Deep Learning/Double Descent

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MIT

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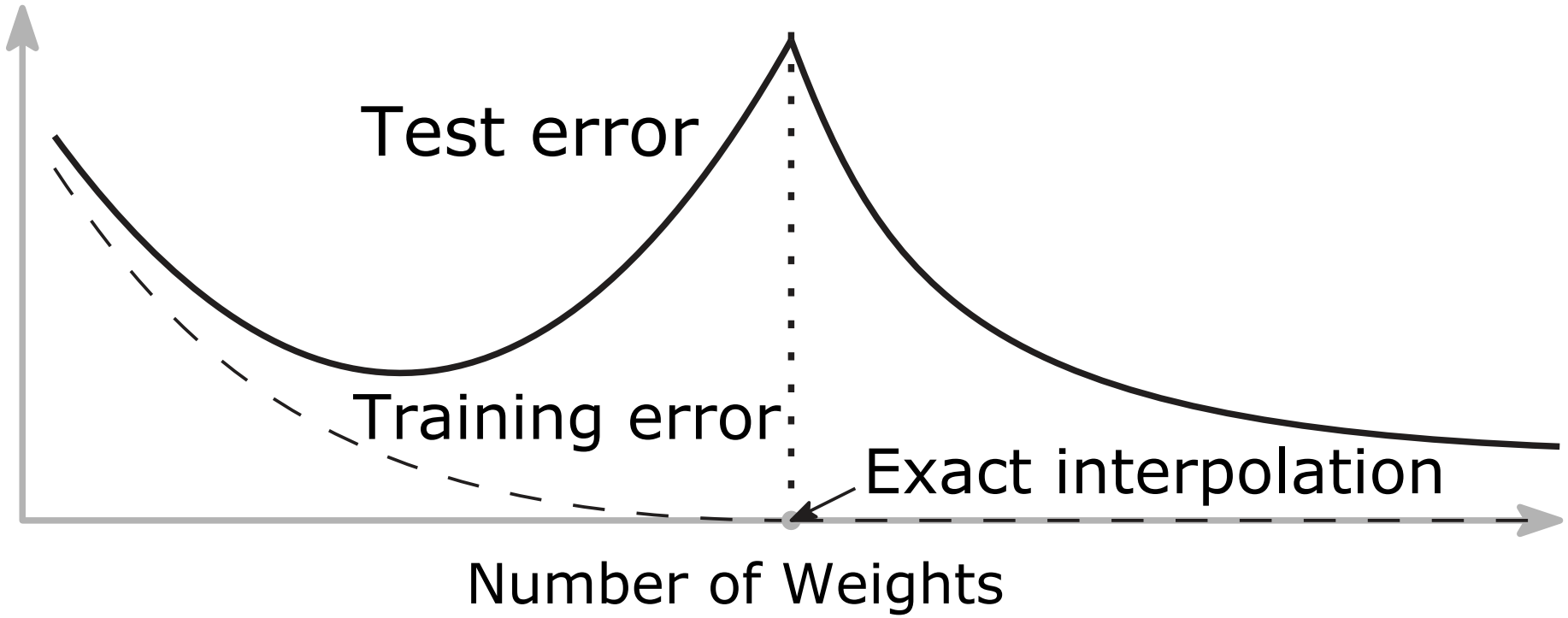
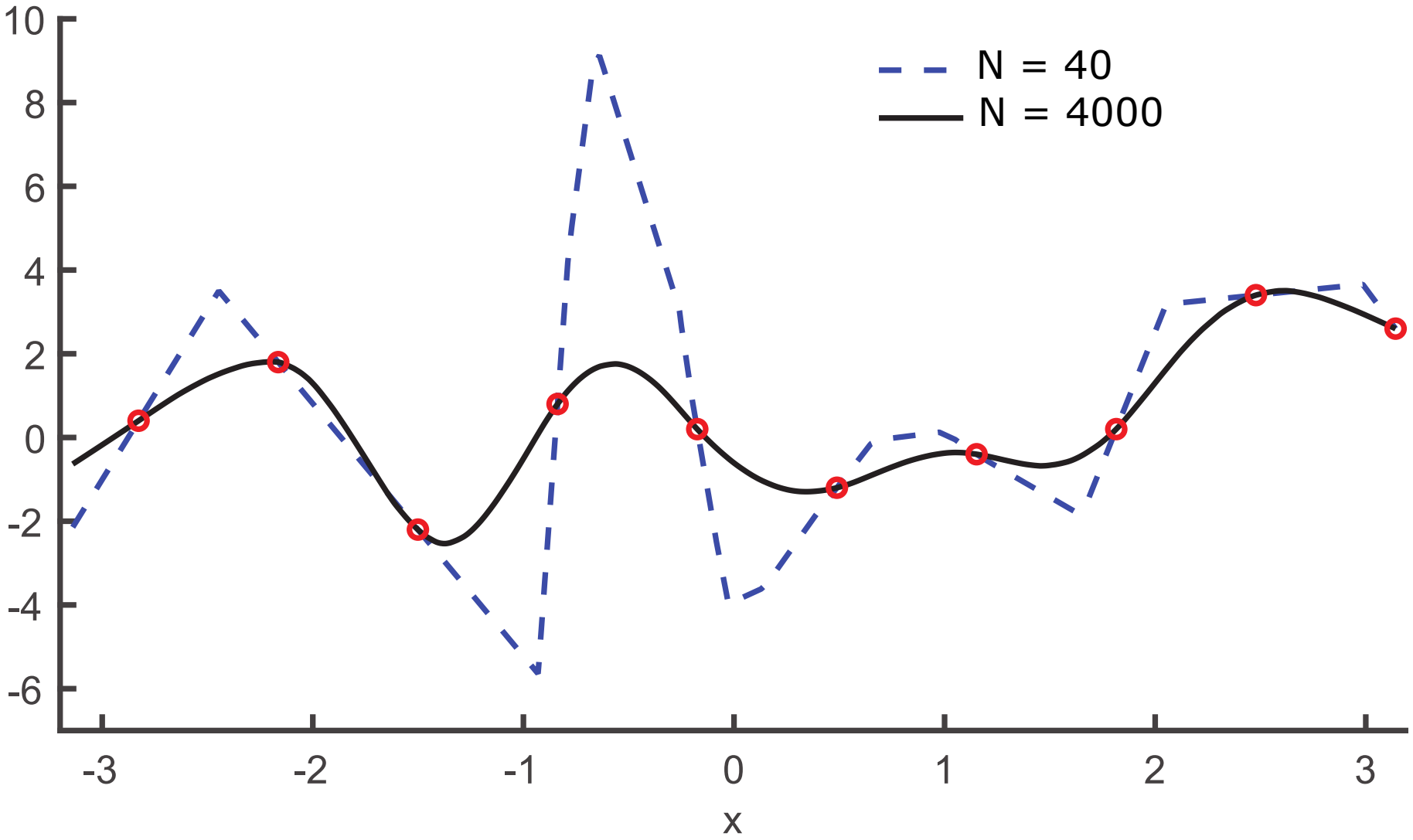

Test error
Training error
Exact interpolation
Number of Weights


N = 40
N = 4000
10
8
6
4
2
0
-2
-4
-6
-3
-2
-1
0
1
2
3
x

Fit training data by a Learning function F

We are given training data : **Inputs v, outputs w**

Example Each v is an image of a number
$w = 0, 1, \ldots, 9$

The vector v describes each pixel in the image

We want to create a **learning function** so that
$F(v) \approx w$

math.mit.edu/learningfromdata

Deep Neural Networks

1	Key operation	Composition $F = F_3(F_2(F_1(x, v_0)))$
2	Key rule	Chain rule for x-derivatives of F
3	Key algorithm	Stochastic gradient descent to find x
4	Key subroutine	Backpropagation to compute grad F
5	Key nonlinearity	ReLU $(y) = \max(y, 0) =$ ramp function

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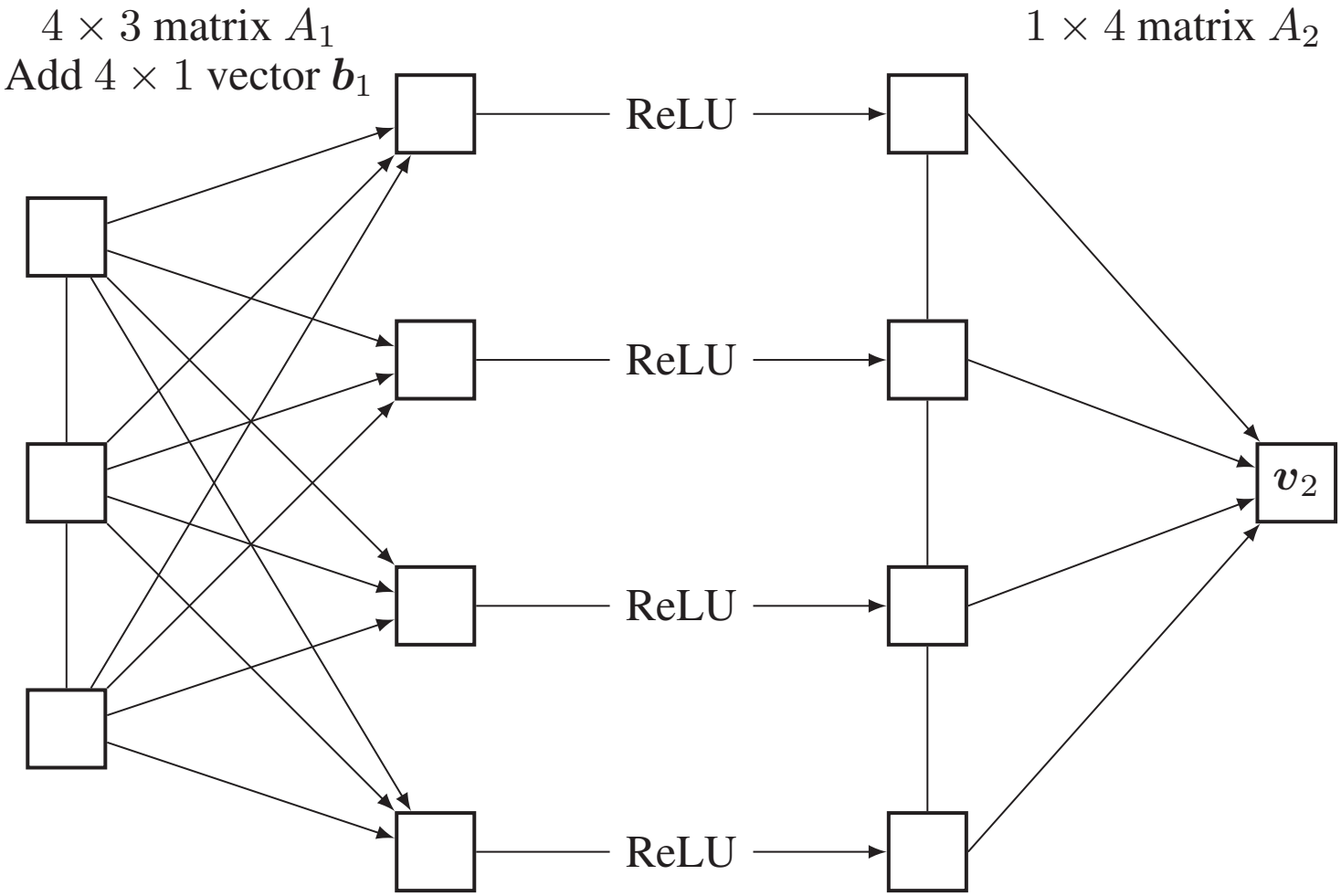
Weights for layer k $\quad A_k =$ matrix and $b_k =$ offset vector

$v_0 =$ training data / $v_1, \ldots, v_{\ell-1}$ hidden layers / $v_\ell =$ output

Figure from math.mit.edu/learningfromdata



Feature vector v_0
Three components for each training sample

$y_1 = A_1 v_0 + b_1$
y_1 at layer 1

v_1 at layer 1
$v_1 = \text{ReLU}(y_1)$

Output $w = v_2$
$v_2 = A_2 v_1$

Four components of y_1 and v_1

Key computation: Weights $\boldsymbol{x}$ minimize overall loss $L(x)$

$$L(x) = \frac{1}{N} \sum_{j=1}^{N} \text{ loss } \ell\left(\boldsymbol{x}, \boldsymbol{v}_0^j\right) \text{ on sample } j$$

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"Square loss" = error $\ell\left(\boldsymbol{x}, \boldsymbol{v}_0^j\right) = \left|\left|F\left(\boldsymbol{x}, \boldsymbol{v}_0^j\right) - \text{true}\right|\right|^2$

Cross-entropy loss, hinge loss,...

Classification problem : true $= 1$ or -1

Regression problem : true = vector

Gradient descent $x_{k+1} = \arg \min ||x_k - s_k \nabla L(x_k)||$

Stochastic descent $x_{k+1} = \arg \min \left|\left|x_k - s_k \nabla \ell\left(x_k, v_0^k\right)\right|\right|$

Key Questions

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2. Convergence rate of descent and accelerated descent (when $\boldsymbol{x}_{k+1}$ depends on $\boldsymbol{x}_k$ and $\boldsymbol{x}_{k-1}$: momentum added)

3. Do the weights $A_1, b_1 \ldots$ generalize to unseen test data ? (Early stopping / Do not overfit the data)

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   $F_1(\boldsymbol{v}_0) = \max(A_1\boldsymbol{v}_0 + b_1, 0) = \text{ReLU} \circ \text{affine map}$

   $F(\boldsymbol{v})$ is continuous piecewise linear : how many pieces?

   This measures the "expressivity" of the network

   Assume 1 hidden layer with N neurons

v_0 has m components / v_1 has N components / N ReLU's

The number of flat regions in $\mathbf{R}^m$ bounded by the N hyperplanes

$$r(N, m) = \sum_{i=0}^{m} \binom{N}{i} = \binom{N}{0} + \binom{N}{1} + \cdots + \binom{N}{m}$$

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$N = 3$ folds in a plane will produce $1 + 3 + 3 = 7$ pieces

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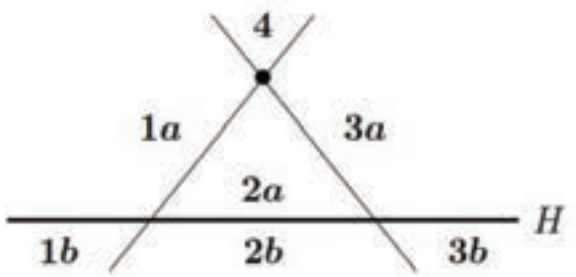

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$\leftarrow r(2,2) = 4$
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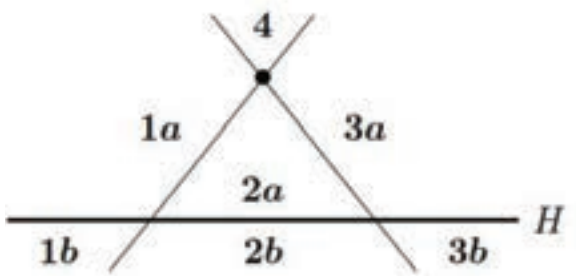

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Recursion $r(N,m) = r(N-1,m) + r(N-1,m-1)$

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Big problems are **underdetermined** [# weights $>$ # samples]

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Stochastic Gradient Descent finds weights that generalize well

Convolutional Neural Nets (**CNN**)

$$A = \begin{bmatrix} x_1 & x_0 & x_{-1} & 0 & 0 & 0 \\ 0 & x_1 & x_0 & x_{-1} & 0 & 0 \\ 0 & 0 & x_1 & x_0 & x_{-1} & 0 \\ 0 & 0 & 0 & x_1 & x_0 & x_{-1} \end{bmatrix}$$

$N + 2$ inputs and N outputs

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$$\frac{\partial \boldsymbol{y}}{\partial x_1} = L\boldsymbol{v} \qquad \frac{\partial \boldsymbol{y}}{\partial x_0} = C\boldsymbol{v} \qquad \frac{\partial \boldsymbol{y}}{\partial x_{-1}} = R\boldsymbol{v}$$

Convolutions in Two Dimensions

Weights $\begin{bmatrix} x_{11} & x_{01} & x_{-11} \\ x_{10} & x_{00} & x_{-10} \\ x_{1-1} & x_{0-1} & x_{-1-1} \end{bmatrix}$

Input image v_{ij} i, j from $(0, 0)$ to $(N+1, N+1)$

Output image y_{ij} i, j from $(1, 1)$to (N, N)

Shifts L, C, R, U, D = **L**eft, **C**enter, **R**ight, **U**p, **D**own

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9 weights instead of n^2 weights in A

Allows the neural net to have more width and depth

Computing the weights $\boldsymbol{x}$ = matrices A_k, bias vectors b_k

Choose a loss function ℓ to measure $\boldsymbol{F(x, v)}-$ **true output**

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Choose a loss function ℓ to measure $\boldsymbol{F(x, v)}-$ **true output**

Total loss $\boldsymbol{L} = \frac{1}{N}$ (sum of losses for all N samples)

Compute weights $\boldsymbol{x}$ to minimize the total loss $\boldsymbol{L}$

Here are three loss functions—Cross-entropy is a favorite loss function for neural nets

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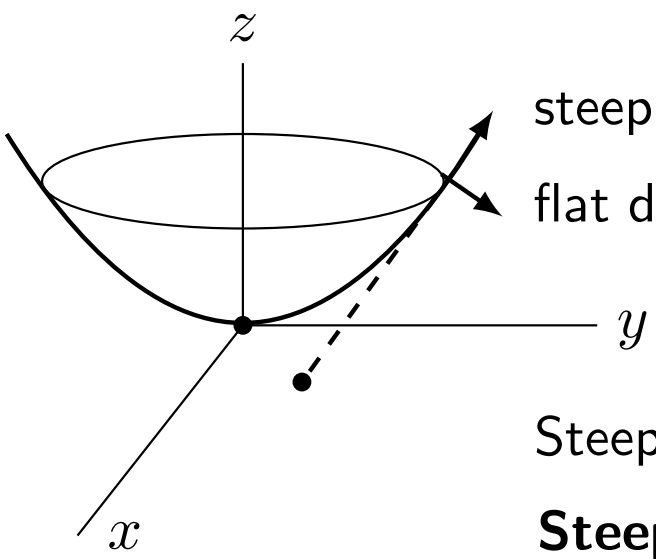
1 **Square loss** $L(\boldsymbol{x}) = \frac{1}{N}\sum_{1}^{N} ||F(\boldsymbol{x}, \boldsymbol{v}_i) - \text{true}||^2$: sum over samples $\boldsymbol{v}_i$

2 **Hinge loss** $L(\boldsymbol{x}) = \frac{1}{N}\sum_{1}^{N} \textbf{max}\,(0, 1 - t\,F(\boldsymbol{x}))$ for **classification**

3 **Cross-entropy loss** $L(\boldsymbol{x}) = -\frac{1}{N}\sum_{1}^{N} [y_i \log\, \widehat{y_i} + (1 - y_i) \log\,(1 - \widehat{y_i})]$

Steepest Descent = Gradient Descent $f = x^2 + by^2$



steepest direction ∇f up and down the bowl

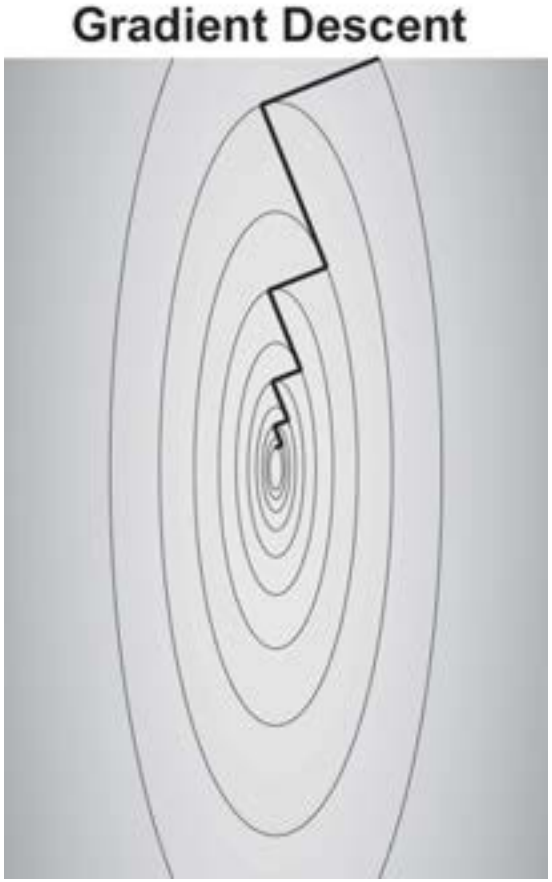
flat direction $(\nabla f)^\perp$ along the ellipse $x^2 + by^2 =$ constant

Steepest direction is perpendicular to the flat direction

Steepest direction is not aimed at the minimum

Steepest descent moves in the gradient direction $\begin{bmatrix} -2x \\ -2by \end{bmatrix}$.

$$x_k = b\left(\frac{b-1}{b+1}\right)^k \quad y_k = \left(\frac{1-b}{1+b}\right)^k \quad f(x_k, y_k) = \left(\frac{1-b}{1+b}\right)^{2k} f(x_0, y_0)$$



The first descent step starts out perpendicular to the level set. As it crosses through lower level sets, the function $f(x, y)$ is decreasing. **Eventually its path is tangent to a level set L.**

Slow convergence on a zig-zag path to the minimum of $f = x^2 + by^2$.

Momentum and the Path of a Heavy Ball

Descent with momentum

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Following the eigenvector q

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It seems a miracle that this problem has a beautiful solution.
The optimal s and β are

$$s = \left(\frac{2}{\sqrt{\lambda_{\max}} + \sqrt{\lambda_{\min}}} \right)^2 \quad \text{and} \quad \beta = \left(\frac{\sqrt{\lambda_{\max}} - \sqrt{\lambda_{\min}}}{\sqrt{\lambda_{\max}} + \sqrt{\lambda_{\min}}} \right)^2$$

Key difference: b is replaced by $\sqrt{b}$

Ordinary descent factor	$\left(\frac{1-b}{1+b}\right)^2$	**Accelerated descent factor**	$\left(\frac{1-\sqrt{b}}{1+\sqrt{b}}\right)^2$

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Steepest descent $\left(\frac{.99}{1.01}\right)^2 = \mathbf{.96}$

Accelerated descent $\left(\frac{.9}{1.1}\right)^2 = \mathbf{.67}$

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Notice that $\lambda_{\mathsf{max}}/\lambda_{\mathsf{min}} = 1/b = \kappa$ is the **condition number of S**

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Choosing a polynomial of degree 60 *to fit* 61 *data points*

Stochastic Descent Using One Sample Per Step

Early steps of SGD often converge quickly toward the solution x^*

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Convergence at the start changes to large oscillations near the solution

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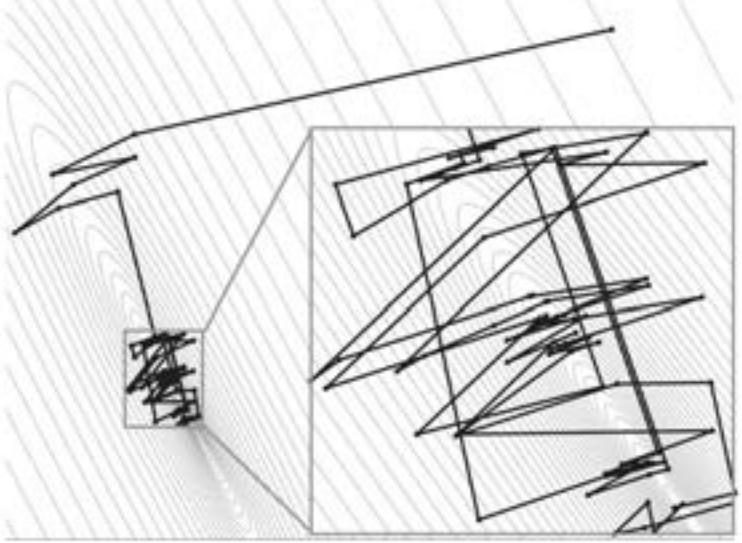

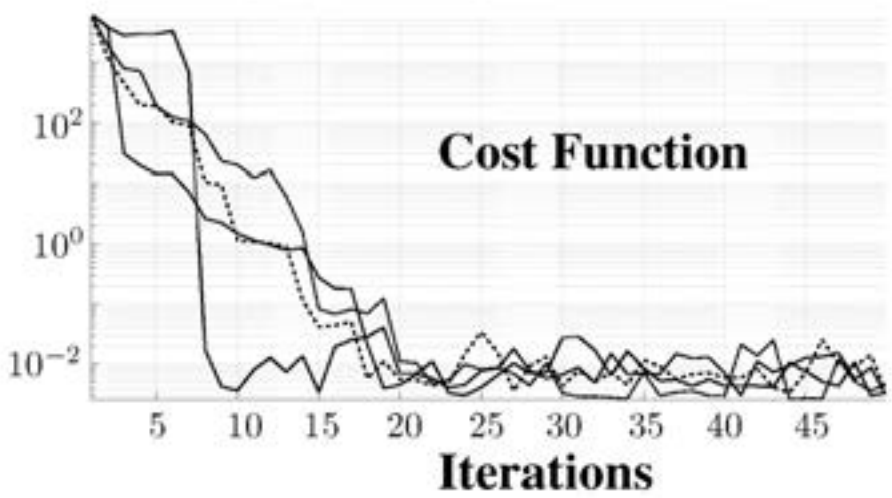

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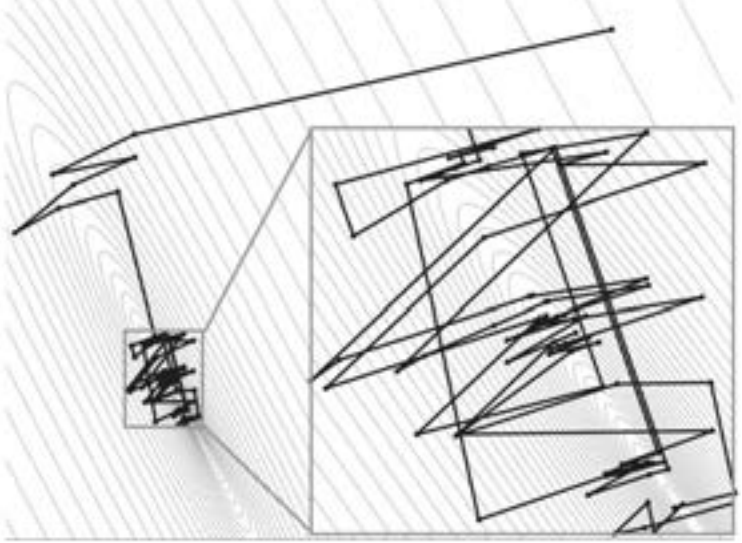

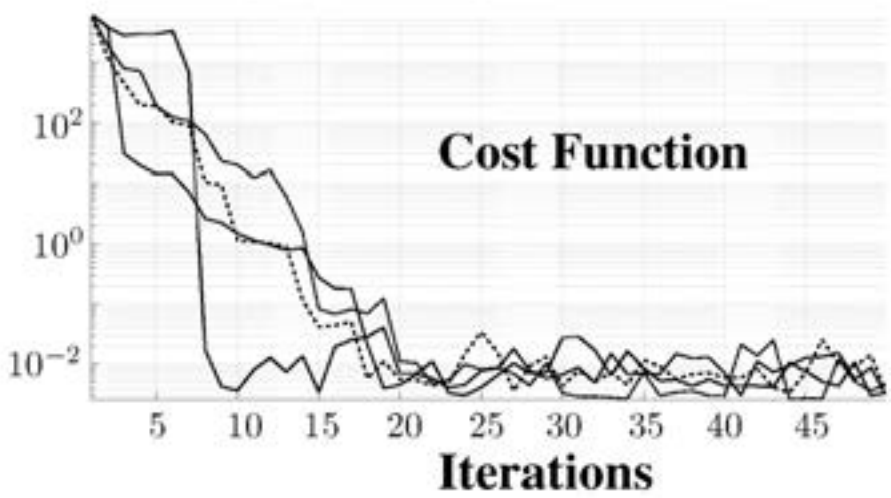

Kaczmarz for $Ax = b$ with random $i(k)$ $\quad \boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \dfrac{b_i - \boldsymbol{a}_i^{\mathrm{T}} \boldsymbol{x}_k}{||\boldsymbol{a}_i||^2} \boldsymbol{a}_i$

Adaptive Methods Using Earlier Gradients (**ADAM**)

Adaptive Stochastic Gradient Descent $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - s_k \boldsymbol{D}_k$

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$$\boldsymbol{D}_k = \delta \boldsymbol{D}_{k-1} + (1-\delta)\boldsymbol{\nabla L}(\boldsymbol{x}_k) \qquad s_k^2 = \beta s_{k-1}^2 + (1-\beta)\,||\boldsymbol{\nabla L}\,(\boldsymbol{x}_k)||^2$$

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Why do the weights generalize well to unseen test data ?

Computation of $\boldsymbol{\partial F/\partial x}$: Explicit Formulas

$\boldsymbol{v}_L = \boldsymbol{b}_L + A_L \boldsymbol{v}_{L-1}$ or simply $\boldsymbol{w} = \boldsymbol{b} + A\boldsymbol{v}$.

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Fully connected layer

Independent weights A_{jk}

$$\frac{\partial w_i}{\partial b_j} = \delta_{ij} \quad \textbf{and} \quad \frac{\partial w_i}{\partial A_{jk}} = \delta_{ij} v_k$$

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Computation of $\partial F/\partial x$: Explicit Formulas

$\boldsymbol{v}_L = \boldsymbol{b}_L + A_L \boldsymbol{v}_{L-1}$ or simply $\boldsymbol{w} = \boldsymbol{b} + A\boldsymbol{v}$.

The output w_i is not affected by b_j or A_{jk} if $j \neq i$

Fully connected layer

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$$\frac{\partial w_1}{\partial b_1} = \mathbf{1}, \quad \frac{\partial w_1}{\partial b_2} = \mathbf{0}, \quad \frac{\partial w_1}{\partial a_{11}} = \boldsymbol{v_1}, \quad \frac{\partial w_1}{\partial a_{12}} = \boldsymbol{v_2}, \quad \frac{\partial w_1}{\partial a_{21}} = \frac{\partial w_1}{\partial a_{22}} = \mathbf{0}.$$

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$$\frac{d}{dx}(F_3(F_2(F_1(x)))) = \left(\frac{dF_3}{dF_2}(F_2(F_1(x)))\right)\left(\frac{dF_2}{dF_1}(F_1(x))\right)\left(\frac{dF_1}{dx}(x)\right)$$

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Which order (**forward or backward** along the chain) is faster ?

Backward-mode AD is faster for $M_1 M_2 \boldsymbol{w}$

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Backward $M_1(M_2(\dots(M_L\boldsymbol{w})))$ needs LN^2

The Multivariable Chain Rule

$$\frac{\partial \boldsymbol{w}}{\partial \boldsymbol{v}} = \begin{bmatrix} \dfrac{\partial w_1}{\partial v_1} & \cdots & \dfrac{\partial w_1}{\partial v_n} \\ & \cdots & \\ \dfrac{\partial w_p}{\partial v_1} & \cdots & \dfrac{\partial w_p}{\partial v_n} \end{bmatrix} \qquad \frac{\partial \boldsymbol{v}}{\partial \boldsymbol{u}} = \begin{bmatrix} \dfrac{\partial v_1}{\partial u_1} & \cdots & \dfrac{\partial v_1}{\partial u_m} \\ & \cdots & \\ \dfrac{\partial v_n}{\partial u_1} & \cdots & \dfrac{\partial v_n}{\partial u_m} \end{bmatrix}$$

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$$\frac{\partial w_i}{\partial u_k} = \frac{\partial w_i}{\partial v_1}\frac{\partial v_1}{\partial u_k} + \cdots + \frac{\partial w_i}{\partial v_n}\frac{\partial v_n}{\partial u_k} = \left(\frac{\partial w_i}{\partial v_1}, \ldots, \frac{\partial w_i}{\partial v_n}\right) \cdot \left(\frac{\partial v_1}{\partial u_k}, \ldots, \frac{\partial v_n}{\partial u_k}\right)$$

Multivariable chain rule: Multiply matrices! $\dfrac{\partial \boldsymbol{w}}{\partial \boldsymbol{u}} = \left(\dfrac{\partial \boldsymbol{w}}{\partial \boldsymbol{v}}\right)\left(\dfrac{\partial \boldsymbol{v}}{\partial \boldsymbol{u}}\right)$

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Cross-validation Divide the available data into K subsets

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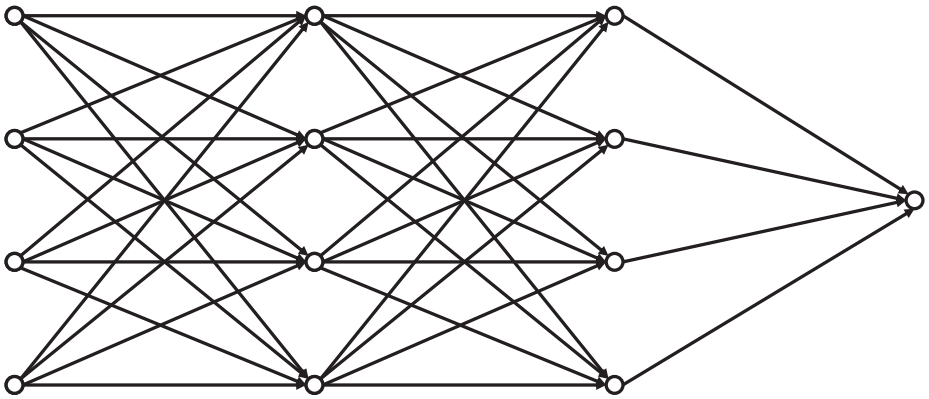

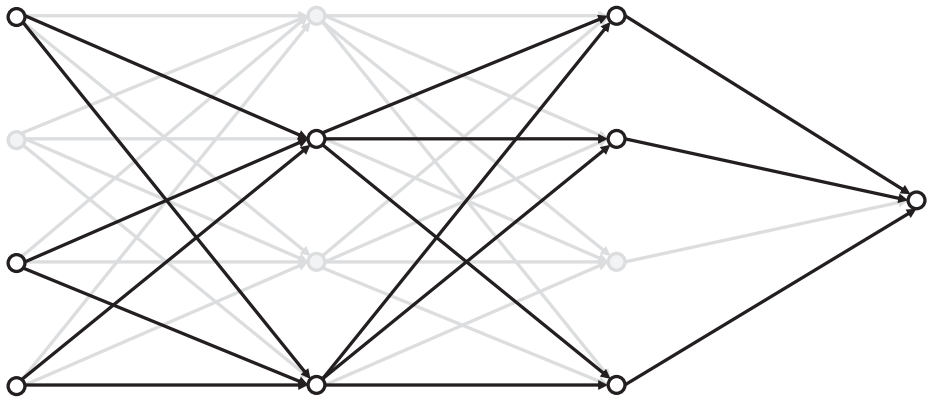

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Residual Networks (ResNets) "*skip connections*"

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Deep networks give **closer approximation** than splines or shallow nets

Counting Flat Pieces in the Graph

Theorem For $\boldsymbol{v}$ in $\mathbf{R}^m$, suppose the graph of $F(\boldsymbol{v})$ has folds along N hyperplanes $H_1, \ldots, H_N$. Those come from N linear equations $\boldsymbol{a}_i^{\mathrm{T}} \boldsymbol{v} + b_i = 0$, in other words ReLU at N neurons. F has $r(N, m)$ linear pieces :

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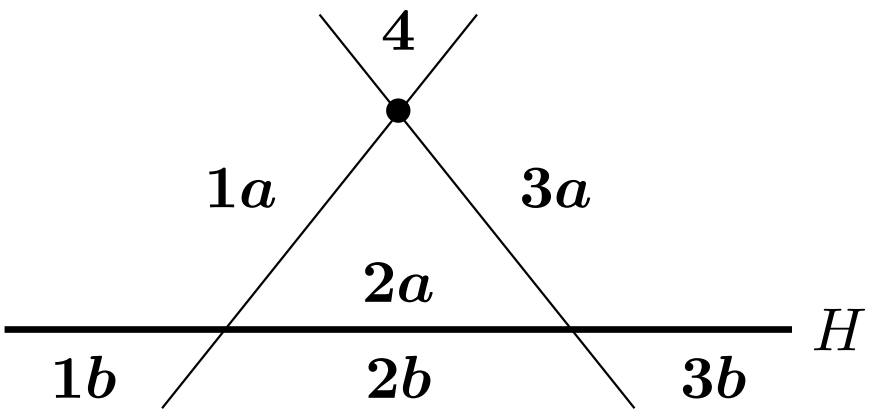

Start with 2 planes

$\leftarrow r(2,2) = 4$

Add new plane H

$\leftarrow r(2,1) = 3$

Continuous Piecewise Linear Function

How many linear pieces with more layers ?

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Now ReLU is folding **piecewise linear** functions

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Hanin-Rolnick : Still $r(N, m) \approx cN^m$ pieces from N neurons

18.085 Computational Science and Engineering I

Summer 2020