The mathematics of machine learning and deep learning

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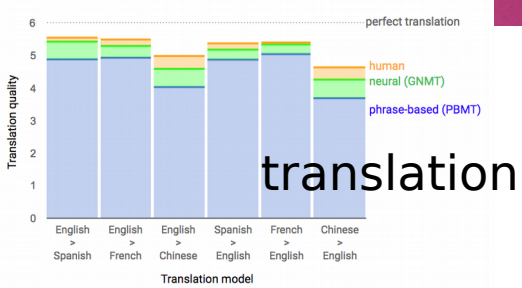
Machine learning (ML): A new kind of science

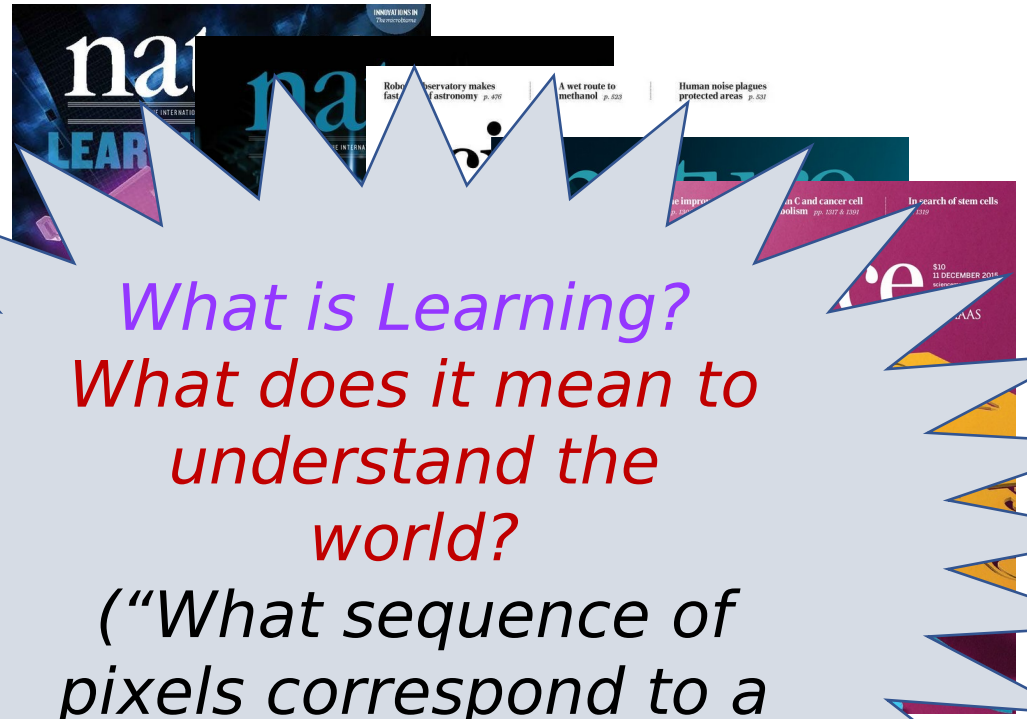


translation

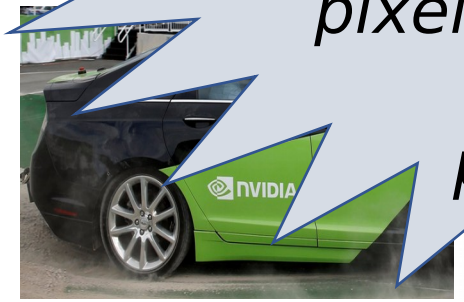
"Science of creating machines/programs that improve from experience and interaction."

(Imitating human intelligence not an explicit

Machine learning (ML): A new kind of science



What is Learning?
What does it mean to understand the world?
("What sequence of pixels correspond to a scene with a pedestrian?")



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Talk overview

- Part 1: Mathematical formulation of Machine Learning (ML).
- Part 2: ML in action (unsupervised, sequential decision-making)
- Part 3: Toward mathematical understanding of deep learning
- Part 4: Taking Stock/Concl[illegible]s

"A tour with many stops…"

Part 1

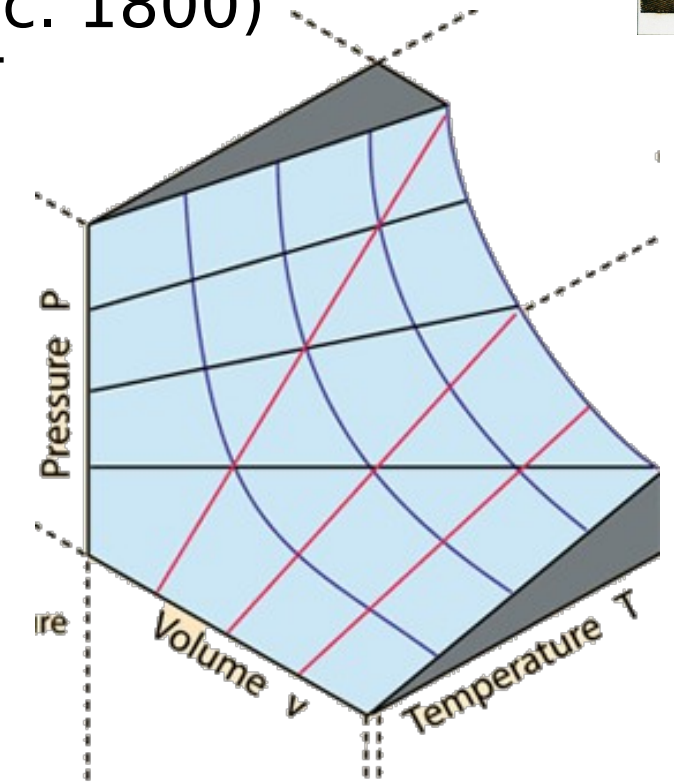
Mathematical formalization of Machine Learning (ML)

(Operationally speaking, boils down to learning patterns in data.)

Old Idea: Curve fitting (Legendre, Gauss, c. 1800)

Phillips curve (1958):

Gas Law (c. 1800)
PV = nRT



Machine Learning uses surface fitting, with many more variables (eg 2
("Learning patterns in data.")

Example: Learning to sco reviews

Score = −1.5
“Slow moving. Couldn’t get into this movie despite all the awards it has won.”

Score = 2.5
“Wow! Did not know what to expect and was delighted! Loved the homage paid to the musicals of old. “

Given: Reviews for different movies and rating score (-3 to +3).
Task: Learn to predict rating score given text of a new review.

The “law” of movie review scores??

Example: Learning to rate reviews (contd)

“Slow moving. Couldn’t get into this movie despite all the awards it has won.”

100,000 words in English dictionary.

Hypothesized “law” (simple linear model):

- Each word w has sentiment score $\theta_w \in R$

  Review score ≈ total sentiment score of all words in it

nding sentiment score for 100,000 words ≡ Surface fitting with 100,000 variable

R^{10000}

100,000 words in English dictionary.

Hypothesized “law” (simple linear model):

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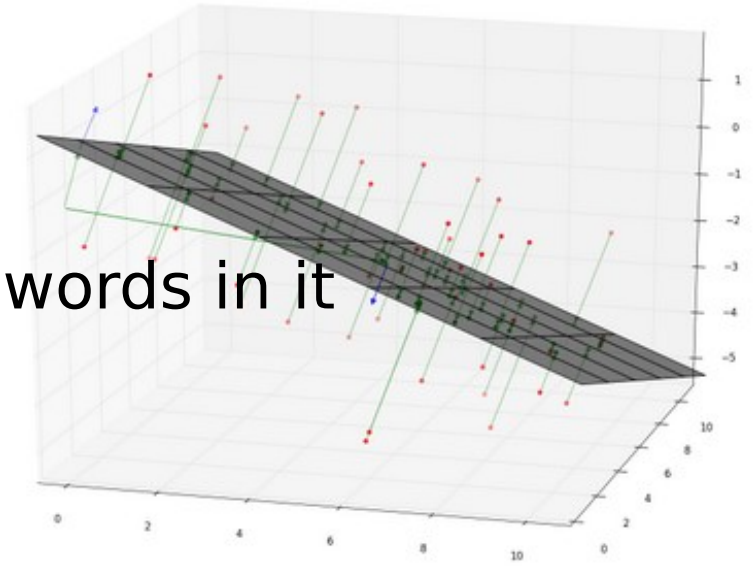


$$Min \sum_{review} \left(Score - \sum_{w \in review} \theta_w \right)^2$$

“Loss function”

Algorithm: “Gaussian Least Square Fit”
(Solvable in seconds given few million ranked reviews.)

Hypothesized law:

- Each word w has sentiment score θ_w

  Review rating ≈ total sentiment score of all words in it

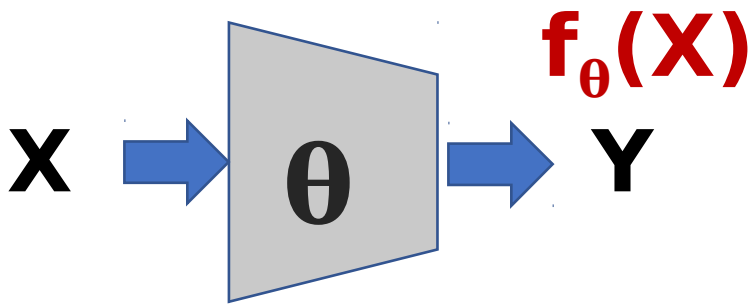
Word	Score
as	+0.1
good	+0.6
homage	0.0
loved	+1.1
musicals	+0.1
of	-0.1
old	-0.4
paid	-0.3
story	+0.3
the	+0.1
to	-0.1
was	-0.2
well	+1.4
⋮	⋮

"Loved the homage paid to the musicals of old. Story was good as well."

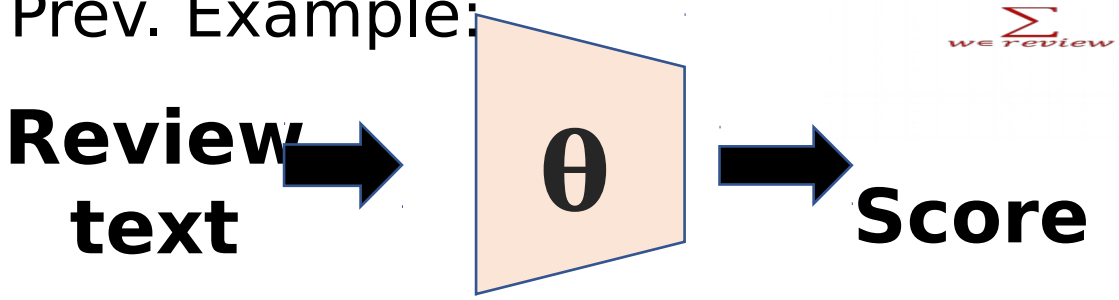
Loved	the	homage	paid	to	the	musicals	of	old.	Story	was	good	as	well.		
+1.1	+0.1	+0.0	-0.3	-0.1	+0.1	+0.1	-0.1	-0.4	+0.3	-0.2	+0.6	+0.1	+1.4	=	**2.7**

"Discovered Patterns"
= How words correlate with positive score

ML ≈ finding suitable function ("model") given examples of desired input/output behavior



Prev. Example:



$\theta \in R^d$

(trainable parameters)

(X, Y) : (Input, Output) pair

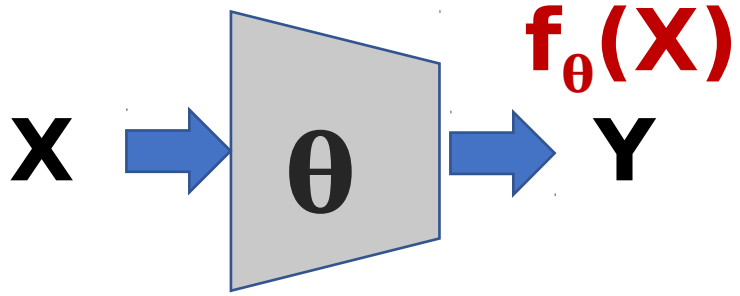
Training method:

$$Min \sum_{review} \left(Score - \sum_{w \in review} \theta_w \right)^2$$

Desired output

Model's output

ML ≈ finding suitable function ("model") given examples of desired input/output behavior



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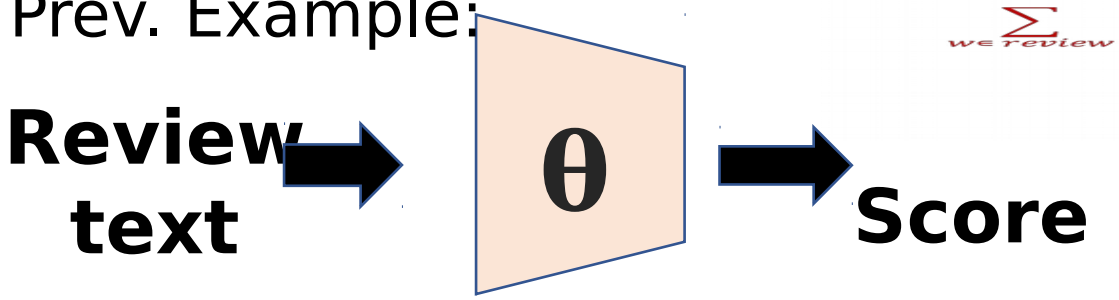


$\theta \in R^d$

(trainable parameters)

Training data: $\{(X_1^{(i)}, Y^{(i)}): i=1,..,N\}$

"Loss" $\ell(\theta) = \sum_{i=1}^{N} (f_\theta(X_1^{(i)}) - Y^{(i)})^2$

(Many other loss formulations exist….)

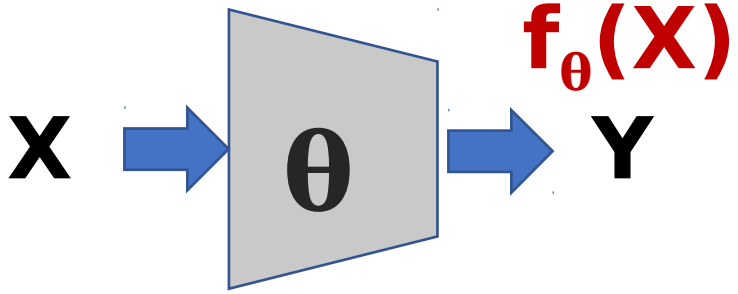
Training method:

$$Min \sum_{review} \left(Score - \sum_{w \in review} \theta_w \right)^2$$

Desired output

Model's output

Formal framework (inherited from classical statistics)



$\theta \in R^d$
(trainable parameters)

Training data: $\{(X_1^{(i)}, Y^{(i)}): i=1,..,N\}$

Assumption: Samples $(X^{(i)}, Y^{(i)})$ drawn from a probability distribution D (e.g., distribution on pairs "(movie review, rating score)")

TRAINING: Optimize loss $\ell(\theta)$.

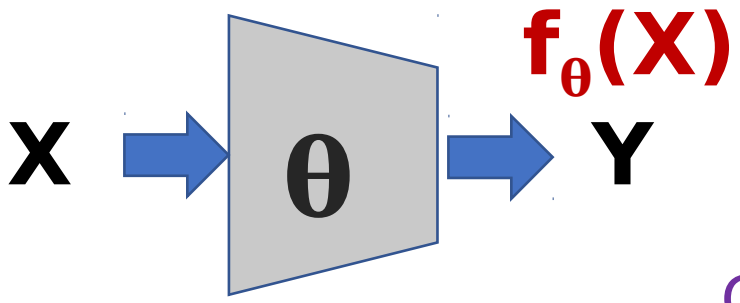
TESTING: Take new X's and see how well the trained model predicts the missing Y (e.g., "given review, predict rating score")

"Loss" $\ell(\theta) = \sum_{i=1}^{N} (f_\theta(X_1^{(i)}) - Y^{(i)})^2$

In practice: TRAIN on 80% of data; TEST by evaluating loss on remaining 20%

(Many other loss formulations exist....)

Formal framework



$f_\theta(X)$

$\theta \in R^d$

(trainable parameters)

Assumption: Samples $(X^{(i)}, Y^{(i)})$ drawn from a probability distribution D (e.g., distribution on pairs "(movie review, rating score)")

Comment: Fourier analysis allows learning f from (x, f(x)) examples….
(under reasonable assumptions on f)….

Training data: $\{(X_1^{(i)}, Y^{(i)}): i=1,..,N\}$

"Loss" $\ell(\theta) = \sum_{i=1}^{N} (f_\theta(X_1^{(i)}) - Y^{(i)})^2$

But practically infeasible: If $X \in R^n$, need exp(n) samples of (X, f(X)) and also exp(n) computation

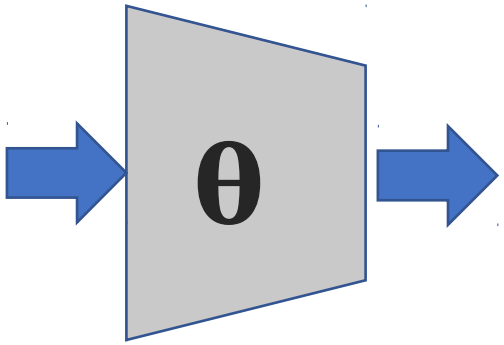
(In practice n =10^4 say, and # samples = 10n)

(Many other loss formulations exist….)

Training via Gradient Descent ("natural algorithm")

$\theta \in \mathbf{R}^d$

trainable parameters

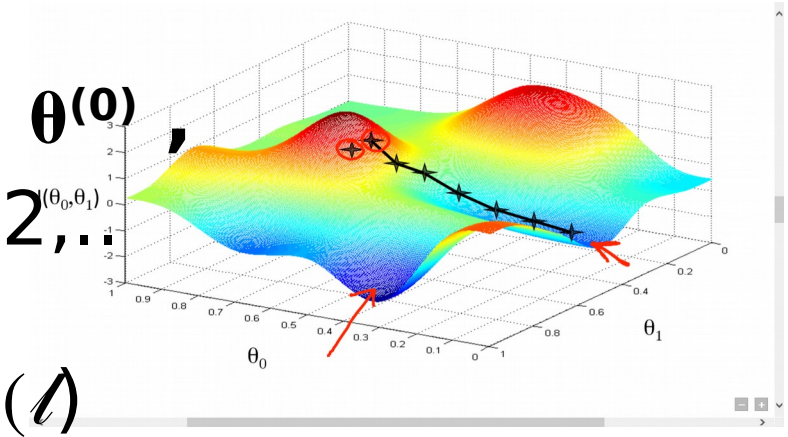


Loss $\ell(\theta)$

deficiency in desired

Often nonconvex, esp. in deep learning.

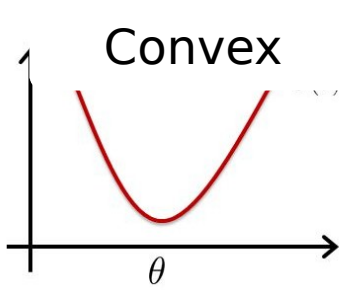
Starting with some $\theta^{(0)}$, compute for t=0,1,2,..

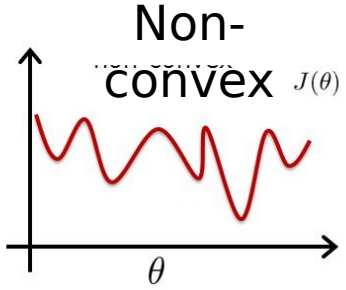


$$\theta^{(t+1)} = \theta^{(t)} - \eta \nabla (\ell)$$

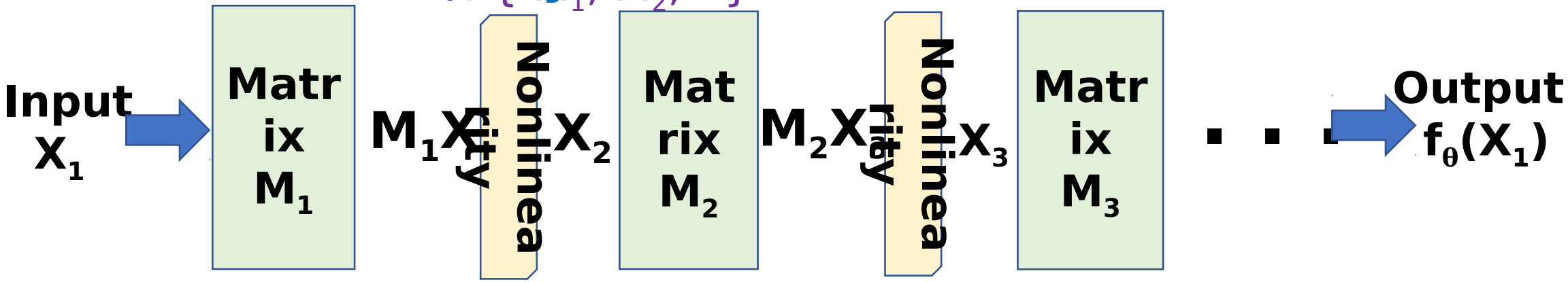
($\eta \in \mathbf{R}$ is "learning rate", say, 0.01)

In practice can improve GD with tricks: time-varying η, past gradients ("momentum"), "regularization", ..





Subcase: deep learning* (deep models = "multilayered")



"Nonlinearity": Given a vector, output same vector but negative entries turned to zero.

Training data: $\{(X_1^{(i)}, Y^{(i)}): i=1,..,N\}$

$$\ell(\theta) = \sum_{i=1}^{N} (f_\theta(X_1^{(i)}) - Y^{(i)})^2$$

bute gradient of Loss??

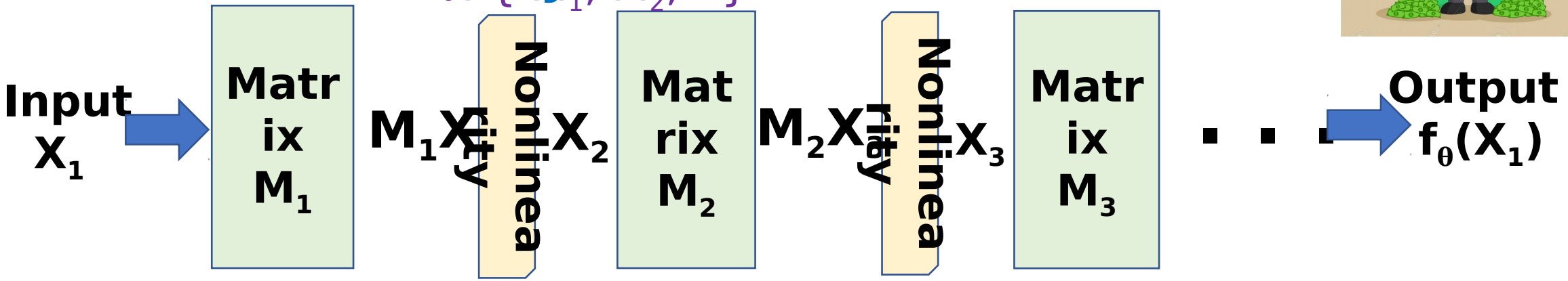
ation Algorithm does it fast; clever application of chain rule [Werbos'77,

hly simplistic: could have "convolution", "bias", "skip connections", other loss fr

Subcase: deep learning* (dee

models = "multilayered")

θ: $\{M_1, M_2, \ldots\}$



"Nonlinearity": Given a vector, output same vector but negative entries turned to zero.

Training data: $\{(X_1^{(i)}, Y^{(i)}): i$

N

$Y^{(i)})^2$

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[Werbos'77,

Nonlinear enough to express many things; linear enough to allow quick optimization on today's computers

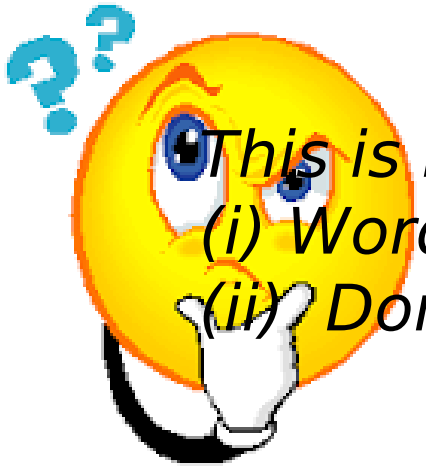
hly simplistic: could have "convolutio", "b", "s connections", other loss fr

Part 2

Machine Learning in Action (Unsupervised, Interactive, etc.)

(Key idea: need to define “loss function” creatively….)

Review rating = total sentiment score of all words in it



This is not how we humans do it!
(i) Word order in text matters. ("No good" vs "Good, no?")
(ii) Don't need millions of examples. (Because we understand languag

Science has long tried to understand and formalize language
+ semantics
(using logic, grammars, model theory,…)

How can machines "understand" language?

(Arguably, more general-purpose than rating reviews!)

Unsupervised learning (no human-supplied labels)

- Key idea: Using large corpus (eg, Wikipedia), train model to predict part of text from adjacent text.

Example: *"I went to a café and ordered a…. "*

del learns to do such completions by training on huge amounts of te

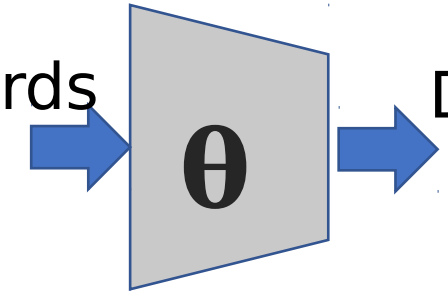
the process, implicitly picks up on grammar rules, common sense et

Used in: Machine Translation, Question-Answering (e.g. Siri, Alexa..)

"I went to a café and ordered a…. "

A Language model (baby "word2vec" [Mikolov et al'13])

Preceding words
$w_1, w_2, .., w_5$



Distribution on all English words

$$\Pr[w|w_1 \dots w_5] \propto \exp\left(\frac{1}{5}\sum_i \langle v_w, v_{w_i} \rangle\right)$$

(implicit normalizing term; will ignore for simplicity)

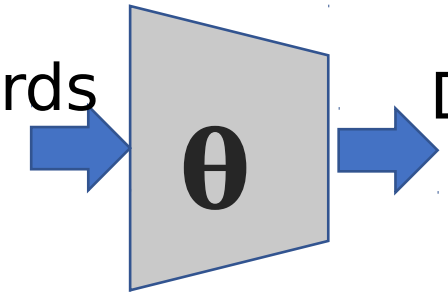
$\theta = \{ v_w \in R^{300} : w$ an English word$\}$
("semantic vectors")

	M	T	W	TH	F	S	S
Chance of rainfall	70%	80%	90%	80%	60%	20%	0%
							

Measure of goodness of fit? (i.e., loss function)?

A Language model (baby "word2vec" [mikolov et al'13])

Preceding words
$w_1, w_2, .., w_5$



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θ = { $v_w \in R^{300}$: w an English word}
("semantic vectors")

oss $\ell(\theta)$: Reciprocal of Probability assigned
y model to Wikipedia = $w_1 w_2 w_3 \dots w_N$

$$\prod_{i=6}^{N} \Pr[w_i|w_{i-5}, \dots, w_{i-1}]$$

$$= \exp(\sum_{i=6}^{N}\sum_{j=1}^{5} \frac{1}{5}\langle v_{w_i}, v_{w_{i-j}} \rangle)$$

(* Omitting negative sampling term...)

Properties of semantic word vectors

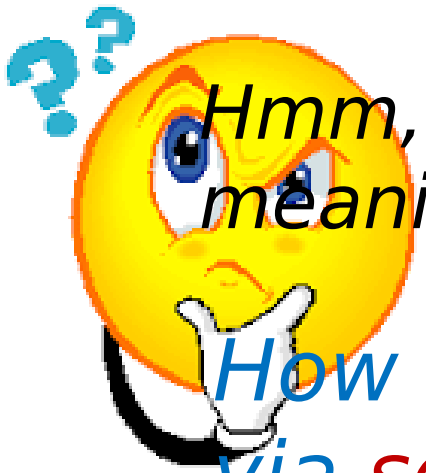
Cosine of angle captures human estimates of "similarity"[Deerwester et al'90]

Possible to use word vectors to define sentence/paragraph vectors that capture sentence/paragraph similarity ["SIF embeddings" [A., Liang, Ma,'17])

Later!

Incorporating semantic vectors improves movie rating task …

Word vector space for different languages (e.g., English, French) can be meaning aligned via a linear transformation [Lample et al'18, Arttextxe et al'18]



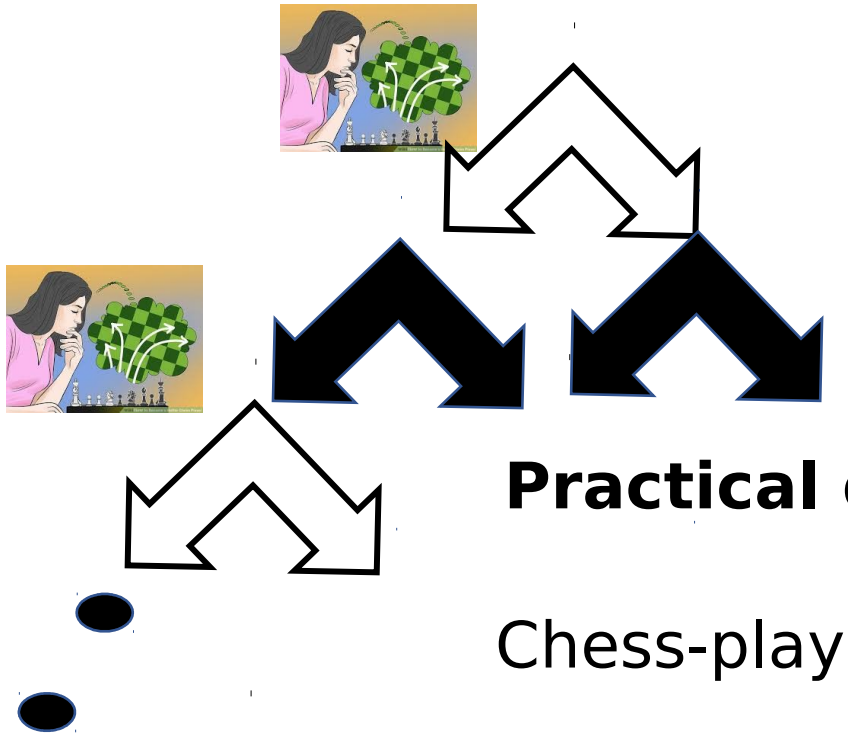
Hmm, predicting review scores, passively understanding wo
meaning…

How can machines actively interact with the world,
via sequence of intelligent decisions ….?

20th century antecedents

Probability Theory: Betting/gambling games (eg martingales)…
Economics: managing stock portfolios; playing repeated games,..
Control theory for power plants/machines,..

Sequential decision-making: framework (uses: robotics, exploration..)



1=LOSE
0 = WIN

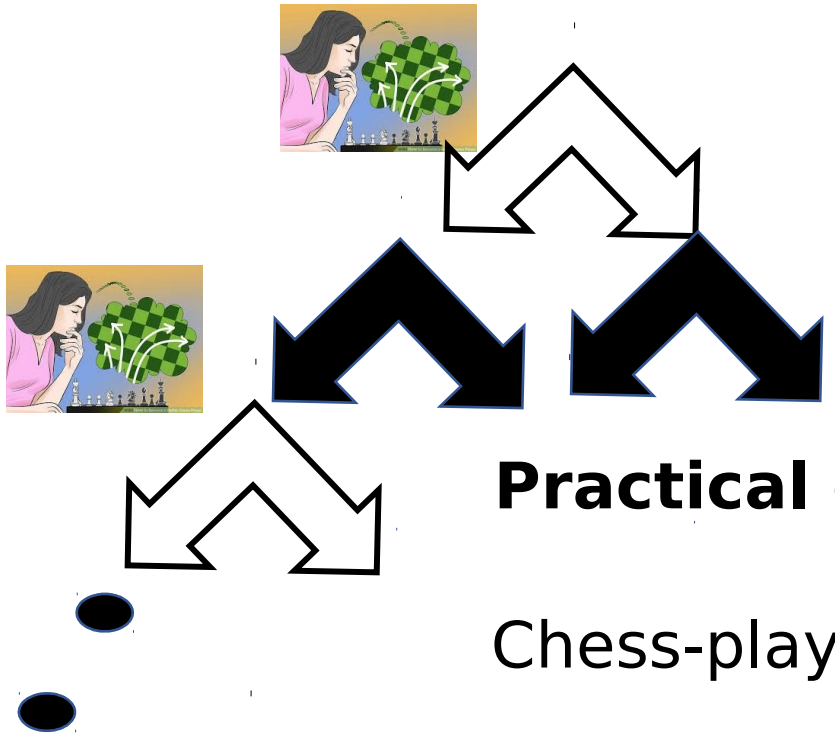
- Tree of all possible action/interactions. (responses can be stochastic)
- Optimum move = one that minimizes expected loss

Practical difficulty: tree too large to allow full evaluatio

Chess-playing software (circa 1990s): Decision-maker is

list of handcrafted rules
+
move evaluation algorithm
(approximate; limited lookahead)

Sequential decision-making (framework)



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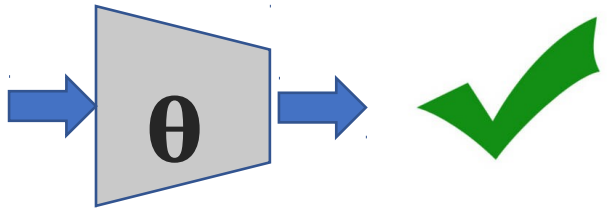
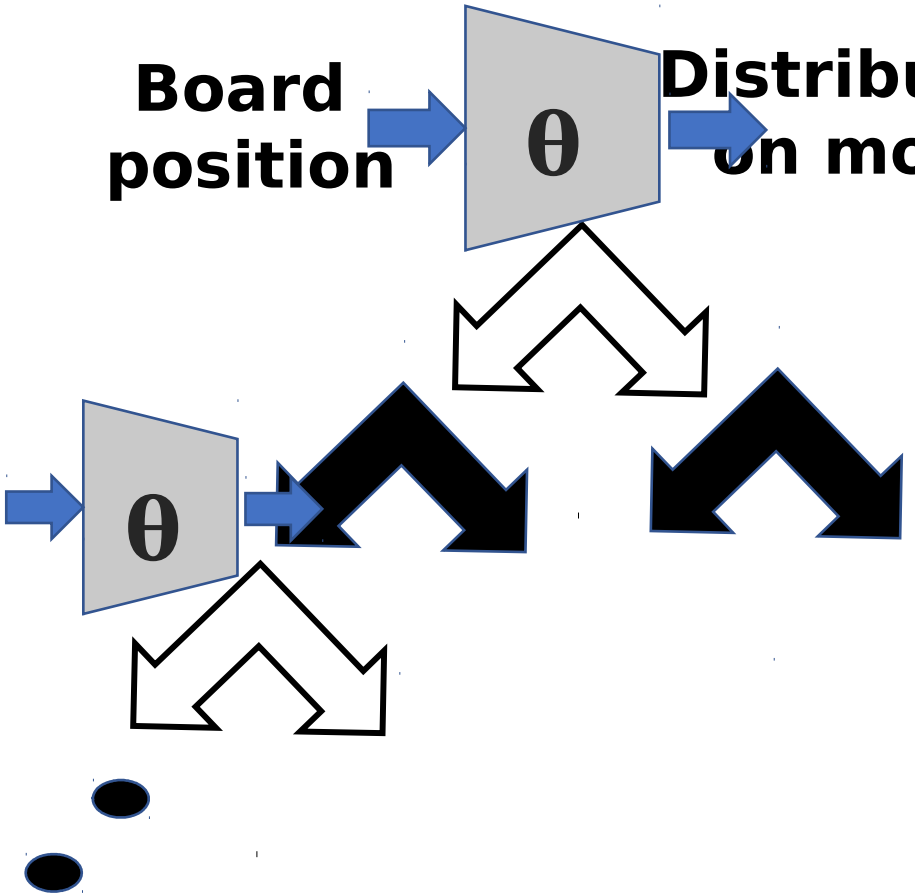


Game-playing via Deep Learning
(crude account of Alpha-Go Zero)



Use move evaluation algorithm to evaluate $\ell(\theta)$ = Pr[loss]

Estimate gradient of ℓ and improve θ !

Crude method:

$$\ell(\theta + \eta) \approx \ell(\theta) + \eta \nabla \ell|_{\theta}$$

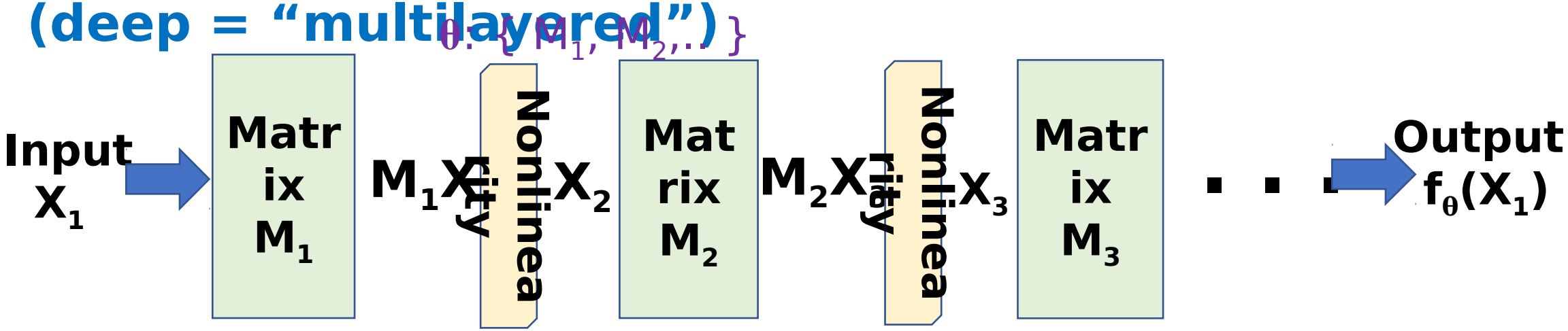
Can "read off" $\nabla \ell|_{\theta}$ using enough η's

Part 3

Toward mathematical understanding of Deep Learning

Special case: deep learning

(deep = "multilayered")



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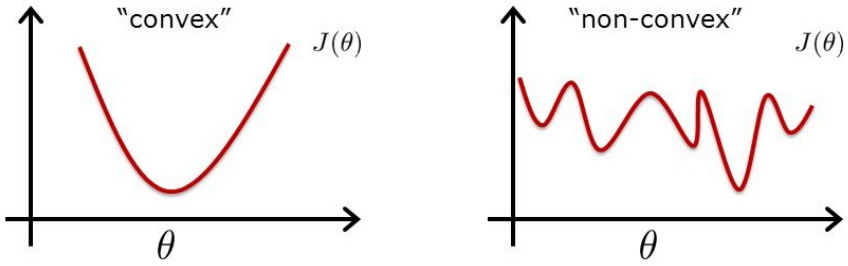
Training data: $\{(X_1^{(i)}, Y^{(i)}) : i=1,..,N\}$

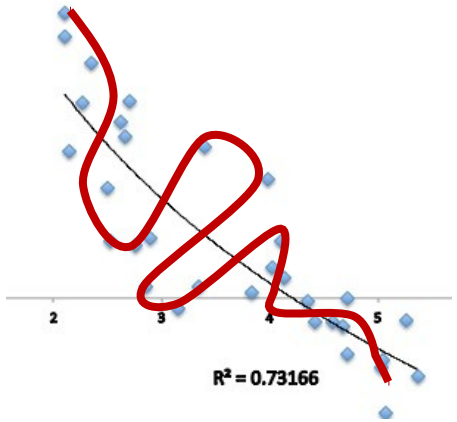
$$\ell(\theta) = \sum_{i=1}^{N} (f_\theta(X_1^{(i)}) - Y^{(i)})^2$$

Some key questions



- Why/when does gradient descent work and how fast? (Nonconvex loss!)

- Why deep (and not shallow)?



- Why doesn't training overfit to training data? (# parameters >> # training samples). Current deep models capable of achieving zero loss on random data [Zhang et al'17])

- How to interpret the trained model's inner workings?

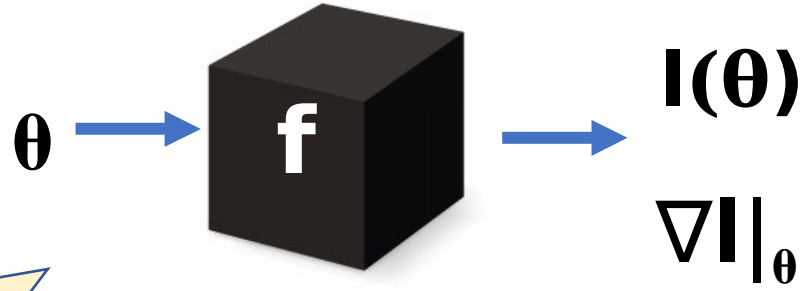
Analysis of optimizat

Before I work on an object I like it to be well-defined at least...

Hurdle 1: Nonconvex optimization is NP-hard. No efficient algorithm if P ≠ NP.)

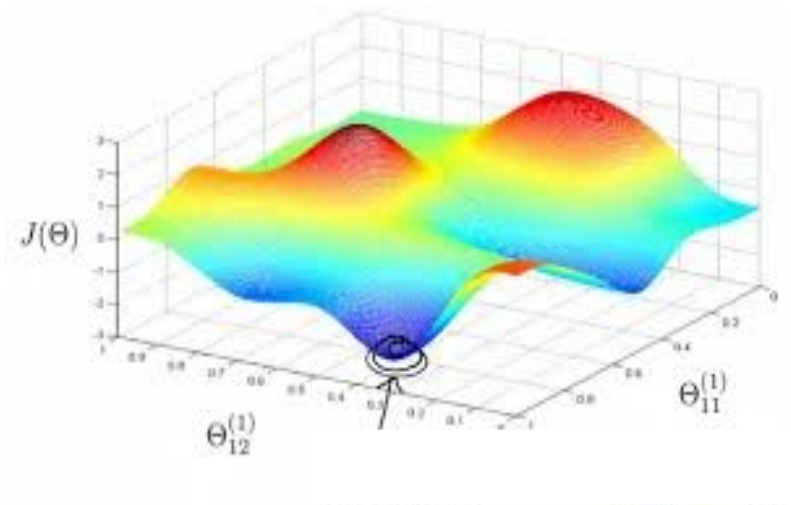
Hurdle 2: Loss $\ell(\theta)$ is essentially a black box to us.

$$\ell(\theta) = \frac{1}{N}\sum_{i=1}^{N}(f_\theta(X_1^{(i)}) - Y^{(i)})^2$$



Lack mathematical description of data ($X^{(i)}$, $Y^{(i)}$). "What makes a bunch of pixels an image of a dog?"

Black box analysis (sketch)



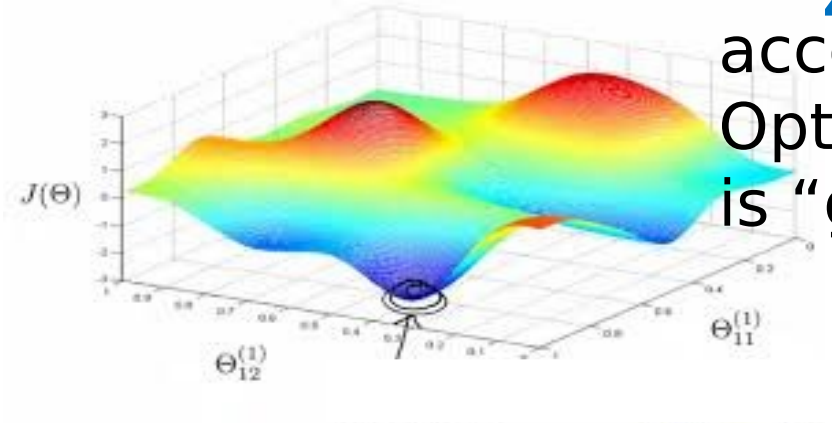
More complicated analyses shows Gradient Descent finds "2nd order local minima" [Ge et al.'15]. (Bottom of valley)

- $\nabla \neq 0 \Rightarrow \exists$ descent direction
- But if Hessian (∇^2) "large", allows ∇ to fluctuate a lot!

  ⇒ To ensure descent, take small enough steps determined by smoothness (norm of $\nabla^{2)}$
- Guaranteed to get close to point with $\nabla \approx 0$ (speed determined by norms of ∇^2 and ∇). "Stationary point"

ysis of optimization algorithms extensively discussed in Michael Jordan's plenary lecture!)

Analyses of nonconvex opt. : nonblack box



"Inverse problems": Assume data generated according to some clean mathematical model. Optimization landscape understood; desired solut is "ground truth" model.

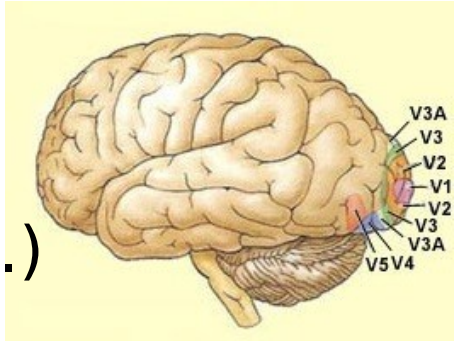
- Phase retrieval, Matrix Completion, Topic Modeling, Sparse coding, Tensor Decomposition, HMM learning,.. Amount to learning special neural nets

Idea in analysis: Prove direction of movement at current point θ is positively correlated with desired direction $(\theta - \theta^*)$ where θ^* = global optimum ("Lyapunov function")

[See "Framework for analyzing nonconvex optimization" by A. + Ma, offconvex.org)

Why deep? (Maybe, more expressive? Composition!)

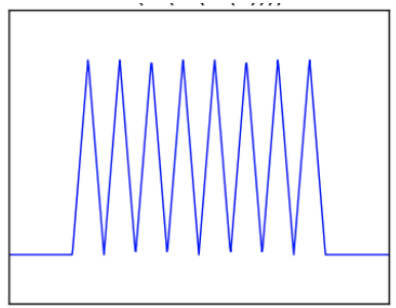
(e.g., If p, q are cubic polynomials, p(q(x)) is degree 9.)



Human Visual Cortex; 6+ levels

[Eldan-Shamir'16], [Telgarsky'17]: ∃ function computable with depth d+1 net of size S which is not approximable by depth d nets of size S^2

Pf Sketch: Characterize max. # of "oscillations" in function computed by depth d net.



Open: Exhibit above for a natural learning problem. (Currently out of reach, since we lack good mathematical characterization of "natural".)

Why deep? (Maybe, helps optimization [A., Cohen,Hazan'18].)

l_4 regression. $\ell(\theta) = \sum_{i=1} (\langle X^i, \theta \rangle - Y^{(i)})^4$ **X → <X, θ>**

Replace with depth-2 linear deep net $\ell(\theta) = \sum_{i=1} (\langle X^i, \beta\theta \rangle - Y^{(i)})^4$ **X → <X, θ> → β <X, θ>**

(= <X, β θ>)

Unchanged??

No! Gradient Descent changes $\theta^{(t+1)} = \theta^{(t)} + \rho^{(t)} \nabla_{\theta^{(t)}} + \sum_{i=1}^{t-1} \mu^{(t,i)} \nabla_{\theta^{(i)}}$

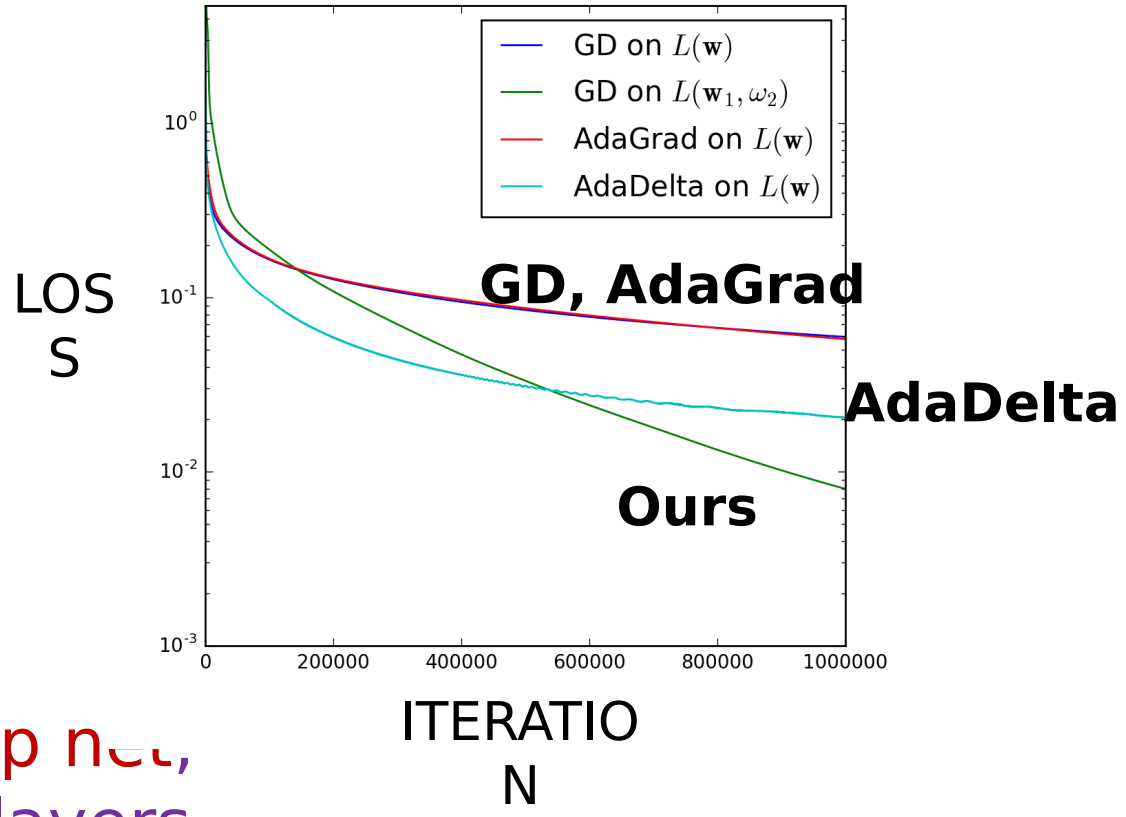
"Acceleration"?

Adaptive learning rate + "memory" of past gradients!

Acceleration effect of increasing depth

(UCI regression task…)

l_4 regression,



Similar effects observed in nonlinear deep net,
eg replace fully connected layer by two layers.

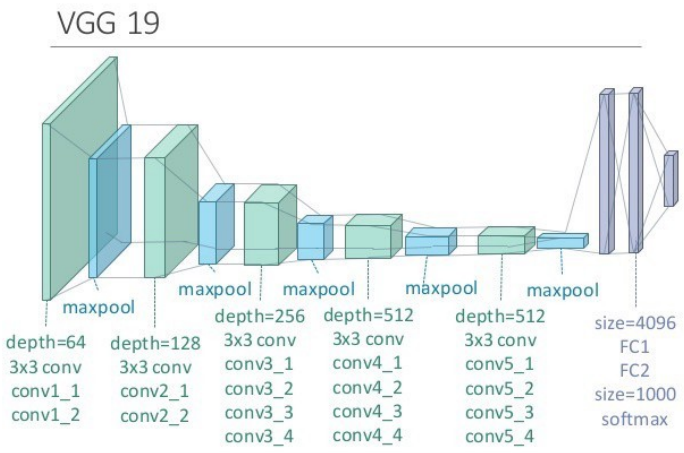
Some theoretical analysis for multilayer linear nets.

Proof that acceleration effect due to increase of depth
not obtainable via any standard manipulation of original loss function

Why no overfitting? Verified for nets with 20M parameters trained on 50k sam

opular conjecture: When trained on realistic data, the net's parameters are onstrained ---by problem and/or training ---- to be highly interdependent (e.g., e on manifold of much lower dimension)

Next few slides: A partial realization of this suggestion

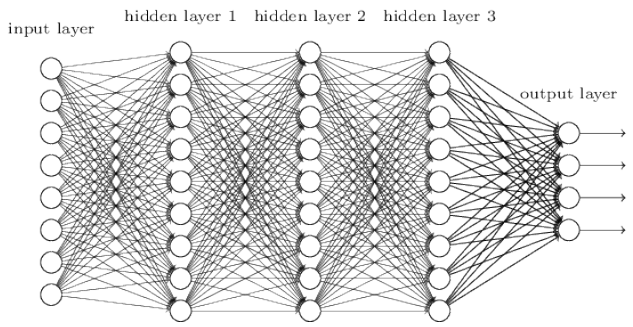


Properly trained nets have "noise stability" property. We prove theorem showing this implies their parameters lie in a lower-dimensional subspace

("dimension reduction" also appears in Assaf Naor's plenary lecture!)

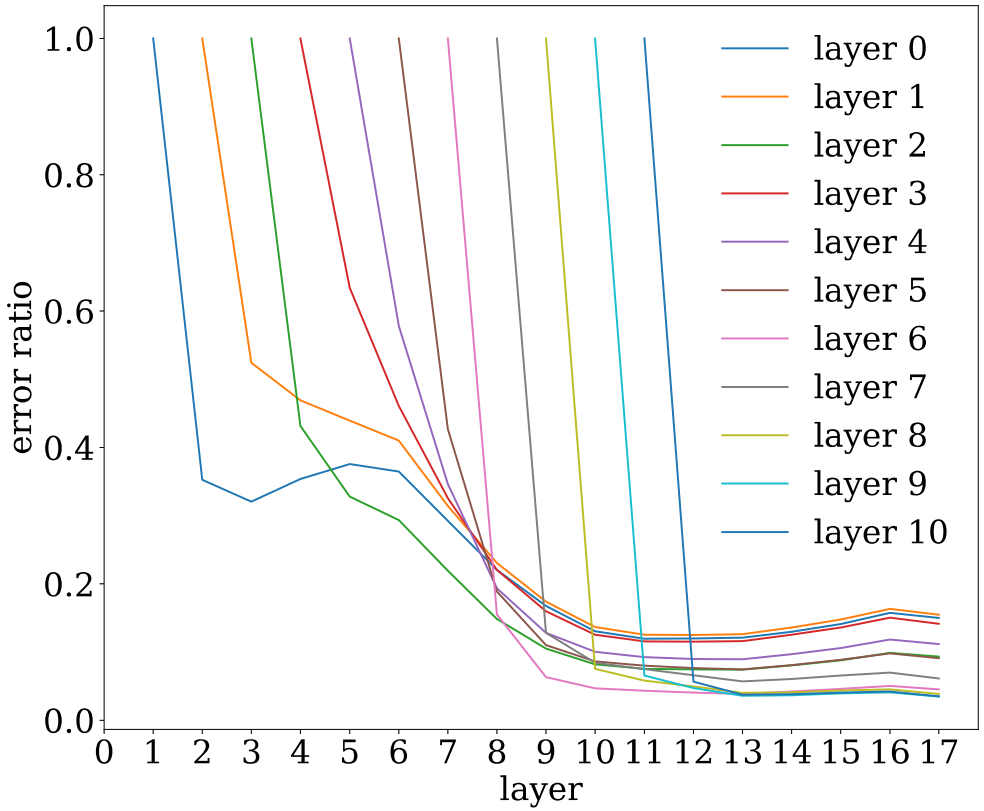
Noise stability experiment

[A., Ge, Neyshabur, Zhang IC

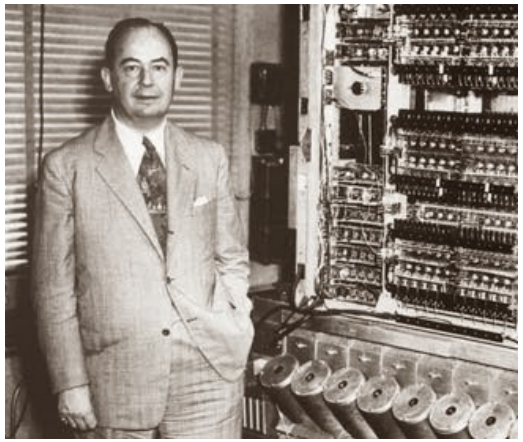


Noise injection: Add gaussian η to outpu of a layer ($|\eta|$ = |x|)

Measure percent change in higher layer (If small, then net is noise stable.)



Results for VGG19 (19 layers)



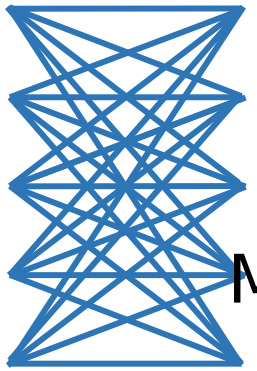
Von Neumann, J. (1956).
Probabilistic logics and the synthesis of reliable organisms from unreliable components.

Key Idea: Can improve reliability of circuits by allowing redundancy.

("noise stability" notion also appears in Gil Kalai's plenary lecture!)

Noise stability: understanding one layer (no nonlinearity)

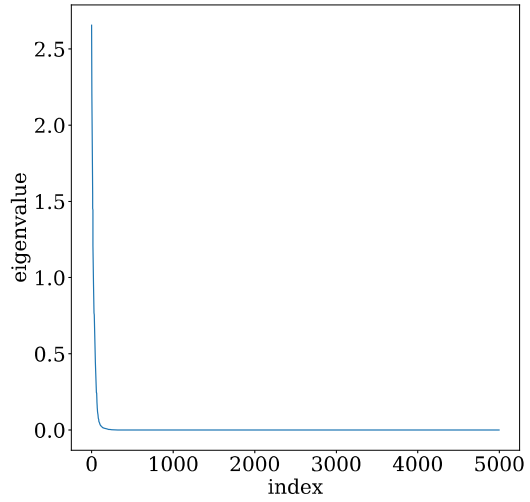
η : Gaussian noise



$|Mx|/|x| \gg |M\,\eta|/|\eta|$

$\sigma_{max}(M)$ ≪ $(\sum_i \sigma_i(M)^2)^{1/2}/\sqrt{n}$

Layer Cushion = ratio (roughly speaking..)

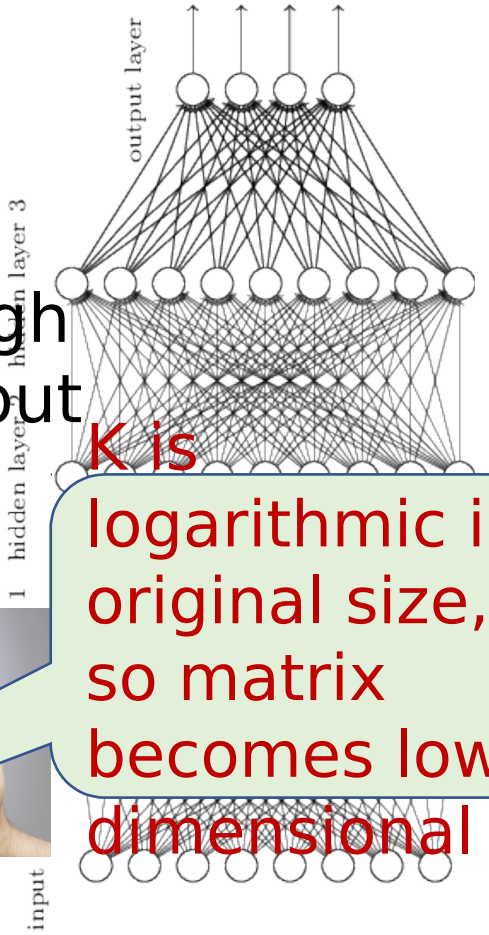


Distribution of singular values in a filter of layer 10 of VGG19.
Such matrices are compressible...

Proof sketch : Noise stability ⇒ deep net can be made low-dimensional (minimal change to training error)

Idea 1: Compress a layer (randomized; errors introduced are “Gaussian like”)

Idea 2: Errors attenuate as they go through network, due to noise stability. So output changed not much.



K is logarithmic in original size, so matrix becomes low-dimensional

Compression:

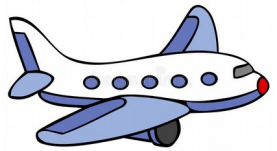
(1) *Generate k random sign matrices $M_1, \dots, M_k$ (impt: picked before seeing data)*

(2) $\hat{A} = \frac{1}{k}\sum_{t=1}^{k}\langle A, M_t\rangle M_t$

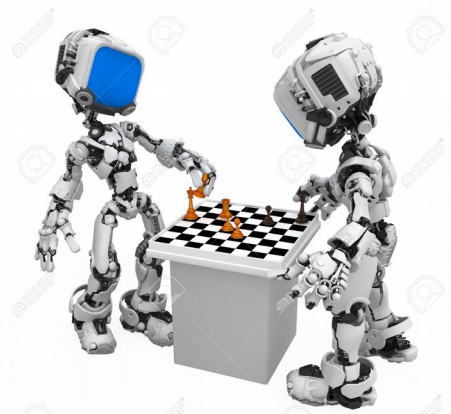
Part 4

Taking stock, wrapping up

"Mindless" model-fitting…
None of this is remotely how humans think!



1. Imitation approach has not worked well in the past: airplanes, chess/go etc.



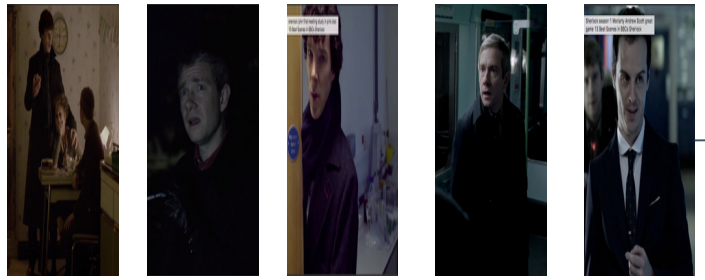
2. Machines' advantage lies precisely in ability to crunch data.

3. We have little idea at an operational level h humans think.

In fact, machine learning is currently the best hope figuring out how humans think...

Sample Task: “Decoding” Brain fMRI [Vodrahalli et al NeuroImage’17]

Movie scenes



Annotations of movie scenes

Sherlock and John talk about the murder in an old room with Mrs. Hudson.

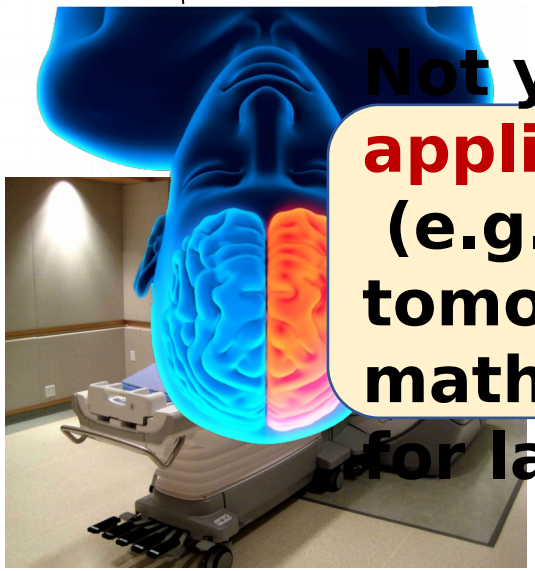
John is worried as Sherlock runs off.

Sherlock enters the door to the chemistry lab, saying “John, I was here the whole time.”

Once they get on the subway, John exclaims, “No

Moriarty arrives and says, “Hello Sherlock, John.”

“Decode?? ”

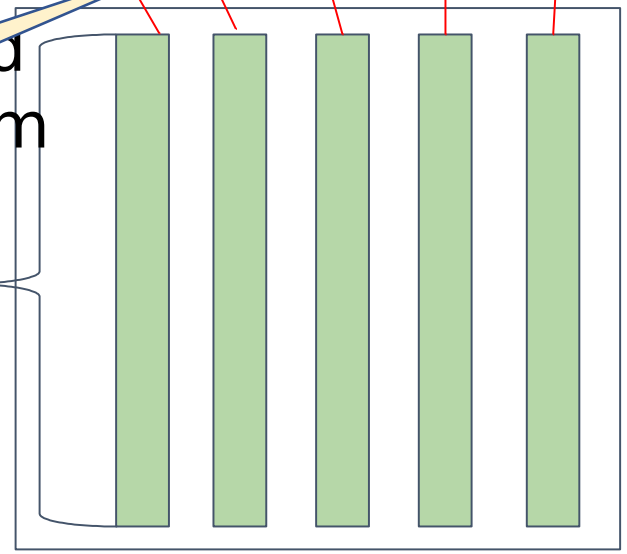


fMRI Machine

Not your typical applied math problem (e.g., x-ray tomography). No mathematical model for language!!

Each movie scene paired with text description from

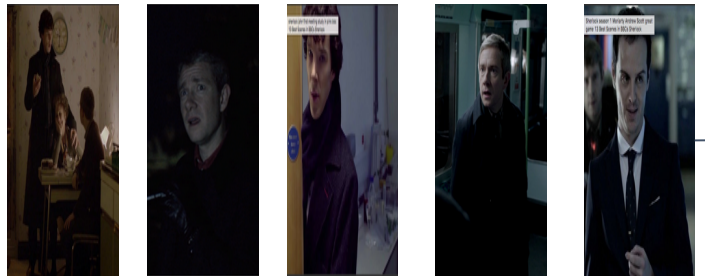
Voxel vector per time step ∈ $R^{50,000}$



fMRI responses

Sample Task: “Decoding” Brain fMRI [Vodrahalli et al NeuroImage’17]

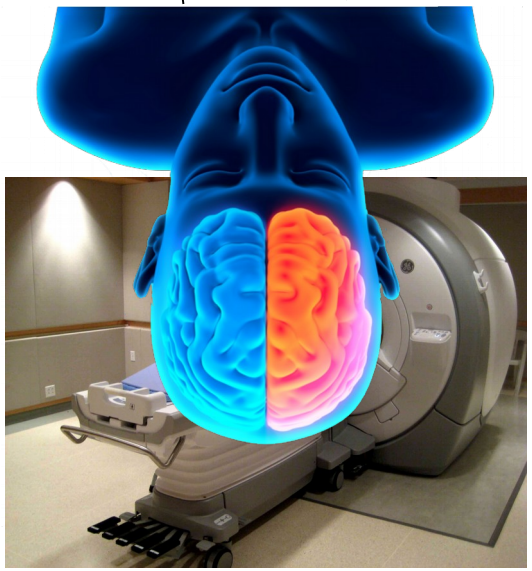
Movie scenes



semantic embeddings of text (“SiF’) from [Arora et al’17]

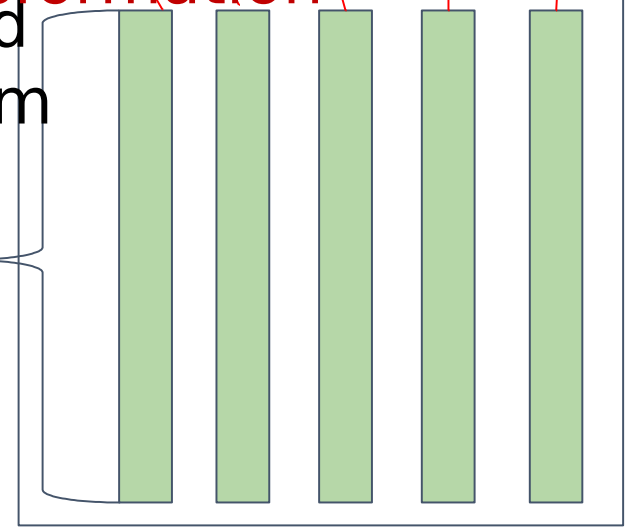
Learnt“ Linear transformation”

Each movie scene paired with text description from external party.



fMRI Machine

Voxel vector per time step ∈ $R^{50,000}$



fMRI responses

Hottest trend in academia…

Apply Machine Learning to Discipline X

(X = Physics, Biology, Chemisty, Medicine, Engineering, Neuroscience, Economics/Finance, History, Comparative Literature,….)

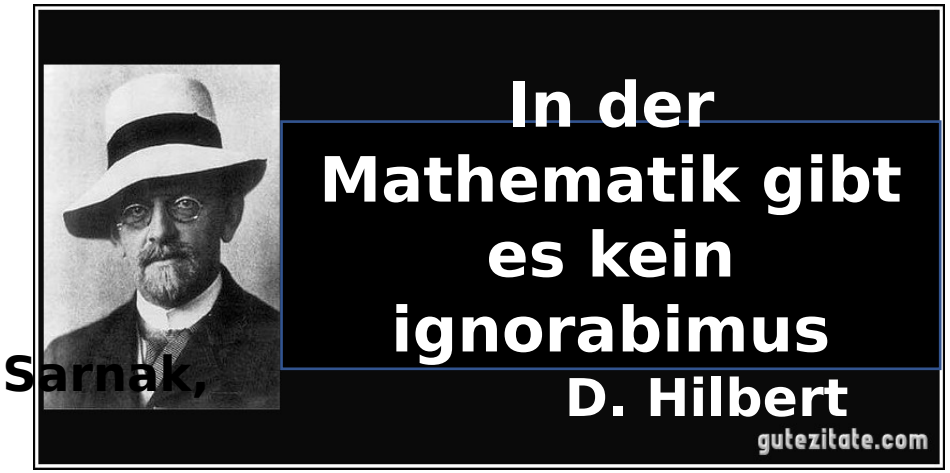
Hope mathematics will join in this development!

oncluding thoughts on ML

What is Learning?
What does it mean to understand the world?

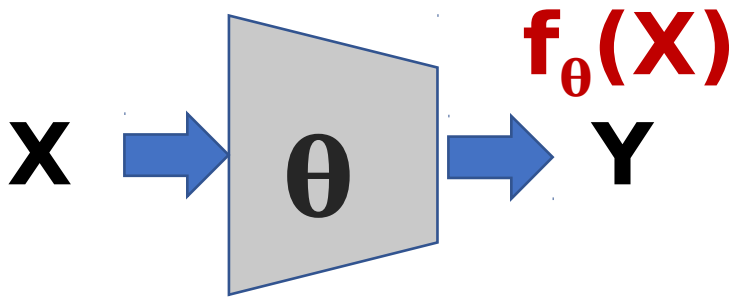
- Speaks to age-old wonders/mysteries
- New way of looking at the world (via complicated inexact descriptions)
- A new frontier for science and math
- I am optimistic that deep learning methods can be mathematically understood and/or simplified.

THANK YOU!!



s for feedback: M. Goresky, A. Ionescu, J. Kollar, P. Sarnak, T. Spencer A. Wigderson.

Formal framework (inherited from classical statistics)



$\theta \in R^d$

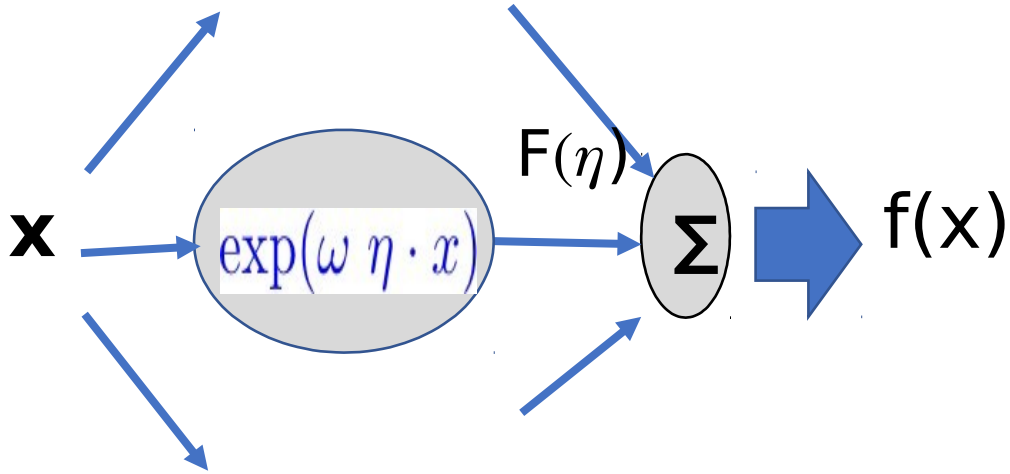
(trainable parameters)

Training data: $\{(X_1^{(i)}, Y^{(i)}): i=1,..,N\}$

"Loss" $\ell(\theta) = \sum_{i=1}^{N} (f_\theta(X_1^{(i)}) - Y^{(i)})^2$

Many other loss formulations exist....)

A classical analog: Fourier Transform of periodic f: $R^n \rightarrow R$



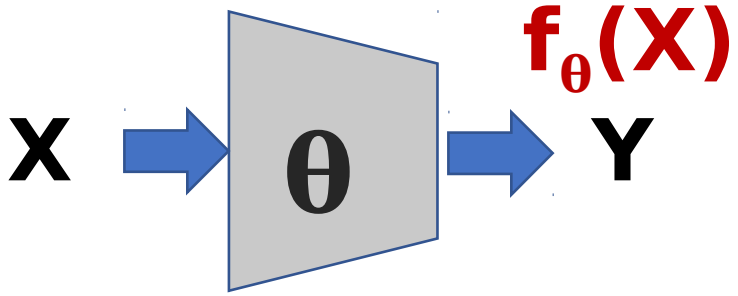
$$f(x) = \sum_{\eta} F(\eta) \exp(\omega\ \eta \cdot x)$$

$$F(\eta) = \int f(x) \exp(-\omega\ \eta \cdot x) dx$$

"Learning from (x, f(x)) pairs"

L_2 Loss function

Formal framework (inherited from classical statistics)



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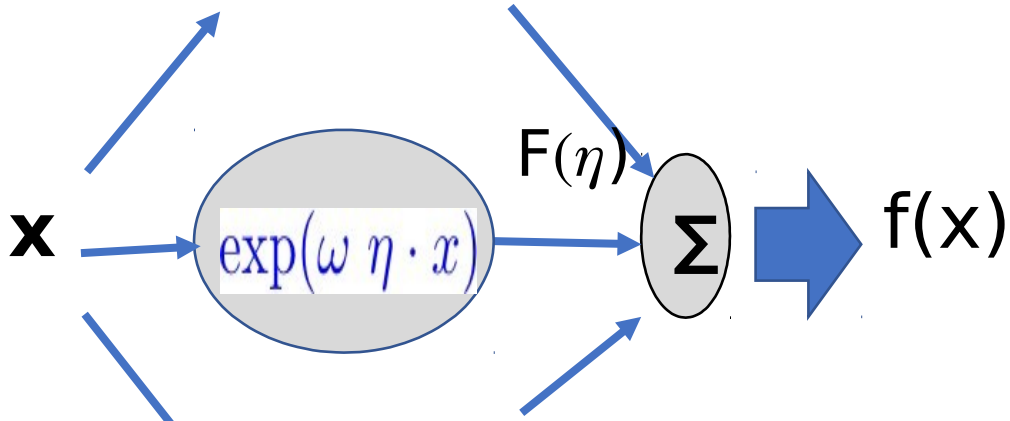

Training data: $\{(X_1^{(i)}, Y^{(i)}): i=1 \ldots N\}$

"Loss" $\ell(\theta) = \sum_{i=1}^{N} (f_\theta(X_1^{(i)}) -$

Many other loss formulations exist...)

Practically Infeasible: Needs exp(n) samples of (x, f(x)) for even modest accuracy.

(Real life: n = 10^4 and 10n samples.)