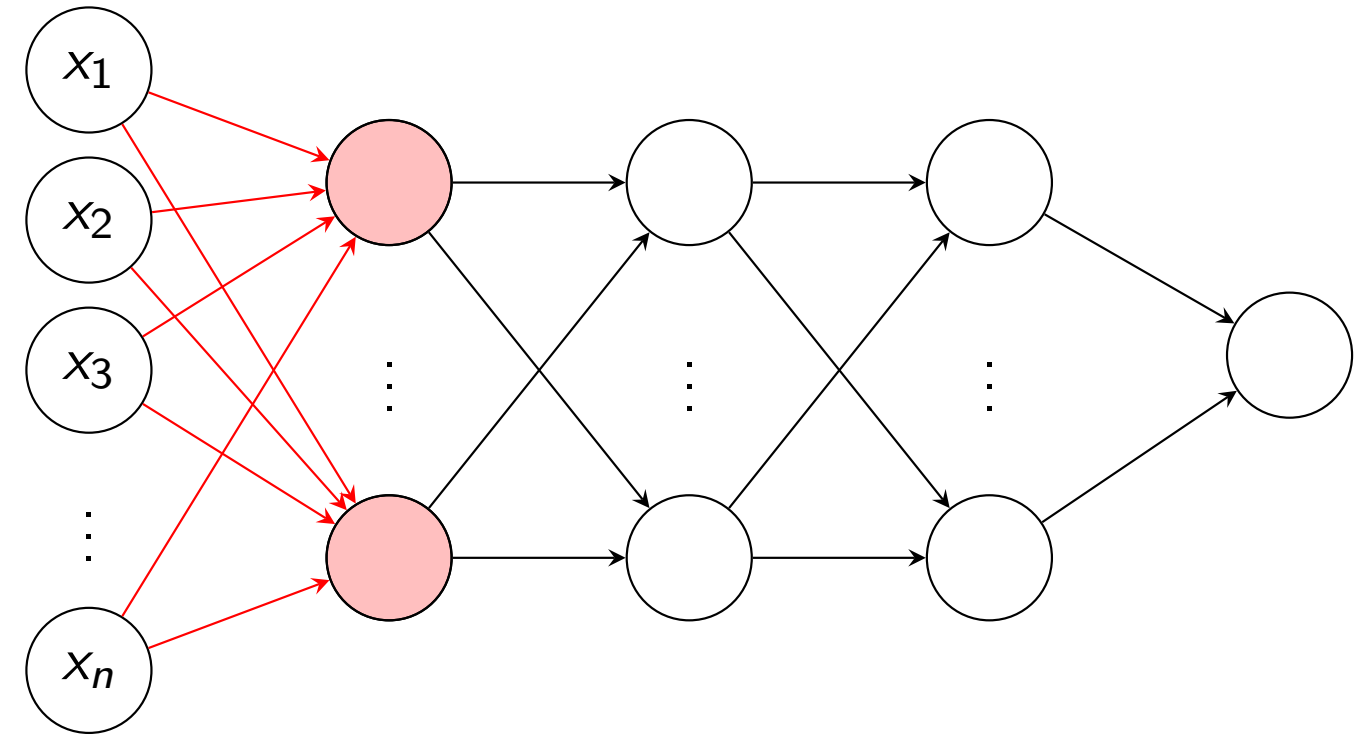
Previous SVD based lower bound technique of [WV05]

- \+ Holds for any expansion
- – Only for single linear neuron
- – Can't go beyond 2 layer linear
- – Restricted to square loss

NEW: Hold for any GD trained any neural net **of any depth** with a fully connected input layer

- – Does not hold for any expansion (essentially Hadamard or Gaussian)
- \+ Holds for single target such as constant feature $\boldsymbol{e}_1$
- \+ Very general losses

Crux: GD trained w. fully connected input layer implies rotational invariance of the predictions



- fully connected input layer with rotation invariant initialization at 1st hidden layer
- weights of first hidden layer trained with GD, any learning rates
- one output node, any initialization
- otherwise any architecture and initialization
- any differentiable transfer functions at the internal nodes
- very general loss function

Minimal loss function assumptions

$L(y, \hat{y})$ differentiable in $\hat{y}$ and
$\min_{\hat{y}} \frac{L(-1,\hat{y})+L(+1,\hat{y})}{2}$ is some positive constant c

Simplifying assumption for the talk: loss is **convex**

Then for proving lower bounds, any randomized algorithm $\hat{y}$ can be turned into a **deterministic algorithm** $\hat{y}_{\text{det}}$:

$$\hat{y}_{\text{det}}(\boldsymbol{x}|(\boldsymbol{X}_{\text{tr}}, \boldsymbol{y}_{\text{tr}})) = \mathbb{E}\left[\hat{y}(\boldsymbol{x}|(\boldsymbol{X}_{\text{tr}}, \boldsymbol{y}_{\text{tr}}))\right]$$

which by Jensen's inequality has loss no greater than the expected loss of $\hat{y}$ on any instance

For simplicity we use **square loss**, i.e. $c = 1$

It's all about rotation invariance of the predictions

A prediction algorithm $\hat{y}(\boldsymbol{x}|(\boldsymbol{X}_{\text{tr}}, \boldsymbol{y}_{\text{tr}}))$ is called **rotation invariant** if

$$\hat{y}(\boldsymbol{U}\boldsymbol{x}|(\boldsymbol{X}_{\text{tr}}\boldsymbol{U}^{\top}, \boldsymbol{y}_{\text{tr}})) = \hat{y}(\boldsymbol{x}|(\boldsymbol{X}_{\text{tr}}, \boldsymbol{y}_{\text{tr}})), \text{ for any orthogonal matrix } \boldsymbol{U}$$

GD trained neural nets with fully connected input layers are rotation invariant because gradients/weights at input nodes are linear combinations of the training instances

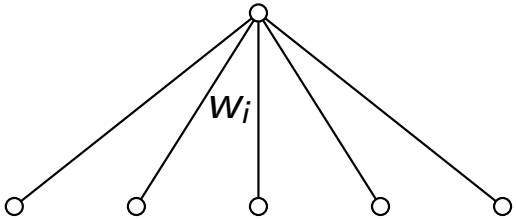
$$\frac{\partial f(\boldsymbol{x} \cdot \boldsymbol{w})}{\partial \boldsymbol{w}} = f'(a)|_{a=\boldsymbol{x}\cdot\boldsymbol{w}}\, \boldsymbol{x}$$

Crux: Any input node that receives an input feature, must receive all input features

Newton, versions of AdaGrad & Adam, ..., also rotation invariant

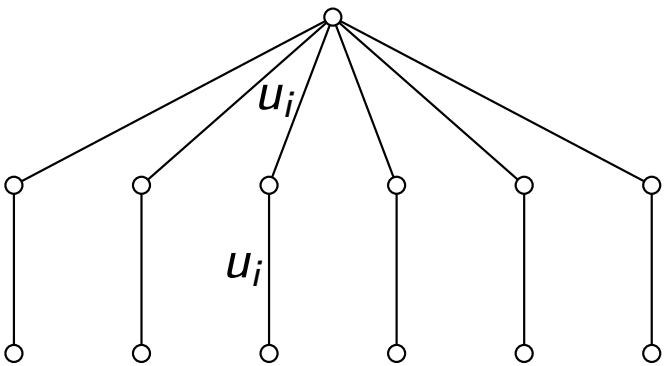
Interlude

EGU on single neuron



$$w_{t+1,i} = w_{t,i} \exp\left(-\eta\, \boldsymbol{x}_{t,i}(\boldsymbol{x}_t^\top \boldsymbol{w}_t - y_t)\right)$$

and GD on spindly network



$$u_{t+1,i}^2 = u_{t,i}^2 \left(1 - \eta/2\, \boldsymbol{x}_{t,i}(\boldsymbol{x}_t^\top \boldsymbol{w}_t - y_t)\right)^2$$

both decidedly not rotation invariant:

- access individual features
- rank grows exponentially fast

Hardness for any rotation invariant algorithm

Initial problem $(\underset{d,d}{\boldsymbol{H}}, \underset{d,1}{\mathbf{1}})$.

Too easy

For each sign pattern $\boldsymbol{s} \in \{+1,-1\}^d$ consider problem $(\mathrm{diag}(\boldsymbol{s})\boldsymbol{H}, \boldsymbol{s})$

Define a rotation matrix $\boldsymbol{U_s}$ as $1/\sqrt{d}\,\mathrm{diag}(\boldsymbol{s})\boldsymbol{H}$

The predictions of any rotation invariant algorithm on $(\mathrm{diag}(\boldsymbol{s})\boldsymbol{H}, \boldsymbol{s})$ and $(\mathrm{diag}(\boldsymbol{s})\boldsymbol{H}\boldsymbol{U_s}^\top, \boldsymbol{s}) = (\sqrt{d}\boldsymbol{I}, \boldsymbol{s})$ are the same

Now fix $\boldsymbol{s}_{1:k}$. The algorithm receives the same first k training examples for each problem $(\sqrt{d}\boldsymbol{I}, \boldsymbol{s})$. Also since $\boldsymbol{s}_{(k+1):d}$ is chosen uniformly, each of the $d-k$ unseen examples is labeled ± 1 with equal probability. So the best prediction on these $d-k$ examples is 0, incurring square loss at least 1 for each unseen example

Conclusion: Expected average loss on all d examples is at least $(d-k)/d = 1 - k/d$

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Extensions

- Lower bound holds even for rotation invariant initialization of hidden nodes of first layer
  (which must all be connected to all inputs)
- There are versions of the problem where the features are $0/1$ instead of ± 1
- Only minimal requirements on the loss needed:
  $L(y, \hat{y})$ differentiable in $\hat{y}$ and
  $\min_{\hat{y}} \frac{L(-1,\hat{y})+L(+1,\hat{y})}{2}$ is some positive constant c

Extensions cont.

- Only slightly weaker linear lower bound for the case when entries of $\underset{d,d}{\boldsymbol{X}}$ are i.i.d. Gaussian and the target is first column $\boldsymbol{X}\boldsymbol{e}_1$:

  After seeing k examples, the expected average square loss on all d examples is at least $(1 - {}^{k}/_{d})^2 = 1 - 2\,{}^{k}/_{d} + ({}^{k}/_{d})^2$
  (so far only for square loss)

- Experimentally the same lower bound for square loss holds for random ± 1 matrices and single feature targets,
  but no proof yet

Is there a method here?

Structure of neural net / update
$\longrightarrow$ invariance
$\longrightarrow$ lower bound

	additive	multiplicative
rot. invariance	$\hat{y}(\boldsymbol{U}\boldsymbol{x}\|(\boldsymbol{X}_{\text{tr}}\boldsymbol{U}^\top, \boldsymbol{y}_{\text{tr}}))$	$\hat{y}(\boldsymbol{U}\boldsymbol{x}\boldsymbol{z}^\top\boldsymbol{V}^\top\|(\boldsymbol{U}\boldsymbol{X}_{\text{tr}}\boldsymbol{Z}_{\text{tr}}^\top\boldsymbol{V}^\top, \boldsymbol{y}_{\text{tr}}))$
	$= \hat{y}(\boldsymbol{x}\|(\boldsymbol{X}_{\text{tr}}, \boldsymbol{y}_{\text{tr}}))$	$= \hat{y}(\boldsymbol{x}\boldsymbol{z}^\top\|(\boldsymbol{X}_{\text{tr}}\boldsymbol{Z}_{\text{tr}}^\top, \boldsymbol{y}_{\text{tr}}))$
linear comb.	$\boldsymbol{w} = \boldsymbol{X}_{\text{tr}}^\top \boldsymbol{a}$	$\boldsymbol{W} = \boldsymbol{X}_{\text{tr}}\boldsymbol{C}\boldsymbol{Z}_{\text{tr}}^\top$
hard problem	Hadamard	???
lower bound	$1 - {}^{k}/_{d}$	???

[WKZ14]

The future is open

For Hadamard instances:

- We showed above that GD trained neural nets with a complete input layer cannot learn a **single target** sample efficiently.
- However **any single target feature $\boldsymbol{y}$ can** be learned when inputs are transformed by the map $\phi(\boldsymbol{H}) = \boldsymbol{y}$
- **Conjecture: The d target features cannot be learned with any $\phi(\cdot)$ map when we average over targets**

Rotation invariance of on-line Newton

Inductive hypothesis: Under transformation $\boldsymbol{x}_t \mapsto \boldsymbol{U}\boldsymbol{x}_t$ for all t we have $\boldsymbol{w}_t \mapsto \boldsymbol{U}\boldsymbol{w}_t$.

Suppose it holds for $\boldsymbol{w}_j$, $j \leq t$ and we show it holds for $\boldsymbol{w}_{t+1}$.

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t - \eta \boldsymbol{A}_t^{-1} \nabla_t, \quad \boldsymbol{A}_t = \epsilon \boldsymbol{I} + \sum_{j \leq t} \nabla_j \nabla_j^\top, \quad \nabla_t = (\hat{y}_t - y_t)\boldsymbol{x}_t$$

Since $\hat{y}_j = \boldsymbol{w}_j^\top \boldsymbol{x}_j \mapsto \boldsymbol{w}_j^\top \boldsymbol{U}^\top \boldsymbol{U}\boldsymbol{x}_j = \hat{y}_j$, we have $\nabla_j \mapsto \boldsymbol{U}\nabla_j$ for $j \leq t$, so $\boldsymbol{A}_t \mapsto \boldsymbol{U}\boldsymbol{A}_t\boldsymbol{U}^\top$. Therefore:

$$\boldsymbol{w}_{t+1} \mapsto \boldsymbol{U}\boldsymbol{w}_t - \eta \boldsymbol{U}\boldsymbol{A}_t^{-1}\boldsymbol{U}^\top \boldsymbol{U}\nabla_t = \boldsymbol{U}\boldsymbol{w}_{t+1}$$

Versions of Adagrad

- Diagonal version:

$$\boldsymbol{w}_{t+1,i} = \boldsymbol{w}_{t,i} - \frac{\eta}{\sqrt{\epsilon + \sum_{j \leq t} \nabla_{j,i}^2}} \nabla_{t,i}$$

  Clearly not rotation-invariant, but when $\boldsymbol{x}_{t,i} = \pm 1$ for all t, i, then $\nabla_{j,i}^2 = (y_t - \hat{y}_t)^2$, i.e. the effective learning rate is shared among all coordinates and rotation invariance holds.

- Full version:

$$\boldsymbol{w}_t = \boldsymbol{w}_t - \eta \sqrt{\boldsymbol{A}_t} \nabla_t, \qquad \boldsymbol{A}_t = \epsilon \boldsymbol{I} + \sum_{j \leq t} \nabla_j \nabla_j^\top$$

  Rotation invariant, proof analogous to On-line Newton

Adam

- Adagrad with momentum and exponentially decaying memory on the past
- Essentially the same arguments as for diagonal Adagrad: generally not rotation invariant, but for ± 1 valued data it is rotation invariant.

[VAW] and [FW]

$$\boldsymbol{w}_t = \boldsymbol{A}_t^{-1} \sum_{j \le t-1} y_j \boldsymbol{x}_j, \qquad \boldsymbol{A}_t = \epsilon \boldsymbol{I} + \sum_{j \le t} \boldsymbol{x}_j \boldsymbol{x}_j^\top.$$

VAW is also rotation invariant: under transformation $\boldsymbol{x}_t \mapsto \boldsymbol{U}\boldsymbol{x}_t$ for all t, we clearly have $\boldsymbol{A}_t \mapsto \boldsymbol{U}\boldsymbol{A}_t\boldsymbol{U}^\top$, so $\boldsymbol{A}_t^{-1} \mapsto \boldsymbol{U}\boldsymbol{A}_t^{-1}\boldsymbol{U}^\top$, and thus

$$\boldsymbol{w}_t \mapsto \boldsymbol{U}\boldsymbol{A}_t^{-1}\boldsymbol{U}^\top \sum_{j \le t-1} y_j \boldsymbol{U}\boldsymbol{x}_j = \boldsymbol{U}\boldsymbol{A}_t^{-1} \sum_{j \le t-1} y_t \boldsymbol{x}_j = \boldsymbol{U}\boldsymbol{w}_t$$