Effective Theory of Transformers



Emily Dinan, Sho Yaida, Susan Zhang [arXiv:2304.02034]

Meta

(Spinoff from)
Effective Theory of Deep Neural Networks



Dan Roberts, Sho Yaida, Boris Hanin [arXiv:2106.10165; Cambridge University Press]

Meta

(Branch of)
Physics of Machine Learning

Order-one fraction of people in this room

Meta

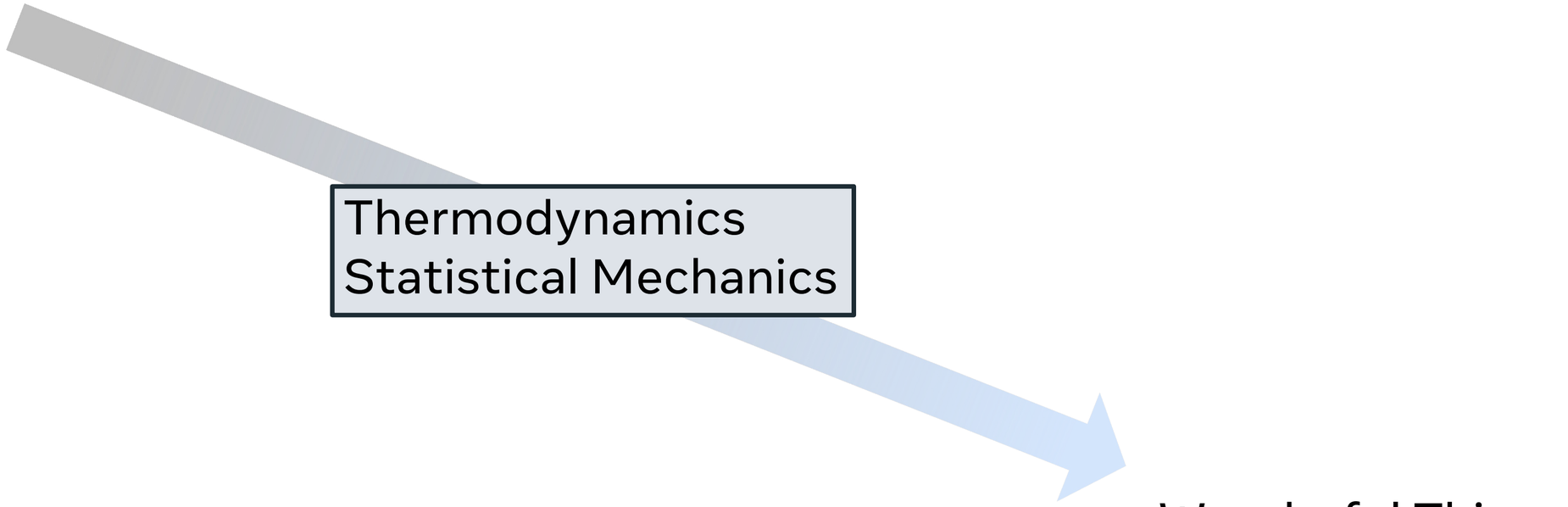
Historical Motivation

Steam Engine

Wonderful Things

Historical Motivation

Steam Engine



Wonderful Things

Historical Motivation

Deep Learning

Wonderful Things

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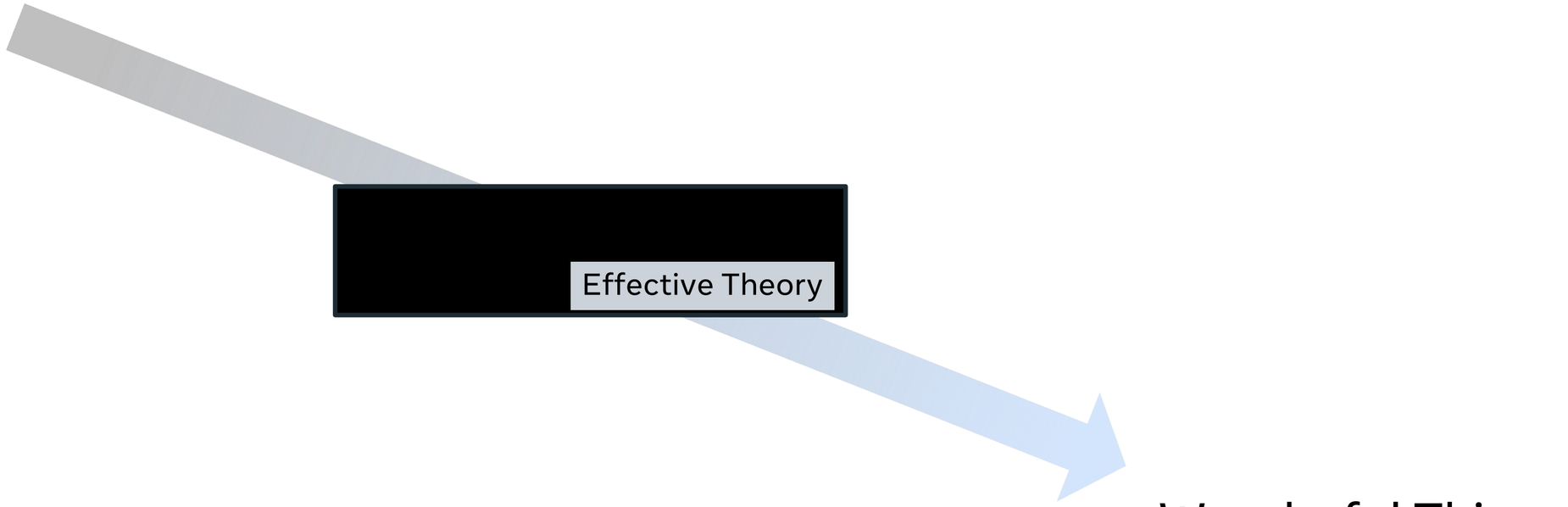


Wonderful Things

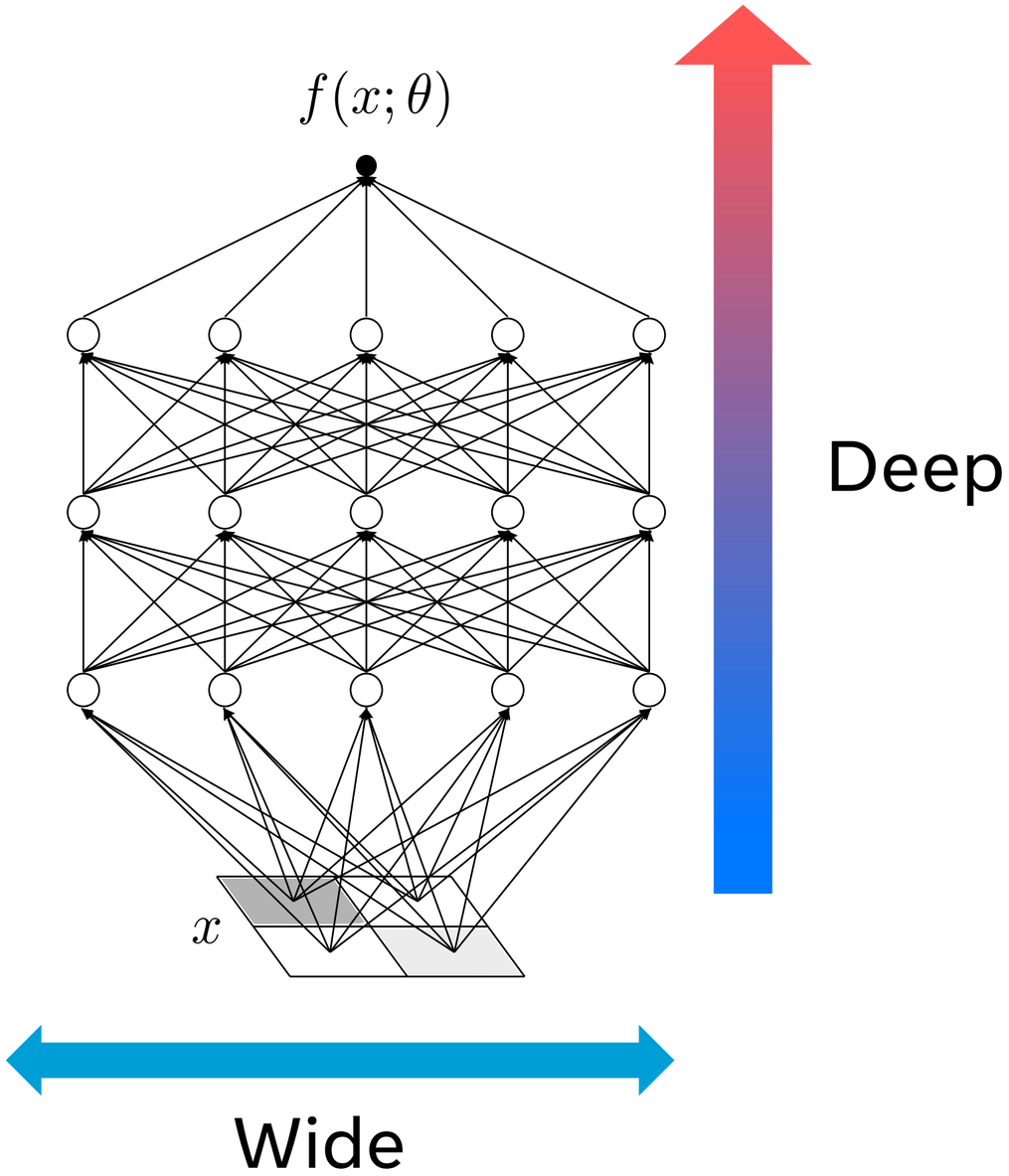
Outline

1. Simplification @Scale

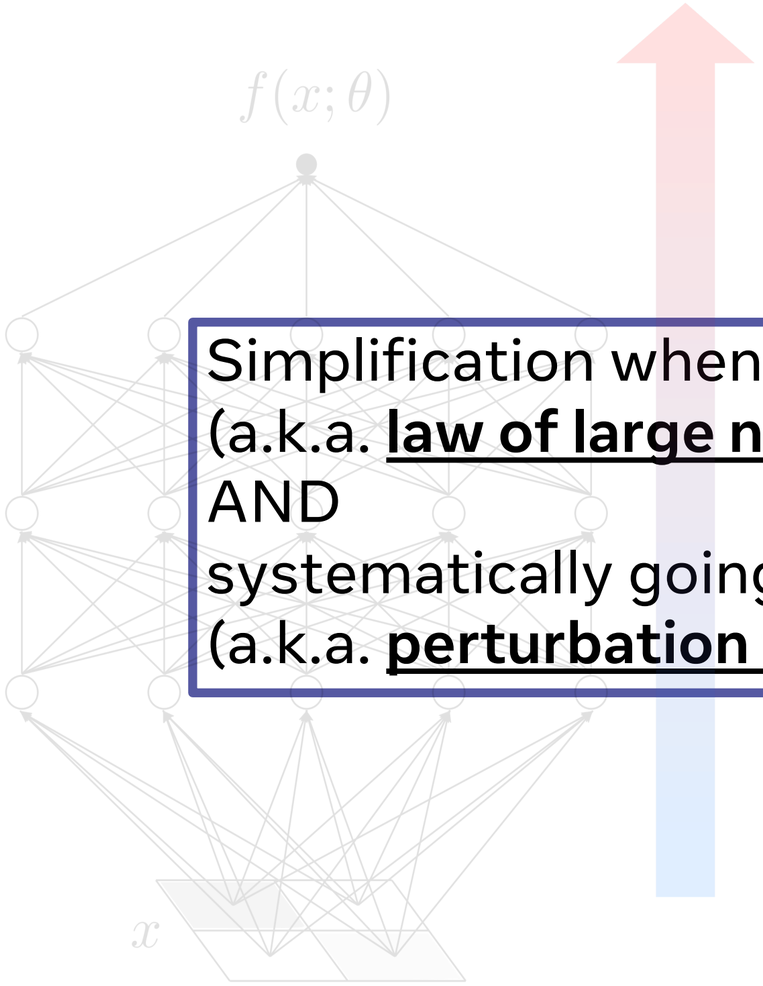
2. Hyperparameter Scaling for Transformers

1. Simplification @Scale

Physics of Wide & Deep Neural Networks



Physics of Wide & Deep Neural Networks

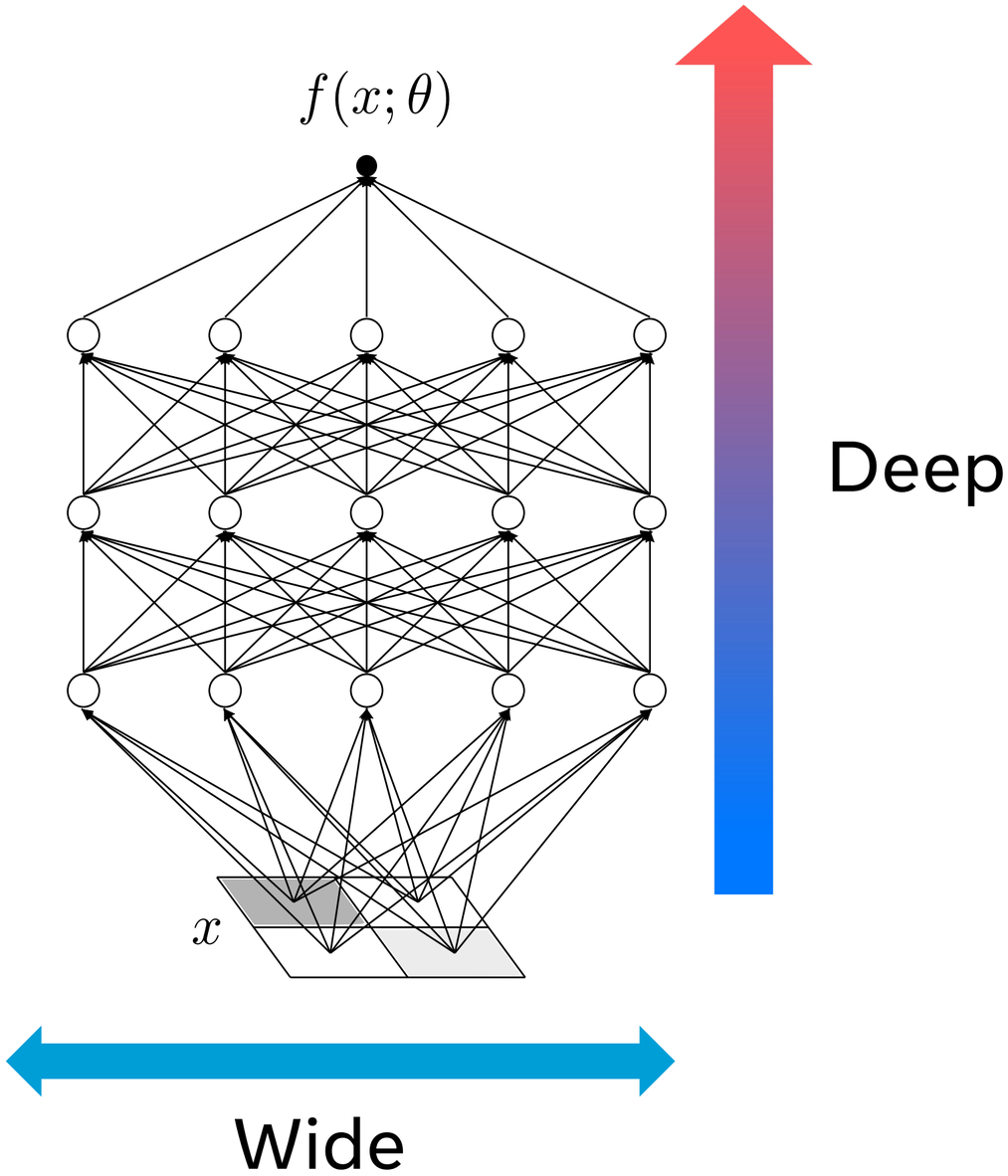


Deep

Wide

Simplification when there are infinitely-many neurons in hidden layers
(a.k.a. **law of large numbers**; a *free theory* at $\text{width} = \infty$)
AND
systematically going beyond that idealized limit
(a.k.a. **perturbation theory**; a *weakly-interacting theory* when $\text{width} \gg \text{depth}$)

Physics of Wide & Deep Neural Networks



Effective theory works well when

$$\text{width}, \text{depth} \gg 1 \quad \& \quad \text{“}\frac{\text{depth}}{\text{width}} \ll 1\text{”}$$

i.e., typical large-scale setups!

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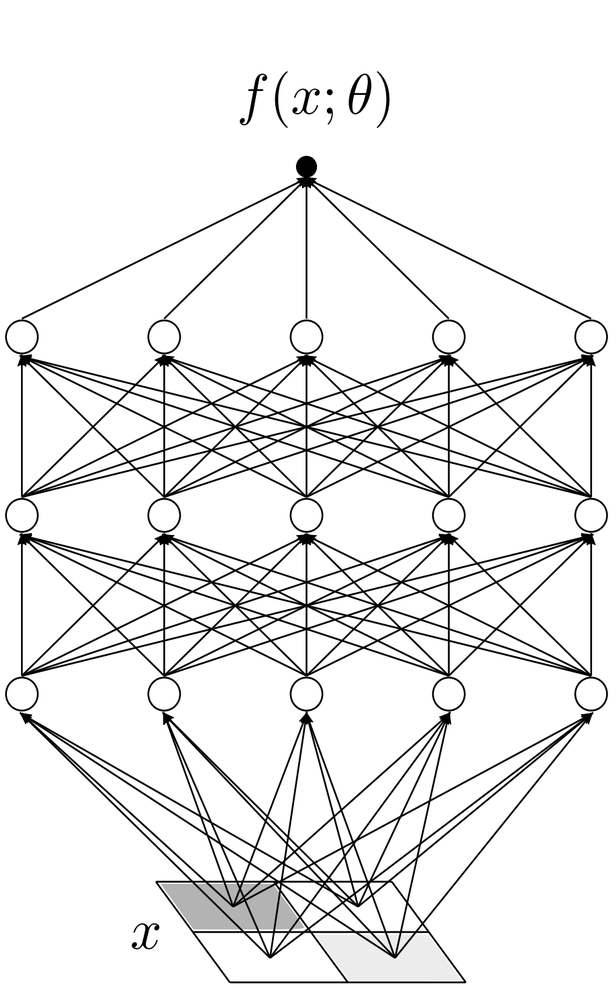

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[D. Roberts, S. Yaida, B. Hanin: arXiv:2106.10165; Cambridge University Press
+many many many others]

Applied Physics of Wide & Deep Neural Networks

Effective theory ⇨ how to scale initialization/training hyperparameters

⇨ Bringing theory & practice closer together @ large scales

Applied Physics of Wide & Deep Neural Networks

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⇒ Bringing theory & practice closer together @ large scales

- For Transformers: w/ Emily Dinan and Susan Zhang [arXiv:2304.02034]

- …

#TL;DR

- **(Meta-)Principle of Criticality**:

  “every preactivation/activation should be of order one, i.e., not too big, not too small”

  → `stddev ~ np.sqrt(1.0/fan_in)` for weights @ initialization

`fan_in` = number of signals coming into a layer

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- **(Meta-)Principle of Equivalence**:

  “every layer should contribute equally to learning (that is, to the neural tangent kernel)”

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* Caveat 1: we need to be careful with “`fan_in`” for sparse inputs.
* Caveat 2: stem—head weight tying requires us to rescale output logits.
* Caveat 3: we can further fine-tune “1.0” but that’s largely moot due to `LayerNorms`.

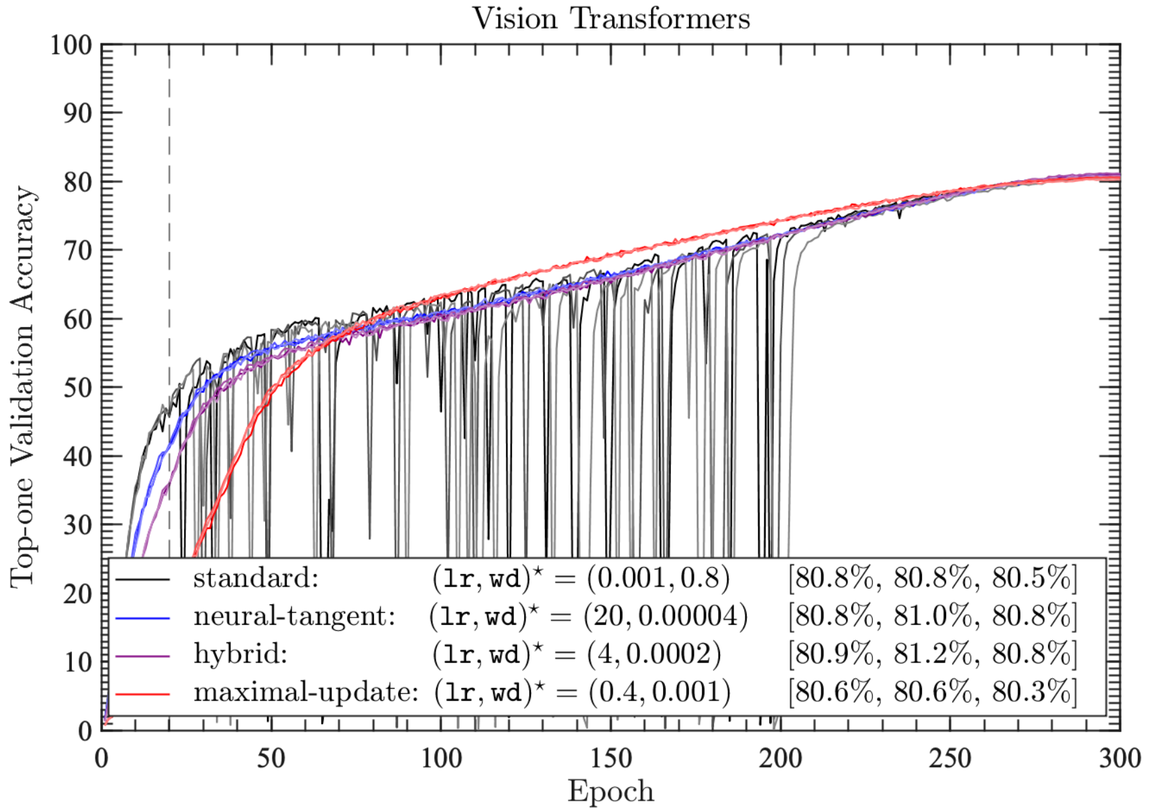
* Meta-Caveat:
preceding and following discussions assume the *neural-tangent* scaling of various hyperparameters;
for more general cases including the *maximal-update* scaling (proposed by Greg Yang & Edward Hu), see

arXiv:2210.04909 (S. Yaida, “Meta-Principled Family of Hyperparameter Scaling Strategies”)
or
various footnotes in our paper [arXiv:2304.02034] under presentation

2. Hyperparameter Scaling for Transformers

`bias=elementwise_affine=False`

Does it work?



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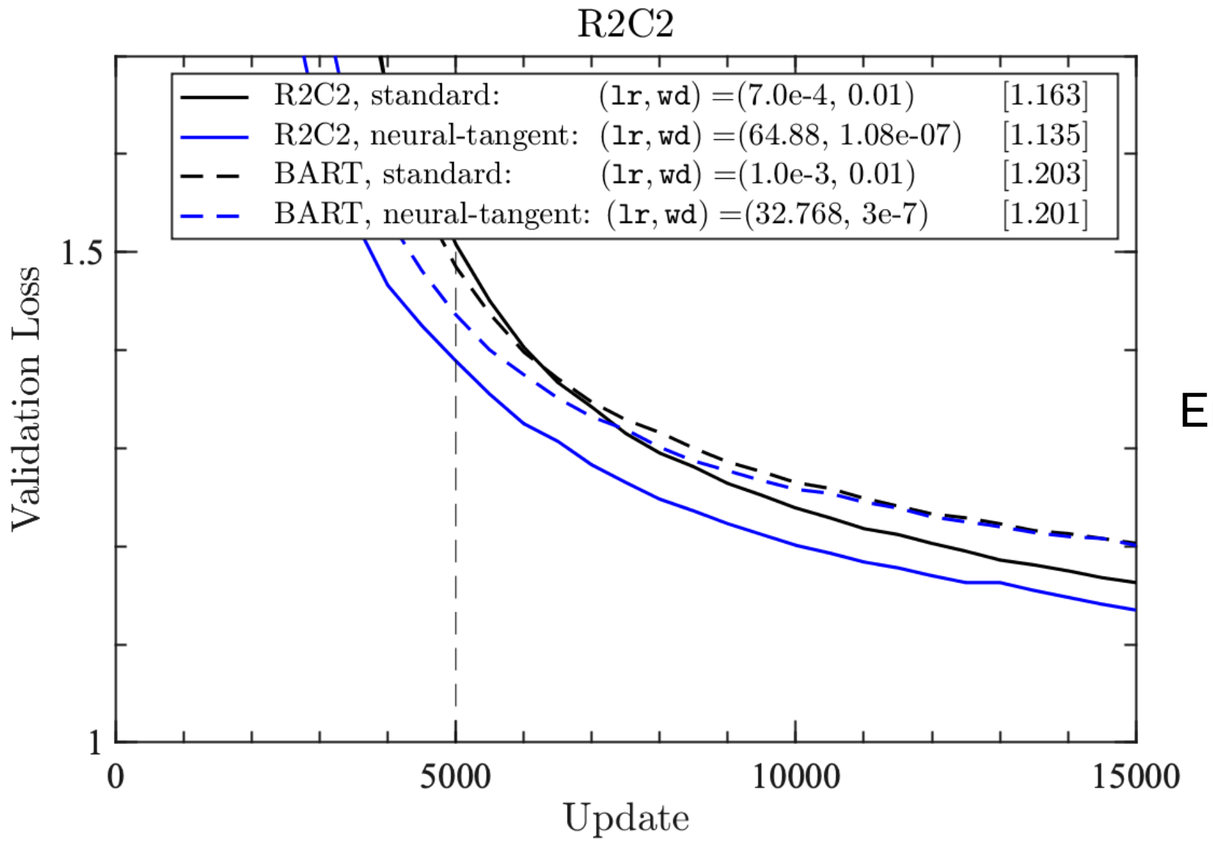
One curious observation:
neural-tangent scaling *increases* the learning rate for positional-embedding parameters by ~*1000 relative to the standard uniform scaling, and it makes the training *stabler*.

Does it work?



Encouraging but not conclusive…

Technical-looking Summary 1: Initialization Hyperparameters

`stddev ~ np.sqrt(1.0/fan_in)`

that their covariances should be scaled as

$$\mathbb{E}\left[W^{\text{patch}}_{i_1 j_1} W^{\text{patch}}_{i_2 j_2}\right] = \left(\frac{C_{\text{patch}}}{n_{\text{patch}}}\right) \delta_{i_1 i_2} \delta_{j_1 j_2} \quad \Big|\Big| \quad \mathbb{E}\left[W^{\text{WE}}_{i_1 j_1} W^{\text{WE}}_{i_2 j_2}\right] = \left(C_{\text{WE}}\right) \delta_{i_1 i_2} \delta_{j_1 j_2} \,, \tag{1.25}$$

$$\mathbb{E}\left[b^{\text{PE}}_{t_1;i_1} b^{\text{PE}}_{t_2;i_2}\right] = \left(C_{\text{PE}}\right) \delta_{t_1 t_2} \delta_{i_1 i_2} \,, \tag{1.26}$$

$$\mathbb{E}\left[Q^{h_1}_{c_1 i_1} Q^{h_2}_{c_2 i_2}\right] = \left(\frac{C_Q}{n}\right) \delta_{c_1 c_2} \delta_{i_1 i_2} \delta^{h_1 h_2} \,, \tag{1.27}$$

$$\mathbb{E}\left[K^{h_1}_{c_1 i_1} K^{h_2}_{c_2 i_2}\right] = \left(\frac{C_K}{n}\right) \delta_{c_1 c_2} \delta_{i_1 i_2} \delta^{h_1 h_2} \,, \tag{1.28}$$

$$\mathbb{E}\left[V^{h_1}_{c_1 i_1} V^{h_2}_{c_2 i_2}\right] = \left(\frac{C_V}{n}\right) \delta_{c_1 c_2} \delta_{i_1 i_2} \delta^{h_1 h_2} \,, \tag{1.29}$$

$$\mathbb{E}\left[U^{h_1}_{i_1 c_1} U^{h_2}_{i_2 c_2}\right] = \left(\frac{C_U}{n}\right) \delta_{i_1 i_2} \delta_{c_1 c_2} \delta^{h_1 h_2} \,, \tag{1.30}$$

$$\mathbb{E}\left[W_{i_1 j_1} W_{i_2 j_2}\right] = \left(\frac{C_W}{n}\right) \delta_{i_1 i_2} \delta_{j_1 j_2} \,, \tag{1.31}$$

$$\mathbb{E}\left[X_{i_1 j_1} X_{i_2 j_2}\right] = \left(\frac{C_X}{Mn}\right) \delta_{i_1 i_2} \delta_{j_1 j_2} \,, \tag{1.32}$$

$$\mathbb{E}\left[W^{\text{head}}_{i_1 j_1} W^{\text{head}}_{i_2 j_2}\right] = \left(\frac{C_{\text{head}}}{n}\right) \delta_{i_1 i_2} \delta_{j_1 j_2} \,, \;\; b^{\text{head}}_i = 0 \quad \Big|\Big| \quad \mathcal{N}_{\text{rescale}} = \sqrt{\frac{1}{n}} \,, \tag{1.33}$$

where $\mathbb{E}\left[\cdot\right]$ denotes an expectation value with respect to the initialization distribution, δ_{ij} is the Kronecker delta (i.e., $\delta_{ij} = 1$ when $i = j$ and $\delta_{ij} = 0$ when $i \neq j$), and all the initialization hyperparameters C_G are order-one numbers for each group G of model parameters. Here, by

Technical-looking Summary 2: Training Hyperparameters (LR)

`lr ~ 1.0/(fan_in*np.sqrt(fan_out))`

of $\sim |g^\mu|$ modifies the above relative learning-rate factors to

$$\widetilde{\lambda}_{W^{\text{patch}}} = \left(\frac{1}{n_{\text{patch}}\sqrt{n}}\right)\widetilde{\Lambda}_{W^{\text{patch}}} \quad \Big\| \quad \widetilde{\lambda}_{W^{\text{WE}}} = \left(\frac{1}{\sqrt{n}}\right)\widetilde{\Lambda}_{W^{\text{WE}}}\,, \tag{1.108}$$

$$\widetilde{\lambda}_{b^{\text{PE}}} = \left(\frac{1}{\sqrt{n}}\right)\widetilde{\Lambda}_{b^{\text{PE}}}\,, \tag{1.109}$$

$$\widetilde{\lambda}_{Q} = \left(\frac{1}{n\sqrt{n}}\right)\widetilde{\Lambda}_{Q}\,, \tag{1.110}$$

$$\widetilde{\lambda}_{K} = \left(\frac{1}{n\sqrt{n}}\right)\widetilde{\Lambda}_{K}\,, \tag{1.111}$$

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$$\widetilde{\lambda}_{W} = \left(\frac{1}{n\sqrt{Mn}}\right)\widetilde{\Lambda}_{W}\,, \tag{1.114}$$

$$\widetilde{\lambda}_{X} = \left(\frac{1}{Mn\sqrt{n}}\right)\widetilde{\Lambda}_{X}\,, \tag{1.115}$$

$$\widetilde{\lambda}_{W^{\text{head}}} = \left(\frac{1}{n\sqrt{n_{\text{out}}}}\right)\widetilde{\Lambda}_{W^{\text{head}}}\,, \quad \widetilde{\lambda}_{b^{\text{head}}} = \left(\frac{1}{\sqrt{n_{\text{out}}}}\right)\widetilde{\Lambda}_{b^{\text{head}}}\,, \tag{1.116}$$

where – like the order-one initialization hyperparameters C_G's – $\widetilde{\Lambda}_G$'s are order-one training hyperparameters which we could in principle tune but won't.[25]

```
stddev ~ np.sqrt(1.0/fan_in)
```

```
lr ~ 1.0/(fan_in*np.sqrt(fan_out))
```

Attention Blocks

$$\text{stddev} \sim \text{np.sqrt}(1.0/\text{fan\_in})$$

$$\text{lr} \sim 1.0/(\text{fan\_in}*\text{np.sqrt}(\text{fan\_out}))$$

The query, key, value, and out_proj weights all have (*)

$$\text{fan\_in}=\text{embedding\_dim}$$

$$\text{fan\_out}=\text{embedding\_dim}$$

(*Ok, with the traditional usage of terminology, strictly speaking, it depends on how you code QKV, but it doesn't really matter much here.)

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The query, key, value, and out_proj weights all have (*)

```
fan_in=embedding_dim
fan_out=embedding_dim
```

```
stddev=np.sqrt(1.0/embedding_dim)
lr=np.sqrt(1.0/embedding_dim**3)
```

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Attention Blocks

`stddev ~ np.sqrt(1.0/fan_in)`

`lr ~ 1.0/(fan_in*np.sqrt(fan_out))`

One comment about the famous query—key dot product normalization:

$$\frac{1}{\sqrt{C}}\mathbf{q}\cdot\mathbf{k} \quad \text{where} \quad C = \#\ \text{of channels per head} = \frac{\texttt{embedding\_dim}}{\texttt{n\_heads}}$$

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One comment about the famous query—key dot product normalization:

$$\frac{1}{\sqrt{C}}\mathbf{q}\cdot\mathbf{k} \quad \text{where} \quad C = \#\ \text{of channels per head} = \frac{\texttt{embedding\_dim}}{\texttt{n\_heads}}$$

This is theoretically correct (while Tensor Program V paper does something else).

FC Blocks

$$stddev \sim np.sqrt(1.0/fan\_in)$$

$$lr \sim 1.0/(fan\_in*np.sqrt(fan\_out))$$

The 1st layer

```
fan_in=embedding_dim
fan_out=M*embedding_dim
```

The 2nd layer

```
fan_in=M*embedding_dim
fan_out=embedding_dim
```

FC Blocks

$$stddev \sim np.sqrt(1.0/fan\_in)$$

$$lr \sim 1.0/(fan\_in*np.sqrt(fan\_out))$$

The 1st layer

```
fan_in=embedding_dim
fan_out=M*embedding_dim
```

```
stddev=np.sqrt(1.0/embedding_dim)
lr=np.sqrt(1.0/(M*(embedding_dim**3)))
```

The 2nd layer

```
fan_in=M*embedding_dim
fan_out=embedding_dim
```

```
stddev=np.sqrt(1.0/(M*embedding_dim))
lr=np.sqrt(1.0/((M**2)*(embedding_dim**3)))
```

Word-Embedding Parameters

$\texttt{stddev} \sim \texttt{np.sqrt(1.0/fan\_in)}$

$\texttt{lr} \sim \texttt{1.0/(fan\_in*np.sqrt(fan\_out))}$

Naively...,

```
fan_in=n_vocab
fan_out=embedding_dim
```

Word-Embedding Parameters

`stddev ~ np.sqrt(1.0/fan_in)`

`lr ~ 1.0/(fan_in*np.sqrt(fan_out))`

Because of one-hot-ness,

~~`fan_in=n_vocab`~~ `fan_in=1`

`fan_out=embedding_dim`

Word-Embedding Parameters

stddev ~ np.sqrt(1.0/fan_in)

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Because of one-hot-ness,

~~fan_in=n_vocab~~ fan_in=1

fan_out=embedding_dim

stddev=1.0

lr=np.sqrt(1.0/embedding_dim)

Word-Embedding Parameters

`stddev ~ np.sqrt(1.0/fan_in)`

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Because of one-hot-ness,

~~`fan_in=n_vocab`~~ `fan_in=1`

`fan_out=embedding_dim`

```
stddev=1.0
lr=np.sqrt(1.0/embedding_dim)
```

* Lesson 1: be mindful with sparse features.
* Lesson 2: the learning rate is relatively much higher than those for other layers.

(Word-Embedding Parameters)^T

$\texttt{stddev} \sim \texttt{np.sqrt(1.0/fan\_in)}$

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Because of stem—head weight tying,

$$\texttt{logit}_i = \sum_{j=1}^{\texttt{embedding\_dim}} (\texttt{WE.weight})_{ji} (\texttt{last\_features})_j$$

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```
logit=logit/np.sqrt(embedding_dim)
```

Positional-Embedding Parameters

$$\text{stddev} \sim \text{np.sqrt}(1.0/\text{fan\_in})$$

$$\text{lr} \sim 1.0/(\text{fan\_in}*\text{np.sqrt}(\text{fan\_out}))$$

Finally, quickly, for positional-embedding (additive, like bias), we have

```
fan_in=1
fan_out=embedding_dim
```

```
sttdev=1.0 or 0.0 or something
lr=np.sqrt(1.0/embedding_dim)
```

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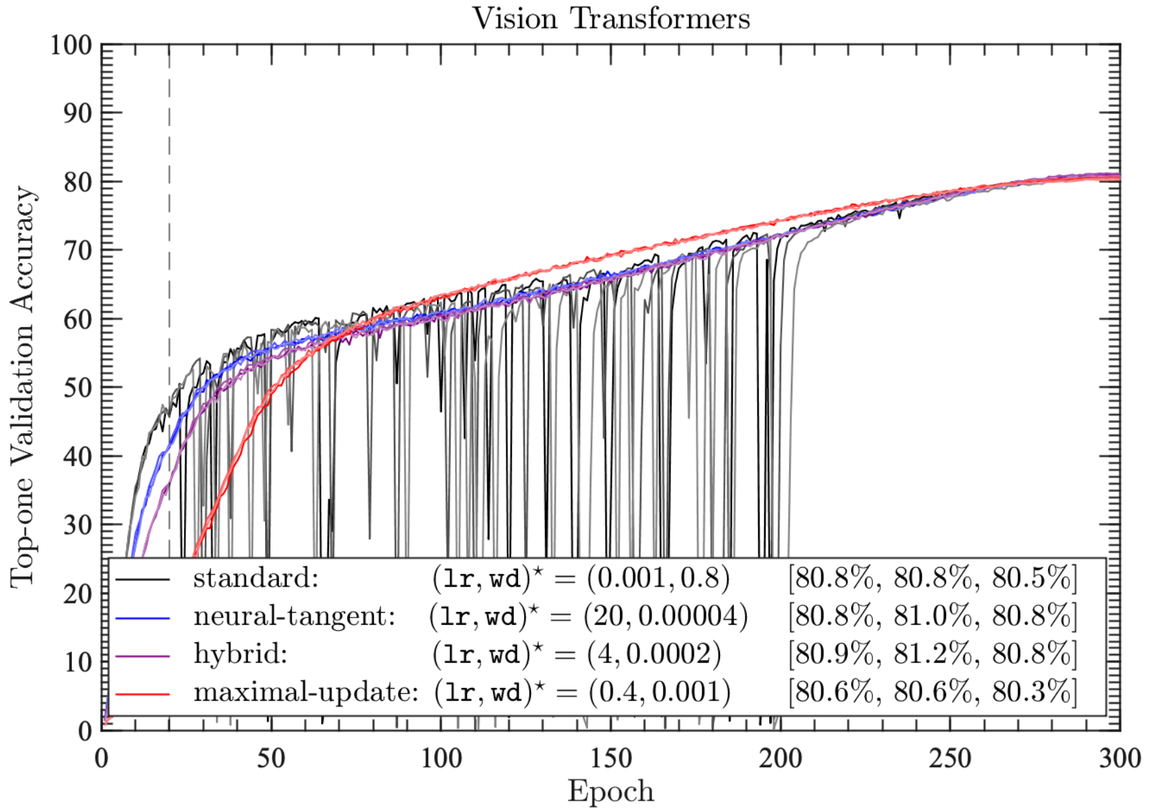

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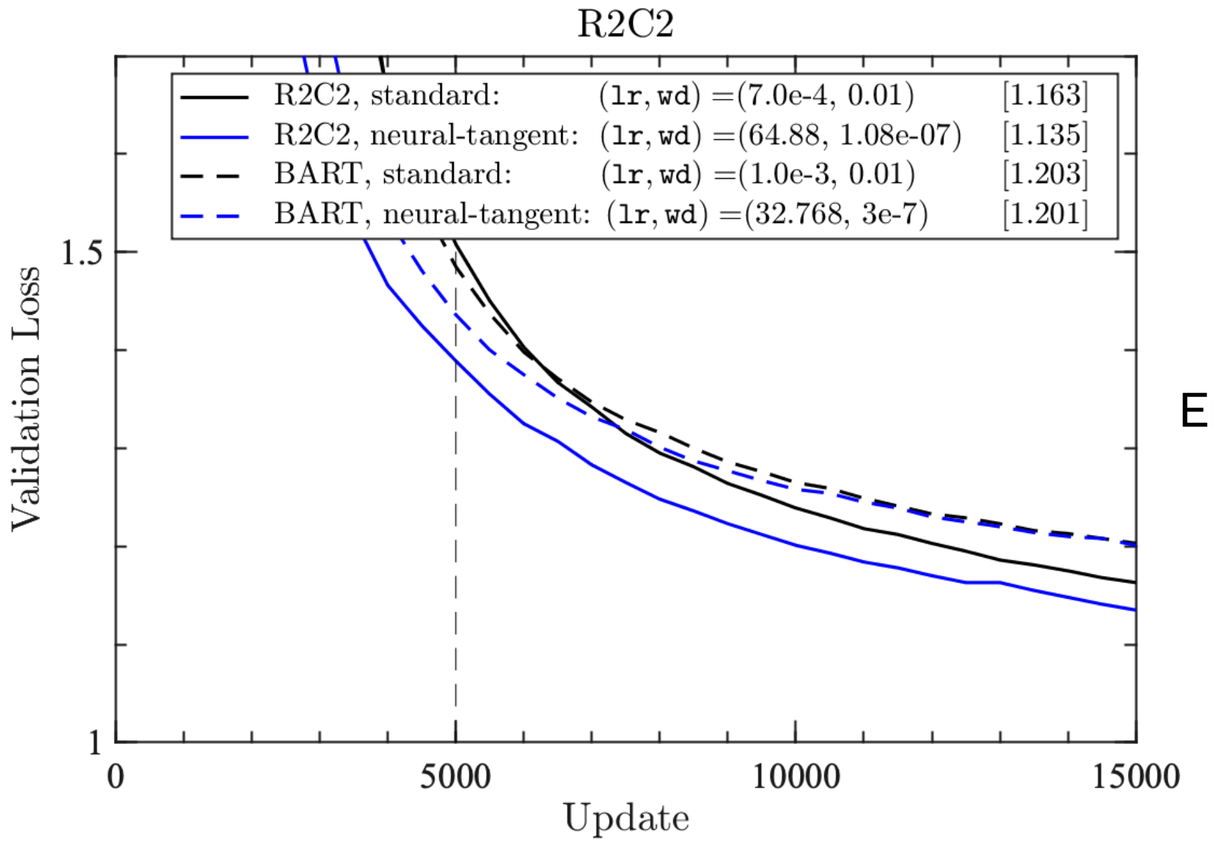

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Does it work?

lots of encouraging/discouraging anecdata to come — from you