PERSONAL NOTES

Principles of Large Scale ML

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2023

Scaling → ML

↑

Principles.

How scale impact performance of ML system.

Data Collection → Data cleaning → Feature Engineering (Embedding) → Training (Robust).

Train / Valide / Test.

Splitting.

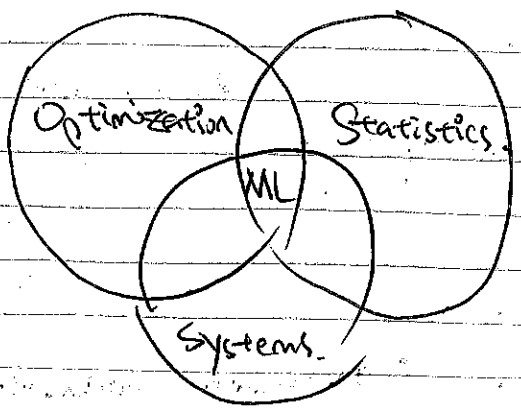
Model selection (Hyperpara. Opt.)

(Online learning)

Deployment

Inference

Monitoring



Principle #1: Optimization. Tasks

Solve it using gradient-base algorithms that are fast & "canned".

backpropagation + numerical linear algebra

- gradient descent.
- empirical risk min.

Principle #2: ✗ whole dataset, → subsample.

- Stochastic gradient d.
  - ↳ subsample the component losses.
  - ↑ compute ↗ faster.
- cross-validation / train / val / test split.
- bagging.
- kernel sampling. → subsample with ~~kernel~~ in CNN
- dropout. - data augmentation.
- VAE. (dimension reduction).

Principle #3 Use algorithms that are compatible w/ hardware. or vice versa.

- batch size. selection.
- numerical precision.
- GPU ↔ NN.
- Caching
  - data loader / streaming
  - ↕
  - GPU.
- using fast numerical linear algebra kernels.
- parallel / distributed computing.
- neuromorphic computing. (chip → NN).

CS.cornell.edu/courses/cs4787.

+ Canvas. + Gradescope → problem.

+ ed discussion. + CMS - programming a. (Python, numpy, torch)

Grading.

Psets

PAs.

Prelims

Final.

Paper reading.

Review sets — linear algebra ..

▷ Vector calculus

▷ Logistics

▷ Computing w/ Python

— office hours

Wednesday · 2-3 pm

Gates 426.

Week 1 . - 2 .

Aug. 24.

Principle 1 : ML as optimization.

↓

Continuous optimization.

↓

optimizing real numbers.

Data.

↳ Embedding steps → $\mathbb{R}^d$

vectors.

eg. pred. ppl.

· 33

· g. avg.

· 2013 . current job / current dun.

· 18,000 / yr.

↳ $\begin{bmatrix} - \\ - \\ - \\ - \end{bmatrix} \Rightarrow \mathbb{R}^4$.

Vector - element in vector space.

$x, y \in V \quad x+y \in V$

+ associated & commutative.

multiplication - -

~~Standard~~ property of a vector space.

Typical example. $\mathbb{R}^n$. $\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}$

e.g. matrix $\mathbb{R}^{n \times n}$.

$\mathbb{R}^{n \times n \times p}$. } can all be interpreted as vectors.

Core idea under: basis in linear algebra.

↓

how many numbers does it take / pinpoint that "vector space".

A basis for V is the subset for

$B = \{x_1, x_2, x_3, \ldots\}$. s.t. for every v in V - v can be written as a linear combination of vectors in B.

exists some $x_1, x_2, \ldots x_n \in B$,

and $a_1, a_2, \ldots a_n$.

s.t. $v = \sum_{i=1}^{n} a_i x_i$ $\quad V = \text{span}(B)$

and $\forall x \in B$,

$|B|$ = "Dimension" $\quad x \notin \text{span}(B / \{x\})$

↓

terminology confusion

↙ numerical linear algebra ↘ numpy, SimPy, ...

$V = \mathbb{R}^2$.

$B = \left\{ \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right\}$

$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = x_1 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + x_2 \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

numpy faster python.

- multiprocessing
- c++
- cache

* & @ easily mapped

↓ ↓

multiply tensor / matrix multiply

per-element.

broadcast → faster than manually comp.

(1.3.7)
(3.1.7)

(3.1.5)
(3.1.6)

X

(1.3.7) ✓ i.e. loop replicate.
(3.1.7)

(3.3.7)

(3.3.7)

numpy broadcasting.

Week 2 (1) Aug. 29

Automatic diff.

Definition - $\nabla f(w)^T$ is a linear map such that: $\Delta \in \mathbb{R}^d$

$$\nabla f(w)^T \Delta = \lim_{a \to 0} \frac{f(w+a\Delta) - f(w)}{a}$$

$f(x) = x^T A x.$

$$\lim_{a \to 0} \frac{(x+a\Delta)^T A (x+a\Delta) - x^T A x}{a}$$

$$\lim_{a \to 0} \frac{x^T A x + a\Delta^T A x + a x^T \Delta x + a^2 \Delta^T A \Delta - x^T A x}{a}$$

$$\lim_{a \to 0} \Delta^T A x + x^T A \Delta + a \Delta^T A \Delta.$$

$$\Delta^T A x + x^T A \Delta$$

$$\Delta^T (A x + A^T x).$$

$$\nabla f(x) = A x + A^T x$$

all elements.

$$f(x) = \|x\|_2^2 = \sum_{i=1}^{d} x_i^2$$

$$\frac{\partial f}{\partial x_i} = \frac{\partial}{\partial x_i} x_i^2 = 2x_i$$

$$\nabla f(x) = 2x. \qquad f(x+\alpha\Delta) = (x+\alpha\Delta)^T (x+\alpha\Delta)$$

Euclidean norm

L_1 Norm.

$$f(x) = \|x\|_1 = \sum_{i=1}^{d} |x_i|$$

$$\frac{\partial f}{\partial x_i} = \frac{\partial}{\partial x_i} |x_i| = \text{sign}(x_i) = \frac{x_i}{|x_i|}$$

$$\nabla f(x) = \text{sign}(x).$$

- Symbolic differentiation.

write function in mathematical expression.

↓

apply chain rule, ...

↓

code.

→ Problems.

had to do it manually.

- converting code into mathe not trivial
- no guarantee → comput. structure.

why important?

differentiating f_x function.

→ Numerical differentiation.

- high-order different.
-
- error accumulating,

Problems.

- numerical imprecision.
  - ↳ number of operations increases.
- f not smooth → wrong results.
- unclear how to setup ε
- for a vector → scalar function, you have to compute each partial individually, meaning $O(d)$ blowup in cost.
- if ε too small, may get zeros or NaN

Automatic differentiation.

- Forward mode
- Reverse mode.

replace y with a tuple & a derivative

* operator overloading

Problems w/ Forward Mode AD.

- Differentiate with respect to one input
- Blow-up proportional to dimension d.

if we are computing a gradient of f:

$\mathbb{R}^d \to \mathbb{R}$.

Week 2 - 2

Aug 31

Backpropagation.

Review for Forward Mode AD.

$x \in \mathbb{R}$.

↓

$\frac{\partial y}{\partial x}$ → Store the tuple: $(y, \frac{\partial y}{\partial x})$.

* Python supports operator overloading

Reverse - Mode AD

→ fix one output l over $\mathbb{R}$.

↳ compute partial derivative $\frac{\partial l}{\partial y}$.

$(y, \nabla_y l)$.

Same shape

- Derive backprop. thru chain rule.

$l = f(u), u = g(y)$

$h = f(u_1, u_2, \dots, u_k)$, $u_i = g_i(y)$

$$\nabla_y h = \sum_{i=1}^{k} Dg_i(y)^T \nabla_{u_i} h$$

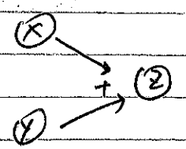
$Dg_i(y)$: derivative

is a Jacobian

compute gradient w.r.t. y.

$$\nabla_y h = \sum_{i=1}^{k} Dg_i(y)^T \nabla_{u_i} h$$

process y — process u_i

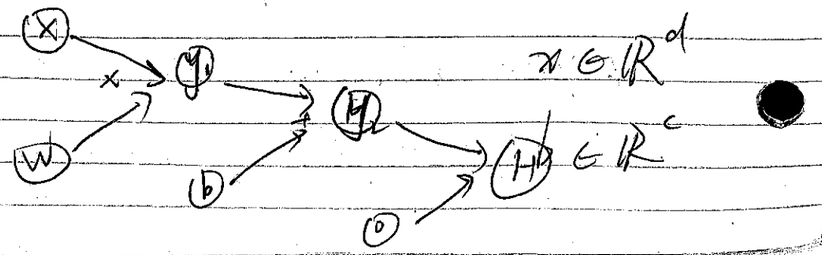


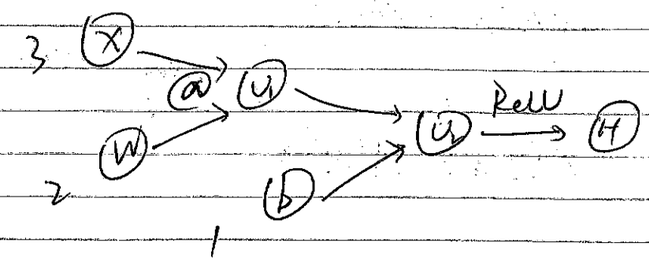
$z = x + y$

$H = \max(0, Wx + b)$. $W \in \mathbb{R}^{c \times d}$

$x \in \mathbb{R}^d$

$H \in \mathbb{R}^c$





$$\nabla_x H = \frac{\partial H}{\partial U_2} \frac{\partial U_2}{\partial g} \frac{\partial g}{\partial U_1} \frac{\partial U_1}{\partial x}$$

$H = f(U_2)$. $U_2 = g(U_1)$, $U_1 = h(x)$.

$\nabla_x H = ReLU'$

initialize

$\nabla_{U_2} H = \nabla_H H = \nabla_W H = \nabla_x H = \nabla_b H = 0$

$\nabla_{U_2} H \mathrel{+}= ReLU'(U_2) \cdot \nabla_H H = 1 \cdot 1 = 1$

Problems

1.2. Derivative of x^TAx.

b. $\Delta^TAx + x^TA\Delta$

↓ why $x^TA\Delta = (x^TA\Delta)^T$?

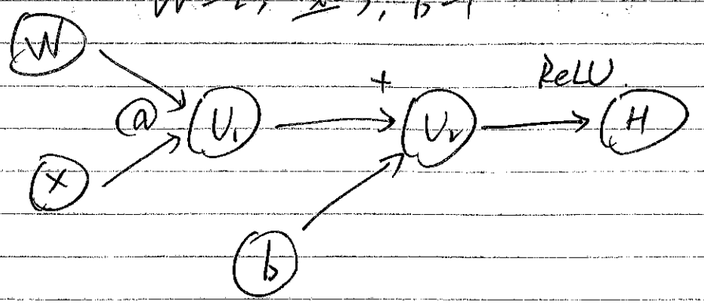
$\Delta^TAx + \Delta^TA^Tx$

d. → a Jacobian.

2.5. why sum(log) in np.

Review: Backprop.

$W=2,\ x=3,\ b=1$



Forward

- $U_1 = W * x = 2*3 = 6$
- $U_2 = U_1 + b = 7$
- $H = ReLU(U_2) = ReLU(Wx+b) = ReLU(7)$

- $\nabla_H H = 1$
- initialize: $\nabla_{U_2} H = \nabla_{U_1} H = \nabla_W H$
  $= \nabla_x H = \nabla_b H = 0$
- $\nabla_{U_2} H \mathrel{+}= ReLU'(U_2)\nabla_H H = 1*1 = 1$
- $\nabla_{U_1} H \mathrel{+}= \nabla_{U_2} H = 1$
- $\nabla_b H \mathrel{+}= \nabla_{U_2} H = 1$
- $\nabla_W H \mathrel{+}= x \nabla_{U_1} H = 3*1 = 3$

- $\nabla_x H += W \nabla_{v_1} H = 2 * 1 = 2$

$F(x) \rightarrow DF(x)$

$\Delta \mapsto$

Λ^{-1}

Labor day.

Week 3 - $\frac{1}{2}$.

Machine learning systems

$f : U \mapsto V$

$Df(x) \quad \mathcal{L}(U, V)$

$f : \mathbb{R}^m \to \mathbb{R}^n$.

$Df(x) \in \mathcal{L}(\mathbb{R}^m, \mathbb{R}^n)$.

$\mathbb{R}^{m \times n}$

If $F(x) = x^2$.

$\lim_{\alpha \to 0} \frac{F(x+\alpha\Delta) - F(x)}{\alpha}$.

$A \in \mathbb{R}^{n \times n}$.

$\lim_{\alpha \to 0} \frac{x^2 + \alpha\Delta x + \alpha x \Delta + \alpha^2\Delta^2 - x^2}{\alpha}$.

$= A x + x \Delta$

$DF(x) = (\Delta \mapsto \Delta x + x \Delta)$

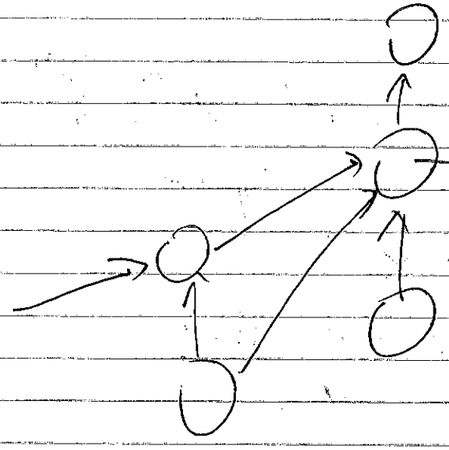
or $(DF(x))(\Delta) = \Delta x + x \Delta$

Why Backprop.

gradient has ↓ output l.

backprop manifest gradient

$\nabla_y l$ for intermediates y.



class / object

↓

knows how

to compute itself

↓

knows its dependencies

+

```
def __add__(self, another):
```

two ways:

(lazy)

EAGER v.s. GRAPH only later

compute immediately — do/can compute, but know the dependencies

Eager

↓ cutoff

↓ error

- take storage

- debugging & development (X).

- if / branch / control flow (✓).

immutabelized

↑

Graph.

- first computation.
- simplification (transform. ✓)
- reuse the graph. (✓)
- good for caching (?).
- memory locality (✓).

- less python overhead (✓)

* Deployment.

↓

convert it into some form that "isn't python"

- optimization

TF —Default→ Graph

PT ⟶ Eager

ML framework.

- numerical linear algebra library.
- hardware accelerator support.
- backprop engine. (gradient auto).
- library for writing Deep Nets.

PyTorch & TensorFlow

MxNet Jax. Flux (Julia)
(C++)

Caffe (ancient) → 1st GPU acc.

```
model = torch.nn.Sequential(
    nn.Linear( ... )
    nn.Linear( ... )
)
```

hardware - accelerator.

```
X. to ("cuda")
X. to ("cpu")
Y. to ("cpu")
Z = X + Y.
```

throw an exception when two diff devs or diff hardwares.

Programming Assignment #1.

def get_next_order
    return to a "+1" order

def to_backprop
    convert array to backprop

* class Backprop Array.

def __init__ (np array).

def __repr__ ( )
    ↦ String.

(1.1)

def all_dependencies( )
    find all the dependencies

use graph search alg.

(1.2)

def backward( )
    backward ⟹ find gradients

Start from the dependencies reverse mode

def grad_fn( )

"Define math operators in backprop"

def add
    → BA_Add( )

def sub
    → BA_Sub( )

def mul
    → BA_Mul( )

def truediv
    → BA_Div( )

def sum ( )
    → BA_Sum( ).

def reshape ( )
    → BA_Reshape( )

def transpose ( )
    → BA_Transpose( )

Different classes

Doesn't matter what tensor operation for (2.2)

Tensor operation

(2.1)

(2.3)

Compare "grad"

implement for scalar-arrays.

(1.3)

compare ad, nd, sd

(1.5)

global funs.

- def numerical_diff( ).
- def numerical_grad( ).
- def backprop_diff( ).

(2.3) (2.4) (2.5) (2.6)

Store test functions in a class:

class TestFxs( ):

def {f1, df1dx, f2, ...}

test implementation: TestFxs.df3dx (1.4)

wish'd input

if __name__ = "__main__":

scalar output

write the script to execute main functions.

for #3:

$$\lim_{\alpha \to 0} \frac{\log(x+\alpha\Delta) - \log(x)}{\alpha} = D(f(x))\Delta$$

$$\frac{\exp(x+\alpha\Delta) - \exp(x)}{\alpha}$$

$$= \frac{\exp(x)\cdot\exp(\alpha\Delta) - \exp(x)}{\alpha}$$

$$= \frac{\exp(x)(\exp(\alpha\Delta) - \exp(0))}{\alpha \cdot \exp(0)}$$

$$=$$

Week 4 - Lecture 7.

GD

we compute gradient in large-scale opt. problem to solve learning task

Examples will most be on supervised learning. but not limited to ...

in SL : $f(w) = \frac{1}{n} \sum_{x,y \in D} \ell(h_w(x), y)$.

$= \frac{1}{n} \sum_{x \in D} f(w; x)$

n: size of dataset.

in framework, we strive to:

Minimize $f(w)$ over $w \in \mathbb{R}^d$.

computing f takes $O(n)$ time.

Init $w_0 = 0$ (not nec. $= 0$.)

$w_{t+1} = w_t - \alpha \nabla f(w_t)$.

↳ gradient descent.

gradient.

★ How much time does it cost?

→ $O(ndk)$.

★ How much memory required?

→ $O(nd)$ or $O(d)$

↓

• parallel way

running backprop thru whole thg.

in a NAIVE way → $O(nd)$.

Newton's Method

$w_{t+1} = w_t - [\nabla^2 f(w_t)]^{-1} \nabla f(w_t)$

↳ converges faster.

"BUT" more expensive that GD

So, ★ How much time? & ★ How m. mem?

store Hessian matrix.

→ $O(nd^2k)$. → $O(d^2)$

(Q) scared away from Newton's method cuz the large memory required, i.e. quadratic GD.

✡ why are we confident that GD will converge?.

the value of gradient as compared based on particular weight, if move a lil' bit, it will drastically change grad.

we want to make it a bust.

How close GD is?

→ bound. Derivative.

↳ second-order D. is also Bd.

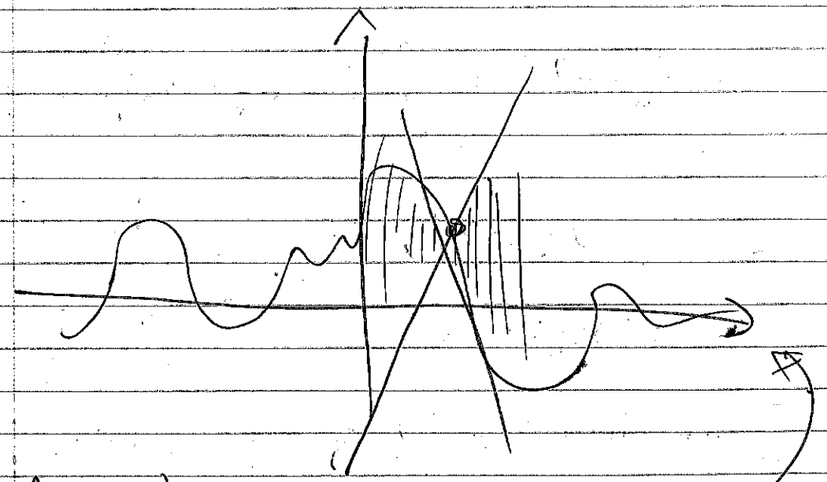
Gradient ∇f is L- Lipshitz continuous

$$\|\nabla f(u) - \nabla f(v)\|_2 \le L\|u-v\|_2$$

Assume $\exists f$ s.t. $f(w) \ge f^*$.

$\forall w, \forall u, \|u\|=1$.

$$\left\| \frac{\partial^2}{\partial \alpha^2} f(w+\alpha u) \right\| \le L.$$



~~AAA~~ Lipshitz continuous

↳ L- smooth.

How to prove GD converges ???

$$f(w_{t+1}) = f(w_t - \alpha \nabla f(w_t))$$

fundamental thm. of calc.

$$= f(w_t) + \int_0^\alpha \frac{\partial}{\partial \eta} f(w_t - \eta \nabla f(w_t))\, d\eta$$

$$f(b) - f(a) = \int_a^b \frac{\partial}{\partial x} f(x)\, dx.$$

$$= f(w_t) + \int_0^\alpha \left(-\nabla f(w_t)\right)^T \nabla f(w_t - \eta \nabla f(w_t))\, d\eta.$$

how? → close to grad.

↳ imagine = 0.

Let $h(\eta) = f(w_t - \eta \nabla f(w_t))$

$$h(\alpha) = h(0) + \int_0^\alpha h'(\eta)\, d\eta$$

Expect η to be small ← expect α small

$$\frac{\partial}{\partial \eta} f(w_t - \eta \nabla f(w_t))$$

$$= \lim_{\delta \to 0} \frac{f(w_t - (\eta+\delta)\nabla f(w_t)) - f(w_t - \eta \nabla f(w_t))}{\delta}$$

$$= \lim_{\delta \to 0} \frac{f(w_t - \eta \nabla f(w_t) - \delta \nabla f(w_t)) - f(w_t - \eta \nabla f(w_t))}{\delta}.$$

$$= \lim_{\delta \to 0} \frac{f(\hat{w} + \delta(-\nabla f(w_t))) - f(\hat{w})}{\delta}$$

$$= -(\nabla f(w_t))^T \nabla f(\hat{w}).$$

⇒ close to norm. → always positive ⇒ gd works to min.

→ cont.

$$= f(w_t) + \int_0^{\alpha} (-\nabla f(w_t)^T \nabla f(w_t))\, d\eta$$

$$+ \int_0^{\alpha} (-\nabla f(w_t))^T (\nabla f(w_t - \eta \nabla f(w_t)) - \nabla f(w_t))\, d\eta.$$

Apply Cau. theorem:

$$A \cdot B \leq \|A\| \|B\|$$

$$\{ \|AB\|, \}$$

$$\leq f(w_t) + \int_0^{\alpha} (-\nabla f(w_t)^T \nabla f(w_t))\, d\eta$$

$$+ \int_0^{\alpha} \|-\nabla f(w_t)\| \, \|\nabla f(w_t - \eta \nabla f(w_t)) - \nabla f(w_t)\|\, d\eta.$$

$$\leq f(w_t) + \int_0^{\alpha} -\|\nabla f(w_t)\|^2 \, d\eta$$

$$\frac{\alpha^2}{2} = \int_0^{\alpha} \eta \, d\eta$$

$$+ \int_0^{\alpha} \|-\nabla f(w_t)\| \cdot L \cdot \|\eta \nabla f(w_t)\|\, d\eta$$

$$\Rightarrow f(w_t) \leq f(w_t) - \alpha \|\nabla f(w_t)\|^2 + \frac{\alpha^2 L}{2} \|\nabla f(w_t)\|^2$$

$$\leq f(w_t) - \alpha\left(1 - \frac{\alpha L}{2}\right) \|\nabla f(w_t)\|^2$$

$\Rightarrow$ How does constant L effect how we learn tasks in scales

$\downarrow$

that's why

Assume: $\alpha L < 1$.

$$\leq f(w_t) - \frac{\alpha}{2} \|\nabla f(w_t)\|^2$$

$$\frac{\alpha}{2}\|\nabla f(w_t)\|^2 \le f(w_t) - f(w_{t+1})$$

↳ Single iteration of GD.

$$\frac{\alpha}{2}\sum_{t=0}^{k}\|\nabla f(w_t)\|^2 \le \sum_{t=0}^{k-1}\left(f(w_t) - f(w_{t+1})\right)$$

↳ k iterations $< f(w_0) - f(w_k)$.

$$\frac{\alpha}{2}\sum_{t=0}^{k-1}\|\nabla f(w_t)\|^2 \le f(w_0) - f(w_t)$$

assume f is bounded from below. ★★★

$$= \le f(w_0) - f^*.$$

$$\frac{\alpha}{2}k \min_{t\in\{0,\dots,k-1\}}\|\nabla f(w_t)\|^2 \le f(w_0) - f(w_t)$$

$$\min_{t\in\{0,\dots,k-1\}}\|\nabla f(w_t)\|^2 \le \frac{2f(w_0) - f^*)}{\alpha k}.$$

↳ require $\alpha k \le 1$.

LHS: run to iteration of GD

return the optimal weights.

RHS upper bound of func.

Step size α → to be large as possible to $\frac{1}{\alpha}$ → small

the largest step

↳ $\le \frac{2(f(w_0) - f^*)}{k}$.

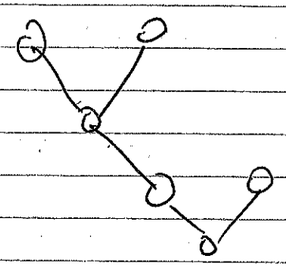
GD only find local opt.

OH (Sep. 13)

(1.1)

- Breadth-first search ?

what are the dependencies



(1.2)

what is the utility of the grad-fn

why zero out ".grad" ?

(1.3)

1.3.4. — why ?

(2)

generally, how write the help function to manipulate the dimensions ?

(2.5) numerical-grad. — hints ?

(2.7).

$\mathbb{R}^d \longrightarrow \mathbb{R}$

confused on the implementation.

② writing a for loop.

while the len

① add empty row / cols. for extra dim. → new axis.

check the dims are targeting the same

⇒ broadcasting.

A: 1 x 6 x 5

↕

B: (1) x 1 x 2

→ iterating over the axis.

1: adding 1.

2: repeating axis (iterating)

helper_fns

BA - And

just recall += helper(a, b)

Lecture 8 . . (Wk. 4).

HW Review:

$\nabla_{\underline{x}} \ell$ has same shape as $\underline{X}$

$\underline{X}$.grad.shape = $\underline{X}$.data.shape.

* "+=" in numpy mutates the vector

self.x.grad += stuff

self.x.grad = self.x.grad + stuff.

* init both as arrays as all zeros

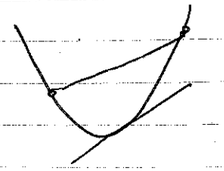
GD continued.

... last time.

$w_{t+1} = w_t - \alpha \nabla f(w_t)$

→ most simple condition - convexity

0th-order convexity



$f((1-\alpha)x + \alpha y) \leq (1-\alpha) f(x) + \alpha f(y)$

for $\alpha \in [0, 1]$

▽ 1st order def. — considering whether func. conv.

$$f(x) + (y-x)^T \nabla f(x) \leq f(y)$$

▽ 2nd order def.

$$\frac{\partial^2}{\partial \alpha^2} f(x + \alpha u) \geq 0 \quad \text{for any } \alpha, u \in \mathbb{R}^d$$

"parabola has a const. sec. deriv."

- Convex has a unique global optimum.

"that's why we care 'bout conv"

Strongly convex function

"a function that can be bounded from below"

μ- strongly convex function.

(scalar positive num.)

$$\frac{\partial^2}{\partial \alpha^2} f(x + \alpha u) \geq \mu \quad (\text{for } \|u\| = 1)$$

e.g. "Strongly convex".

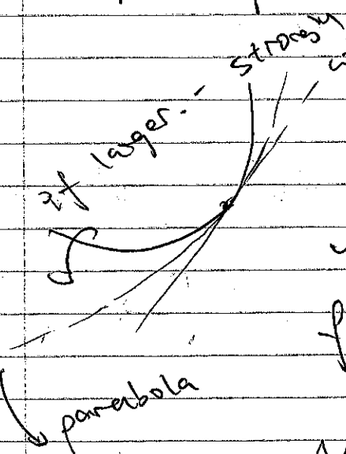
$f(x) = \max(x, 0)$

Convexity: vector space ↦ real num.
i.e. scalar.

Strictly convex vs. Strongly convex

e.g. $f(x) = e^x$ ↳ but not larger than a positive val.

$$f(y) \geq f(x) + (y-x)^T \nabla f(x) + \frac{\mu}{2}\|y-x\|^2$$



f is μ-strongly convex, iff $\exists g$ s.t.

$$f(w) = g(w) + \frac{\mu}{2}\|w\|^2$$

& g is convex.

☆☆☆

Use in a lot of analysis.

Polyak-Łojasiewicz (PL)

... TBC

$$\|\nabla f(w)\|^2 \geq 2\mu \underbrace{(f(w) - f^*)}_{\text{min val.}}$$

Strongly convex.

but does not imply strongly convex

e.g. $f(w) = \frac{\mu}{2}\|w\|^2$.

$\nabla f(w) = \mu w$

$\|\nabla f(w)\|^2 = \|\mu w\|^2 = \mu^2 \|w\|^2$

$= 2\mu \left(\frac{\mu}{2}\|w\|^2\right) = 2\mu (f(w) - f^*)$

☆ the gradient is only close to zero when its only around global optimum.

satisfies PL yet not strongly cv.

$f(w_{t+1}) = f(w_t - \alpha \nabla f(w_t))$

$\leq f(w_t) - \alpha\left(1 - \frac{\alpha L}{2}\right)\|\nabla f(w_t)\|^2$

non-convex of gd.

$\leq f(w_t) - 2\mu\alpha\left(1 - \frac{\alpha L}{2}\right)(f(w_t) - f^*)$

$f(w_{t+1}) - f^* \leq (f(w_t) - f^*) - 2\mu\alpha\left(1 - \frac{\alpha L}{2}\right)(f(w_t) - f^*)$

$= \left(1 - \underbrace{2\mu\alpha\left(1 - \frac{\alpha L}{2}\right)}_{\text{call it } \gamma}\right)(f(w_t) - f^*)$

$\leq \gamma (f(w_t) - f^*)$ ← min, ↳ min is γ

$f(w_k) - f^* \leq \gamma^k (f(w_0) - f^*)$ if $\gamma > 0$.

☆ How should we chose α? ↳ to show $1 - \frac{\mu}{L}$ is min

$$2\mu\alpha - \frac{2\mu\alpha^2 L}{2} \to 0$$

$$1 - \alpha L = 0$$

$$\alpha L = 1$$

$$\alpha = \frac{1}{L}.$$

we got $\gamma = 1 - L\mu\frac{1}{L}\left(1 - \frac{\frac{1}{L}L}{2}\right) = 1 - \frac{\mu}{2}$

$$f(w_k) - f^* \leq \left(1 - \frac{\mu}{L}\right)^k \left(f(w_0) - f^*\right)$$

$$\leq \exp\left(-\frac{\mu k}{L}\right) \cdot \left(f(w_0) - f^*\right)$$

convergence @ a linear rate

even tho is decreasing exponentially

converges with errors a num. of digits.

going to be linear wrt. ...

"roughly linear with digits not. sense".

Goal: output $\hat{w}$ with

$f(\hat{w}) - f^* \in \Sigma \mapsto$ Error tol.

$(\varepsilon \in \mathbb{R},\ \varepsilon > 0)$.

It suffices to run T iterations of (num timestep)

GD, s.t.

$$\exp\left(-\frac{\mu}{L}T\right)\left(f(w_0) - f^*\right) \leq \varepsilon.$$

we can solve this for T

$$\exp\left(\frac{\mu}{L}T\right) \geq \frac{f(w_0) - f^*}{\varepsilon}$$

$$\frac{\mu}{L}T \geq \log\left(\frac{f(w_0) - f^*}{\varepsilon}\right)$$

$$T \geq \frac{L}{\mu}\log\left(\frac{f(w_0) - f^*}{\varepsilon}\right)$$

hessian for sc. pos. def symm.

ratio of largest eigen val of hessian / the smallest val.

$\frac{L}{\mu} = K$ "condition number".

$\|\nabla f(x) - \nabla f(y)\| \le L\|x-y\|$

$\left|\frac{\partial^2}{\partial \alpha^2} f(x+\alpha u)\right| \le L$

(for $\|u\| = 1$)

eqly. $-L I \le H f(x) \le L I$

$\nabla^2 f$

L large → lot of steps

L small → a few steps.

$L \gg 1 \hookrightarrow k = 1$ isotropic quadratic

Condition number ∝ num. of steps

— to solve the opt. problem.

the other thing impact time of GD.

→ size of dataset.

↓

Stochastic GD ← GD goes bad when DS are large.

↓

Subsampling + approx.

↓

Principle #2 of LS ML.

Spoiler: SGD faster than GD.

GD # steps. $\sim \vartheta(K)$.

SGD # time steps. $\sim \vartheta(nK)$

GD

Lecture 7

Week 3.

GD time

Subscription

$O(nk)\ \log\left(\frac{1}{\varepsilon}\right)$

Num. of iterations of GD.

size

training set

$f(w) = \frac{1}{n}\sum_{i=1}^{n} f_i(w)$.

$$\text{GD}\begin{cases} w_{t+1} = w_t - \alpha \nabla f(w_t) \\ = w_t - \frac{\alpha}{n}\sum_{i=1}^{n} \nabla f_i(w_t) \end{cases}$$

SGD: sample a random $i \in \{1, \dots, n\}$.

$w_{t+1} = w_t - \alpha \nabla f_i(w_t)$.

mini-batch SGD: sampling B

$w_{t+1} = w_t - \frac{\alpha}{|B|}\sum_{b=1}^{B} \nabla f_{i_b}(w_t)$

batch size

sample i_b uniformly from $\{1, \dots, n\}$ for each $b \in \{1, \dots, B\}$

Stochastic GD (mini-batch)

$$\mathbb{E}\left[w_{t+1} \mid w_t\right] = w_t - \alpha \nabla f(w_t)$$

$$\mathbb{E}\left[\nabla f_i(w_t) \mid w_t\right] = \sum_{j=1}^{n} P(i=j) \nabla f_j(w_t)$$

$$= \sum_{j=1}^{n} \frac{1}{n} \nabla f_j(w_t).$$

$$= \nabla f(w_t).$$

Assume $\exists L > 0$ s.t.

$$\|\nabla f(w) - \nabla f(v)\| \le L\|w - v\|$$

Assume. $f(w) \ge f^*$

let g_t denote $\frac{1}{B}\sum_{b=1}^{B} \nabla f_{i_b}(w_t) - g_t$

$f(w_{t+1}) = f(w_t - \alpha g_t) = f(w_t) + \int_0^{\alpha} \frac{\partial}{\partial \eta} f(w_t - \eta g_t)\, d\eta = f(w_t) + \int_0^{\alpha} \nabla f(w_t - \eta g_t)(-g_t)\, d\eta$

fwd loss function

$$= f(w_t) - \alpha \nabla f(w_t)^T q_t + \int_0^\alpha (\nabla f(w_t - \eta q_t) - \nabla f(w_t))^T (-q_t)\, d\eta$$

$$\leq f(w_t) - \alpha \nabla f(w_t)^T q_t + \int_0^\alpha \|\nabla f(w_t - \eta q_t) - \nabla f(w_t)\| \, \|q_t\| \, d\eta$$

$$\leq f(w_t) - \alpha \nabla f(w_t)^T q_t + \int_0^\alpha L \eta \|q_t\| \|q_t\| \, d\eta$$

$$\leq f(w_t) - \alpha \nabla f(w_t)^T q_t + \frac{\alpha^2 L}{2} \|q_t\|^2$$

full-batch grad

$$f(w_{t+1}) \leq f(w_t) - \alpha \nabla f(w_t)^T q_t + \frac{\alpha^2 L}{2} \|q_t\|^2$$

$\nabla f(w_t)$ ← Stochastic grad.

$$\mathbb{E}[f(w_{t+1}) | w_t] \leq f(w_t) - \alpha \nabla f(w_t)^T \mathbb{E}[q_t | w_t] + \frac{\alpha^2 L}{2} \mathbb{E}[\|q_t\|^2 | w_t]$$

$$\leq f(w_t) - \alpha_t \nabla f(w_t)^T \nabla f(w_t) + \frac{\alpha^2 L}{2} \mathbb{E}[\|q_t\|^2 | w_t]$$

$$\leq f(w_t) - \alpha \|\nabla f(w_t)\|^2 + \frac{\alpha^2 L}{2} \mathbb{E}[\|q_t\|^2 | w_t]$$

New Assumption (uniform over w_t)

$$\frac{1}{n} \sum_{i=1}^n \|\nabla f_i(w_t) - \nabla f(w_t)\|^2 \leq \sigma^2$$

for any $w \in \mathbb{R}^d$.

$$\mathbb{E}[\|q_t\|^2 | w_t] = \mathbb{E}\left[\left\| \frac{1}{B} \sum_{b=1}^B \nabla f_{i_b}(w_t) \right\|^2 | w_t\right]$$

$$= \mathbb{E}\left[\left(\frac{1}{B} \sum_{b=1}^B \nabla f_{i_b}(w_t)\right)^T \left(\frac{1}{B} \sum_{c=1}^B \nabla f_{i_c}(w_t)\right) \middle| w_t\right]$$

$$= \frac{1}{B^2} \sum_{b=1}^B \sum_{c=1}^B \mathbb{E}[\nabla f_{i_b}(w_t)^T \nabla f_{i_c}(w_t) | w_t]$$

$\mathbb{E}[\ ]$ → samples that $b \neq c$; independent of each other → $b \neq c$

$$= \frac{1}{B^2}(B^2 - B) \|\nabla f(w_t)\|^2 + \frac{1}{B^2} \sum_{b=1}^B \mathbb{E}[\|\nabla f_{i_b}(w_t)\|^2 | w_t]$$

same

$$= \frac{B-1}{B} \|\nabla f(w_t)\|^2 + \frac{1}{B n} \sum_{i=1}^{n} \|\nabla f_i(w_t)\|^2$$

Recall the assumption:

$$\frac{1}{n}\sum_{i=1}^{n} \|\nabla f_i(w_t)\|^2 - \frac{2}{n}\sum_{i=1}^{n} \nabla f_i(w)^T \nabla f(w) + \frac{1}{n}\sum_{i=1}^{n} \|\nabla f(w)\|^2 \le \sigma^2$$

$$-2\|\nabla f(w)\|^2$$

Easy to bound $\|\nabla f(w)\|^2$.

$$\frac{1}{n}\sum_{i=1}^{n} \|\nabla f_i(w)\|^2 - \|\nabla f(w)\|^2 \le \sigma^2$$

$$\le \frac{B-1}{B}\|f(w_t)\|^2 + \frac{1}{B}\left(\sigma^2 + \|\nabla f(w)\|^2\right)$$

$$= \|\nabla f(w_t)\|^2 + \frac{\sigma^2}{B}$$

Coming back to 3rd assumption

$$\mathbb{E}\left[f(w_{t+1}) \mid w_t\right] \le f(w_t) - \alpha \|\nabla f(w_t)\|^2 + \frac{\alpha^2 L}{2}\|\nabla f(w_t)\|^2 + \frac{\alpha^2 \sigma^2 L}{2B}$$

Variance of the square error of SGD

$\mathbb{E}[Y] = \mathbb{E}[\mathbb{E}[Y|X]]$

Also assume: $\|\nabla f(w)\|^2 \ge 2\mu(f(w) - f^*)$

PL condition

$$\le f(w_t) - \alpha\left(1 - \frac{\alpha L}{2}\right) 2\mu (f(w_t) - f^*) + \frac{\alpha^2 \sigma^2 L}{2B}$$

$$\mathbb{E}\left[f(w_{t+1}) - f^* \mid w_t\right] \le \left(1 - \alpha\left(1 - \frac{\alpha L}{2}\right)2\mu\right)(f(w_t) - f^*) + \frac{\alpha^2 \sigma^2 L}{2B}$$

SGD additional "noise" term.

$$\Leftarrow \rho_t = \mathbb{E}\left[f(w_t) - f^*\right]$$

$$\rho_{t+1} \le \left(1 - \alpha\left(1 - \frac{\alpha L}{2}\right)2\mu\right)\rho_t + \frac{\alpha^2 \sigma^2 L}{2B}$$

$\Rightarrow$ Assume $\alpha L \le 1$.

$$\le (1 - \alpha\mu)\rho_t + \frac{\alpha^2 \sigma^2 L}{2B}$$

$$\rho_\alpha = (1-\alpha/\mu)\rho_\alpha + \frac{\alpha^2\sigma^2 L}{2B}$$

$$\alpha/\mu \rho_\alpha = \frac{\alpha\sigma^2 L}{2B}$$

$$\rho_\alpha = \frac{\alpha\sigma^2 L}{2\mu B} = \frac{\alpha\sigma^2 K}{2B}$$

$$\rho_{t+1} - \frac{\alpha\sigma^2 L}{2\mu B} \le (1-\alpha/\mu)\rho_t - \frac{\alpha\sigma^2 L}{2\mu B}$$

$$+ \frac{\alpha^2\sigma^2 L}{2B}$$

$$\le (1-\alpha/\mu)\left(\rho_t - \frac{\alpha\sigma^2 L}{2\mu B}\right)$$

$$\rho_T - \frac{\alpha\sigma^2 L}{2\mu B} \le (1-\alpha/\mu)^T \left(\rho_0 - \frac{\alpha\sigma^2 L}{2\mu B}\right)$$

Step:

$$\le (1-\alpha/\mu)^T \rho_0$$

$$\mathbb{E}[f(w_T) - f^*] \le (1-\alpha/\mu)^T (f(w_0) - f^*)$$

$$+ \frac{\alpha^2\sigma^2 L}{2\mu B} \rightarrow \text{noise wall / noise floor}$$

$$\Rightarrow 1 - x \le \exp(-x) \quad (\text{plug in})$$

$$\text{LHS} \le \exp(-\alpha\mu T)(f(w_0) - f^*) + \frac{\alpha\sigma^2 L}{2\mu B}$$

Lecture 9. Week 5 - 2.

Rev - Last time.

$$\mathbb{E}[f(w_t) - f^*] \le \exp(-\alpha\mu T)(f(w_0) - f^*) + \frac{\alpha L \sigma^2}{2B\mu}.$$

Goal: $\mathbb{E}[f(w_{out}) - f^*] \le \varepsilon$.

suffice for $\varepsilon \ge \exp(-\alpha\mu T)(f(w_0)-f^*) + \frac{\alpha L\sigma^2}{2B\mu}$.

also suffice $\frac{\varepsilon}{2} \ge \exp(-\alpha\mu T)(f(w_0)-f^*)$

and $\frac{\varepsilon}{2} \ge \frac{\alpha L\sigma^2}{2B\mu}$.

$$\Rightarrow \alpha \le \frac{B\mu\varepsilon}{L\sigma^2}.$$

$$\log\left(\frac{\varepsilon}{2(f(w)-f^*)}\right) \ge -\alpha\mu T.$$

$$\Rightarrow T \ge \frac{1}{\alpha\mu}\cdot\log\left(\frac{2(f(w_0)-f^*)}{\varepsilon}\right)$$

also $\alpha L \le 1$.

$$\alpha \le \min\left(\frac{B\mu\varepsilon}{\sigma^2}, 1\right)\cdot\frac{1}{L}$$

$$T \ge \max\left(\frac{\sigma^2}{B\mu\varepsilon}, 1\right)\frac{L}{\mu}\log\left(\cdots \frac{2(f(w_0)-f^*)}{\varepsilon}\right)$$

$$\ge \max\left(\frac{\sigma^2}{B\mu\varepsilon}, 1\right)\cdot K\cdot\log(\cdots)$$

(runtime of SGD): $\mathcal{O}\left(\max\left(\frac{\sigma^2}{B\mu\varepsilon}, 1\right)\right)\cdot K\cdot\log\left(\frac{1}{\varepsilon}\right)$

usually, ε are small

$\tilde{\Theta}\left(\frac{\sigma^2}{B\mu\varepsilon}K\right)$ → batch B cancels

↳ ignoring "log" term.

runtime of GD. $\mathcal{O}(nK\log(\frac{1}{\varepsilon}))$

for GD $n \longrightarrow \frac{\nabla^2}{B\varepsilon}$.

GD	SGD
• convex (strongly).	• non-convex
• Global opt. guaranteed (unique).	• multi-objective
• large memory. (GPU). parallel	• huge dataset • huge n $\varepsilon \rightarrow$ large "noisy" or not too small
• really small ε	
• large ∇^2	

How to set batch size B

⇓

★ Hardware consideration.

eg. $f_i(w) = \frac{1}{2}(x_i^T w - y_i)^2$.

$\nabla f_i(w) = x_i(x_i^T w - y_i)$ → dot, axpy

minibatch $X \in \mathbb{R}^{B\times d}$. $y \in \mathbb{R}^B$

$\nabla f_{batch}(w) = \frac{1}{B} X^T (Xw - Y)$

mmpy $(B,d)\,@\,(d,1)$,

faster

$(d,B)\,@\,(B,1)$

$(1024,1024)\,@\,(1024,1024)$ a lot less than $1024\times$

$(1024,1024)\,@\,(1024,1)$

minibatch size ∝ hardware itself

e.g. $B = 256, 64, \ldots$

SGD → GD: sampling w/o replacement.

$\max(n, 1)$ → is GD scenario

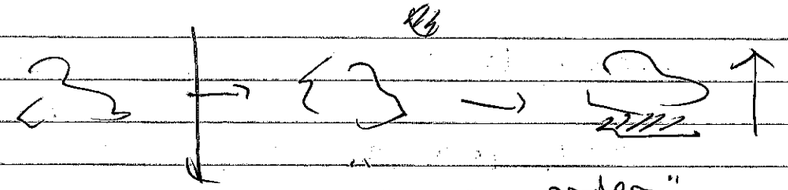
larger, slower

Random reshuffling

sample w/o repl., only reuse example after every example has been used.

epoch ⇒ 1 past thru the training set (e.g. 100 ~ 200).

Shuffle-once



Statistically not -

use a fixed step size.

Diminishing step size (assuming $\alpha_t L \le 1$)

$$\mathbb{E}[f(w_{t+1}) - f^*] \le (1 - \alpha_t \mu)\,\mathbb{E}[f(w_t) - f^*] + \frac{\alpha_t^2 \sigma^2 L}{2B}$$

$$\rho_{t+1} \le (1 - \alpha_t \mu)\rho_t + \frac{\alpha_t^2 \sigma^2 L}{2B}$$

$$\Rightarrow 0 = -\mu \rho_t + \frac{\alpha_t \sigma^2 L}{B}$$

$$\Rightarrow \alpha_t \triangleq \frac{\rho_t \mu B}{\sigma^2 L}$$

$$\rho_{t+1} \le \rho_t - \frac{\mu^2 B}{2\sigma^2 L}\rho_t^2$$

$$\frac{1}{\rho_{t+1}} \ge \frac{1}{\rho_t - \frac{\mu^2 B}{2\sigma^2 L}\rho_t^2} \quad (\text{let } \rho_t)$$

$$= \frac{1}{\rho_t}\left(1 - \frac{\mu^2 B}{2\sigma^2 L}\rho_t\right)^{-1}$$

$$\ge \frac{1}{\rho_t}\left(1 + \frac{\mu^2 B}{2\sigma^2 L}\rho_t\right) = \frac{1}{\rho_t} + \frac{\mu^2 B}{2\sigma^2 L}$$

$$\Rightarrow \frac{1}{\rho_T} \ge \frac{1}{\rho_0} + \frac{\mu^2 B T}{2\sigma^2 L} \Rightarrow \rho_T = \mathbb{E}[f(w_T) - f^*]$$

$$\leq \left(\frac{1}{f(w_0) - f^*} + \frac{\mu^2 BT}{2\sigma^2 L} \right)^{-1}$$

$$= \vartheta^2 \left(\frac{1}{T} \right)$$

$$\simeq \vartheta \left(\frac{\sigma^2 K}{\mu BT} \right)$$

Lecture 11 Week 6.

Momentum.

Rev: $K \sim \frac{L}{\mu}$; grad. noise $\propto \left(\frac{\sigma^2}{\mu} \right)$

Announcement: • Pset 3
• PA 2.

Rev: GD.

$$\ell \to f(w_T) - f^* \leq \exp\left(-\frac{T}{K} \right) (f(w_0) - f^*)$$

gap after T epochs

Q. Simplest model with large K?

a 2D problem → Quadratic

e.g. $f(w) = \frac{1}{2}(w_1^2 L + w_2^2 \mu)$

$$= \frac{1}{2} w^T \begin{bmatrix} L & 0 \\ 0 & \mu \end{bmatrix} w$$

$\nabla^2 f(w)$

$\Rightarrow H(w) = \begin{bmatrix} L & 0 \\ 0 & \mu \end{bmatrix}$ Suppose $L > \mu > 0$

$$\nabla f(w) = \begin{bmatrix} L & 0 \\ 0 & \mu \end{bmatrix} w$$

$$w_{t+1} = w_t - \alpha \nabla f(w_t)$$

$$= w_t - \alpha \begin{bmatrix} L & 0 \\ 0 & \mu \end{bmatrix} w_t$$

$$= \begin{pmatrix} 1-\alpha L & 0 \\ 0 & 1-\alpha\mu \end{pmatrix} w_t$$

power "T"

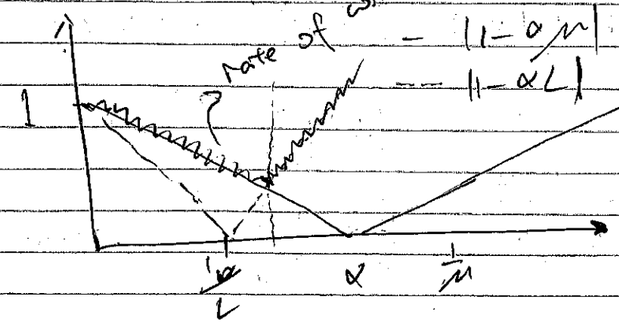
$$\Rightarrow w_T = \begin{bmatrix} 1-\alpha L & 0 \\ 0 & 1-\alpha\mu \end{bmatrix}^T w_0$$

$$= w_T - \begin{bmatrix} (1-\alpha L)^T & 0 \\ 0 & (1-\alpha\mu)^T \end{bmatrix} w_0$$

$$f(w_T) = \frac{1}{2}\left(L(1-\alpha L)^{2T} (w_0)_1^2 + \mu(1-\alpha\mu)^{2T} (w_0)_2^2 \right)$$

rate of convergence $= |1-\alpha\mu|$

$= |1-\alpha L|$



$$\alpha = \frac{2}{L+\mu}$$

$$= \frac{1-\frac{\mu}{L}}{1+\frac{\mu}{L}} = \frac{1-\frac{\mu}{L}}{k+1}$$

$$= 1 - \frac{2}{k+1}$$

$$\Rightarrow f(w_T) = \sigma\left(\left(1-\frac{2}{k+1}\right)^{2T}\right) = \mathcal{O}\left(\exp\left(-\frac{4T}{k+1}\right)\right)$$

$$w_{t+1} = w_t - \alpha \nabla f(w_t) + \beta(w_t - w_{t-1})$$

previous step — the more step, step size too large, overshooting the object.

"Self-tune" the step size

$$w_{t+1} - w_t = \cancel{-\alpha \nabla f(w_t)}$$

$$\beta(w_t - w_{t+1}) - \alpha \nabla f(w_t)$$

we need — particle undergoes "some" force term

$0 < \beta < 1$

"friction" term

- or momentum.

How Polyak momentum applies to 2D system?

$$w_{t+1} = w_t - \alpha \underbrace{\begin{bmatrix} L & 0 \\ 0 & \mu \end{bmatrix}}_{A} w_t + \beta(w_t - w_{t-1})$$

$$\begin{bmatrix} w_{t+1} \\ w_t \end{bmatrix} = \begin{bmatrix} w_t - \alpha A w_t + \beta(w_t - w_{t-1}) \\ w_t \end{bmatrix}$$

$$= \begin{bmatrix} (1+\beta)I - \alpha A & -\beta \\ I & 0 \end{bmatrix} \begin{bmatrix} w_t \\ w_{t-1} \end{bmatrix}$$

$$\begin{bmatrix} w_{T+1} \\ w_T \end{bmatrix} = \begin{bmatrix} (1+\beta)I - \alpha A & -\beta I \\ I & 0 \end{bmatrix}^T \begin{bmatrix} w_1 \\ w_0 \end{bmatrix}$$

4×4 block matrix

$$\begin{bmatrix} (1+\beta) - \alpha L & -\alpha & -\beta & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & (1+\beta) - \alpha\lambda & -\beta \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

Eigenvalue

use χ to find eigenvalues.

$$\begin{vmatrix} (1+\beta) - \alpha\lambda - \chi & -\beta \\ 1 & 0 - \chi \end{vmatrix} \overset{(2a)}{=} \chi^2 - (1+\beta-\alpha\lambda)\chi + \beta$$

$$\chi = \frac{1+\beta-\alpha\lambda \pm \sqrt{(1+\beta-\alpha\lambda)^2 - 4\beta}}{2}$$

complex vals.

Polyak Sives:

$$\alpha = \frac{1+2\beta}{L+\mu}, \quad \sqrt{\beta} = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}$$

$$|\chi|^2 = \frac{1}{4}\left[(1+\beta-\alpha\lambda)^2 + 4\beta - (1+\beta-\alpha\lambda)^2\right]$$

$$T \approx \sqrt{\kappa} \cdot \sqrt{\beta}^T \approx \exp\left(-\frac{L}{\sqrt{\kappa}+1}T\right)$$

$$T \approx \sqrt{\kappa}$$

Works when $L(\beta \geq (1+\beta-\alpha\lambda)^2$

$$|2\sqrt{\beta}| \geq |1+\beta+\alpha\lambda|$$

$$\hookrightarrow 2\sqrt{\beta} \geq 1+\beta+\alpha\lambda \geq -2\sqrt{\beta}$$

$\mu \leq \lambda \leq L$

Lecture 11. - Week 6.

Conditioning

Rev. - momentum.

$T = \mathcal{O}\left(nK \log\left(\frac{1}{\varepsilon}\right)\right)$

$\Uparrow$

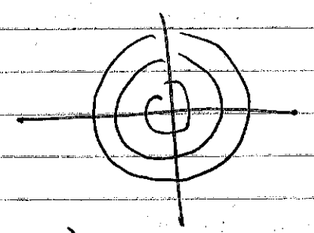
condition num.

Could be too large / too small.

but lec.

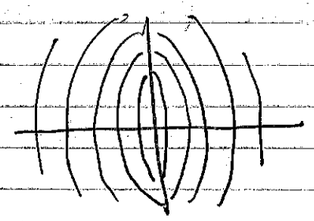
$\hookrightarrow T_{mom} = \mathcal{O}\left(\alpha \sqrt{K} \log\left(\frac{1}{\varepsilon}\right)\right)$.

$f(\omega_1, \omega_2) = \frac{1}{2}\omega_1^2 + \frac{1}{2}\omega_2^2 \quad (K=1)$



$C = \omega_1^2 + \omega_2^2$

$f(\omega_1, \omega_2) = \frac{10}{2}\omega_1^2 + \frac{1}{2}\omega_2^2$



$C = a\omega_1^2 + b\omega_2^2$

"poorly-conditioned" prob.

$w = Pu$

$\min_w f(w) = \min_u f(Pu)$

ALA. $|P| \neq 0$

↙ invertible

$\operatorname{argmin}_w f(w) = P\left(\operatorname{argmin}_u f(Pu)\right)$ ← any matrix, invertible

let $g(u) = f(Pu)$.

graphically, this is essentially "stretching" the poorly-conditioned problem, i.e. apply linear operation

⇓

map back ← reduced K

⇓

solve for optimal

preconditioning.

instead of saying minimize $f(w)$ over w — solve minimize $f(Pu)$ over u (for clever P).

e.g. $f(w) = \frac{1}{2} w^T A w$. $A^T = A$.

- how to set P?.. what cond. can we get?.. (PD, $A > 0$, all eigenval. A are positive)

$P^T A P = I$ ← symmetric.

$2f(Pu) = (Pu)^T A(Pu) = u^T P^T A P u$

$= u^T u = \|u\|^2$

suppose P symmetric, invertible

- $PAP = I$

- $P^{-1}PAPP^{-1} = P^{-1} I P^{-1}$ ← replace eigenval.

$A = P^{-2} = P = A^{-\frac{1}{2}}$

in transformed space.

$$g(w) = f(Pw) \rightarrow \nabla g(w) = P^T \nabla f(Pw)$$

$$u_{t+1} = u_t - \alpha \nabla g(u_t) = u_t - \alpha P^T \nabla f(Pu_t)$$

assume $w = Pu$; $w_t = Pu_t$

$$Pu_{t+1} = Pu_t - \alpha P P^T \nabla f(Pu_t)$$

$$w_{t+1} = w_t - \alpha P P^T \nabla f(w_t)$$

R ← Preconditioner

$$w_{t+1} = w_t - \alpha R \nabla f(w_t)$$

positive, invertible, definite, symmetric.

Preconditioned GD

$R = A^{-1}$

$$x^T R x = x^T P P^T x$$
$$= (P^T x)^T (P^T x)$$
$$= \|P^T x\|^2 > 0$$

chose R to be diagonal preconditioner

R diagonal ⟶ stretch along the coordinates' axis

memory $\mathcal{O}(d)$.

time multiply $\mathcal{O}(d)$.

$$(w_{t+1})_i = (w_t)_i - \alpha R_{ii} (\nabla f(w_t))_i$$

Let $\alpha_i = \alpha R_{ii}$.

$$(w_{t+1})_i = (w_t)_i - \alpha_i (\nabla f(w_t))_i$$

$$w_{t+1} = w_t - \alpha \odot \nabla f(w_t)$$

element-wise

- run GD in implicit scaled space.

AdaGrad

loop

$g \leftarrow \nabla f_i(w)$, random i

$r_i \leftarrow r_i + g_i^2$

$\left((r_i)_t = \sum_{k=0}^{t} (g_i^2)_t\right)$

$w_i \leftarrow w_i \oplus - \frac{\alpha}{\sqrt{r_i}} g_i \quad (\alpha_i = \frac{\alpha}{\sqrt{r_i}})$

- AdaGrad.

↳ "Adaptive Optimization" Alg.

Lecture 12. Week 7.

AdaGrad.

init $w \in \mathbb{R}^d$, $r = 0 \in \mathbb{R}^d$.

loop:

get example grad $g \in \mathbb{R}^d$

$g = \nabla f(w; x)$ minibatch etc

↑ large example

update $r \leftarrow r + g^2$

update $w \leftarrow w - \frac{\alpha}{\sqrt{r} + \varepsilon} \cdot g$

↳ small number.

- done in element-wise

implicitly.

depends too much on the history

infinite memory. ⇐

$r_i \approx \mathbb{E}[g_i^2]$

mul. num. of steps.

↳ $\approx \tau(\mathbb{E}(g_i)^2 + Var(g_i))$

could be dominant

fix this: RMSProp.

RMSProp

hyperparameters $\alpha > 0$, $\rho \in (0, 1)$, ε

init $w \in \mathbb{R}^d$, $r = 0 \in \mathbb{R}^d$

loop:

get gradient sample g at w.

update $r \leftarrow \rho r + (1-\rho) g^2$

update $w \leftarrow w - \dfrac{\alpha}{\sqrt{r} + \varepsilon} g$

$r_i \approx \mathbb{E}[g_i^2]$

typical $\rho = 0.999$

Combining momentum + RMSProp + correction for 0-init

init $w \in \mathbb{R}^d$, $r = 0 \in \mathbb{R}^d$

$s = 0 \in \mathbb{R}^d$

momentum:

$$w_{t+1} = w_t - \alpha g_t + \beta (w_t - w_{t-1})$$

$$(w_{t+1} - w_t) = \beta (w_t - w_{t-1}) - \alpha g_t$$

$$\begin{cases} v_{t+1} = \beta v_t - \alpha g_t \to \beta v_t - (1-\beta)\left[\frac{\alpha}{(1-\beta)} g_t\right] \\ w_{t+1} = w_t + v_t \end{cases}$$

α, β_1, β_2 hyperparam.

loop:

get gradient sample g @ w.

$$s \leftarrow \beta_1 s + (1-\beta_1) g$$

$$r \leftarrow \beta_2 r + (1-\beta_2) g^2$$

update:

$$w \leftarrow w - \frac{\alpha}{\sqrt{\hat{r}} + \varepsilon} \hat{s}$$

$$\hat{s} \leftarrow \frac{s}{1-\beta_1^t}$$

t = # of steps

$$\hat{r} \leftarrow \frac{r}{1-\beta_2^t}$$

if g_t denotes the g drawn at step t, $s_t = \sum_{k=0}^{t-1} \beta_1^k (1-\beta_1) g_{t-k}$

s after t steps

$$\sum_{k=0}^{t-1} \beta_1^k (1-\beta_1)$$

$$= (1-\beta_1)\left(\frac{1-\beta_1^t}{1-\beta_1}\right)$$

SI: exponential MA:

sequence $x_0, x_1, x_2, \ldots$ (recurrence)

$s_0 = 0$; $s_{t+1} = \beta s_t + (1-\beta) x_t$.

Evolving - parameters:

Subsampling - training number n.

momentum - k.

variance of the gradient

↳ avoid having

Variance Reduction

→ SVRG

↳ Strive to behave GD

- yet SGD each steps.

↳ Large-Scale convex optimization

⇒ great !!

for DL - Not so good.

GD SVRG.

$O(nk\log(\frac{1}{\varepsilon}))$ $O((n+k)\log(\frac{1}{\varepsilon}))$

Polyak Averaging

- Output an average:

if W_t is parameters vector after t steps

↳ $\frac{1}{T}\sum_{t=0}^{T-1} W_t$

Stochastic Weight averaging (SWA).

(wed.)

Lecture 15/14. Week 7.

Rev...

$\mathcal{O}(n/\kappa \log(\frac{1}{\varepsilon}))$ - GD.

$\mathcal{O}(\kappa/\varepsilon^2)$ - SGD

Momentum: $\mathcal{O}(n\sqrt{\kappa}\log(\frac{1}{\varepsilon}))$ - MSGD.

$\mathcal{O}((n+\kappa)\log(\frac{1}{\varepsilon}))$ SVRG.

- Polyak averaging / Stochastic weight averaging

$\mathcal{O}(n\kappa \cdot d \cdot \log(\frac{1}{\varepsilon})) \Leftrightarrow \mathcal{O}(\kappa\sigma^2 d/\varepsilon^2)$

$\mathcal{O}(n\sqrt{\kappa} d \log(\frac{1}{\varepsilon}))$

linear model: $w \in \mathbb{R}^d$.

$f(w) = \frac{1}{n}\sum_{x,y\in D} \mathcal{L}(w^T x, y)$.

time to compute an example grad

$\mathcal{O}(d)$

$\nabla^2 f(x)$ → covariance matrix. $(d\times d)$.

computationally expensive

Random Projection. (Johnson-Lindenstrauss

$x \in \mathbb{R}^D \Rightarrow Ax \in \mathbb{R}^d$ (transform)

feature length

$A \in \mathbb{R}^{d\times D}$ random.

$A_{ij} \sim \mathcal{N}(0, \sigma^2)$.

$\|Ax - Ay\|^2 \leq$

$(1-\varepsilon)\|x_i - x_j\|^2 \leq \|Ax_i - Ax_j\|^2 \leq (1+\varepsilon)\|x_i - x_j\|^2$

$\forall x_i, x_j \in D$

$d \geq \frac{8\log(n)}{\varepsilon^2}$.

Why? choose σ^2 s.t.

$\mathbb{E}\left[\|Ax_i - Ax_j\|^2\right] = \|x_i - x_j\|^2$.

$\mathbb{E}[\|A(x_i - x_j)\|^2] = \mathbb{E}[(x_i - x_j)^T A^T A (x_i - x_j)]$

$= (x_i - x_j)^T \mathbb{E}[A^T A] (x_i - x_j)$

↳ Gaussian matrix.

$\mathbb{E}[A^T A]_{ij} = \sum_{k=1}^{d} \mathbb{E}(A_{ki} A_{kj})$

$= \begin{cases} 0 & \text{if } i \neq j \\ \sum_{k=1}^{d} \mathbb{E}[A_{ki}^2] & \text{if } i = j \end{cases}$

σ^2

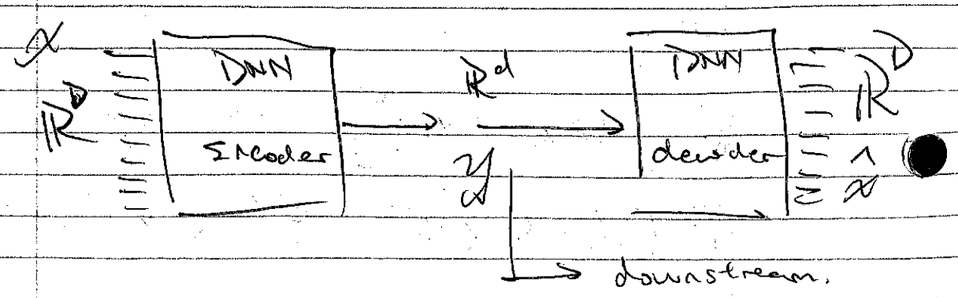
$\mathbb{E}[A^T A] = \sigma^2 d I$

$= (x_i - x_j)^T (\sigma^2 d I)(x_i - x_j)$

$= \sigma^2 d \|x_i - x_j\|^2 \overset{\text{if}}{=} \|x_i - x_j\|^2$

↳ $\sigma^2 = \frac{1}{d}$.

AutoEncoders



$\ell(x, \hat{x})$

e.g. $\frac{1}{|D|} \sum_{x \in D} \|x - \hat{x}\|_2^2$

↑ unsupervised learning.

Sparsity

density of x = $\frac{\#\text{ of nonzero entries } x}{\text{size of } x \cdot d}$

$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 2 \\ 0 \\ 0 \\ 3 \end{bmatrix} = \{(4, 2.0), (7, 3.0)\}$ = indices = [4, 7]

values = [2.0, 3.0]

16 ish

Sparse matrix.

COO

↳ expensive to comp.
Easy to write

$\begin{bmatrix} 0 & .5 & 0 & 0.3 \\ 0 & 1.0 & 0 & 0.0 \end{bmatrix} \mapsto$

row idx. [1, 1, 2]

col. idx. [3, 6, 2]

values [5, 3, 1]

CSR — vs. — CSC

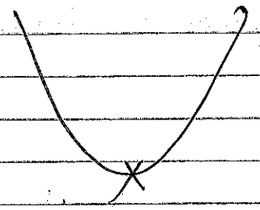
row offsets. [0, 2] [3, 6] [2] ⇒ [3, 6, 2]

col idxs. [5.0, 3.0] [1.0] [5.0, 3.0, 1.2]

values.

Week 8. Lecture 15/16.

Deep learning

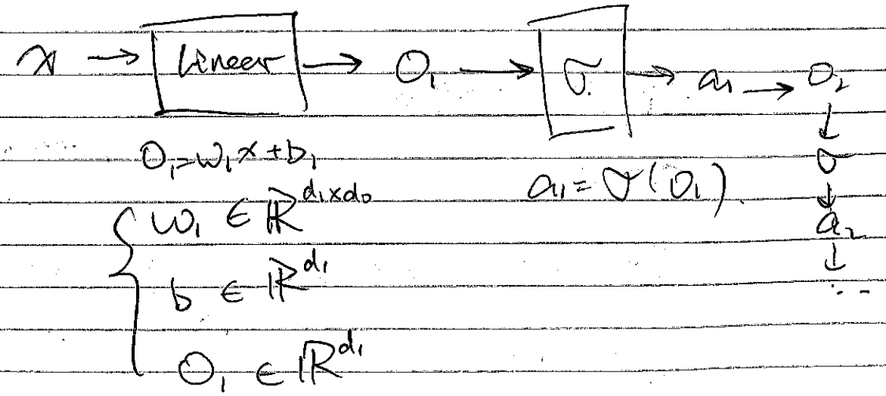


convex opt.

Neural Networks

- MLP

$x \in \mathbb{R}^{d_0}$



Nonlinear: function acts element-wise as the activation function.

$\sigma(x) = ReLU(x) = \max(x, 0)$.

universal: for continuous input → output. there exists a function that approx. with bounded parameters (good recovery).

capacity $\xrightarrow{\text{imply}}$ overfit.

NN tend not to overfit!

→ larger models generalize better.

▷ double-descent.

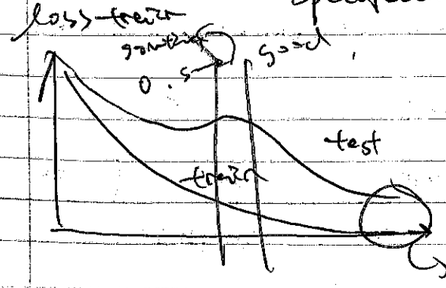
$(x, y) \in \mathbb{R}^d \times \mathbb{R}$.

$|\mathcal{D}| = n$. $n = d$.

$\mathcal{L}(w) = \frac{1}{n} \sum_{i=1}^{n} (x_i^T w - y_i)^2$ + regularization

larger model generalize better

Specifically for SGD, Adam. or sth similar.



"double-descent" phenomenon.

$a_\ell, o_\ell \in \mathbb{R}^{d_\ell}$

$a_\ell = W_\ell \cdot o_{\ell-1} + b_\ell \rightarrow \mathcal{O}(\;)$

$\mathbb{R}^{d_\ell} \quad [\mathbb{R}^{d_{\ell-1}}] \in \mathbb{R}^{d_\ell}$

$o_\ell = \sigma_\ell(a_\ell) \rightarrow \mathcal{O}(\;)$

$d_1(d_0 + d_2 - 1) + d_1$

$3 d_1 \ell.$

$W_1 \in \mathbb{R}^{d_1 \times d_0}$

$b_1 \in \mathbb{R}^{d_1}$

$x \in \mathbb{R}^{d_0}$

Image processing (- CV.

$x \in \mathbb{R}^{C \times W \times H}$ → height of image

→ width of image

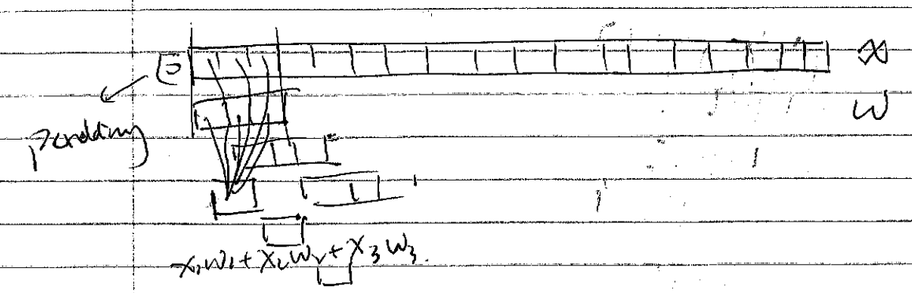
↑ channels.

1) convolutional neural network

- restricted subset

convolutional layers. in place of the linear layers.

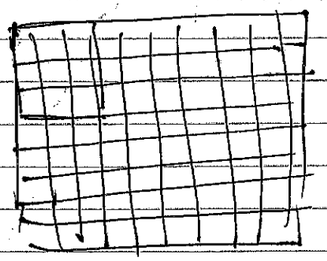
convolution in 1D:



filter: arbitrarily set of parameters.

$x_{k+1} w_1 + x_{k+2} w_2 + x_{k+3} w_3$

in 2D



Conv. layer

diff. channels

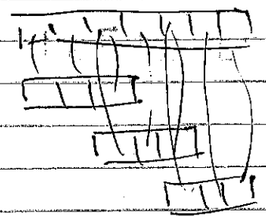
input $x \in \mathbb{R}^{C_0 \times W_0 \times H_0}$ output. $a \in \mathbb{R}^{C_1 \times W_1 \times H_1}$

parameters $W \in \mathbb{R}^{C_1 \times C_0 \times k_W \times k_H}$

$a_i = \sum_{j=1}^{C_0} \text{conv.}(W_{ij}, x_j)$ (W_{ij}: matrix) $W \in \mathbb{R}^{C_1 \times C_0 \times k_W \times k_H}$ ↑ ↑ ↑ ↑ i-th image

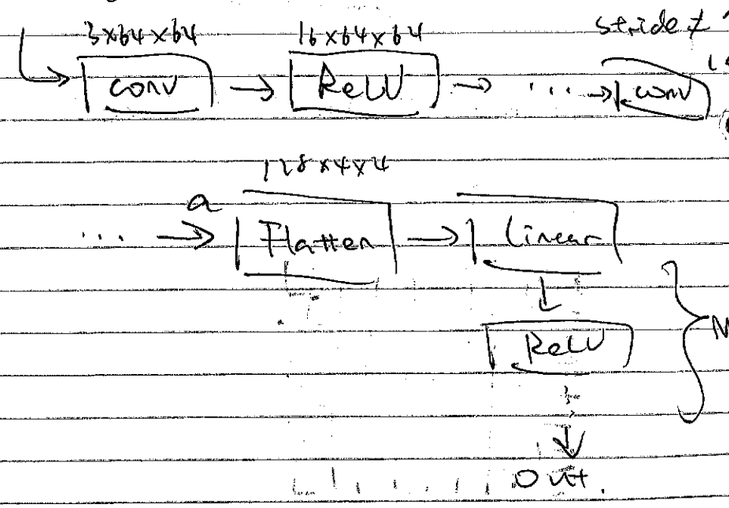
$b \in \mathbb{R}^{C_1}$

• stride.



output: 3

input image:



Week 9. Lecture 17.

Overfitting / Underfitting ← low capacity

↖ model has high capacity.

(overparametrized).

↓

DNNs high ← representational

many weights.

weights coming ← effective.

from the learning algorithm.

Dropout.

↳ increase the representation capacity.

During training → randomly drop

(independently each step) neurons.

↓

forces the learn to employ

more neurons.

Week 9 Lecture 18

Batch Norm.

Let $u \in \mathbb{R}^n$.

$$u \to \frac{u - \mu}{\sqrt{\sigma^2}} = \frac{u - \mu}{\sigma}$$

↳ Instead, look at $u \in \mathbb{R}^B$

— conv. ⇒ image ⇒ per channel

— saves a running [exp.] average,

of the mean & variance

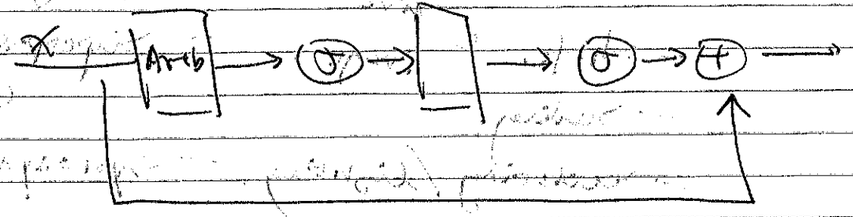
μ , σ.

Model.train() ⇒ turning on/off batch norm.
Model.eval()

$$u \to \frac{u - \mu}{\sigma} \cdot \gamma + \beta$$

broadcast. scalar learned (SGD)

Residual / connections / skip connections



⇒ ResNet.

⇒ DenseNet.

$$\min_w \ell(w) = \frac{1}{n} \sum_{i=1}^{n} \ell(w, x_i, y_i)$$

$(x_i, y_i) \in \mathcal{D} \subseteq \mathcal{X} \times \mathcal{Y}$

▷ sparse data (prob. ρ)

n too small.

☆ Data Augmentation.

randomness.

Aug: function $\mathcal{A} \cdot \mathcal{X} \xrightarrow{r \in [0,1]} \mathcal{X}$. ← random noise

$$w_{t+1} = w_t - \alpha \nabla \ell(w_t; \mathcal{A}(x_t; \eta_t), y_t)$$

example chosen @ t.

IMAGES:

- Translation
- Rotation
- Shift
- Scaling
- recoloring / lighting

make image

- Noise / Anti fact Addition
- Cropping
- Superposition (Mixup)
- synonym swapping
- deletion
- back translations

Semi-supervised learning:

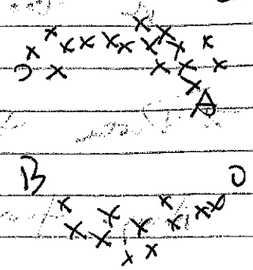
"data-cheap" "label-expens."

lots of data, few labels

assump.

Similar inputs have similar outputs.

↳ (kNN)



clustering → data is clustered

labels by cluster.

Manifold → data lie on low-dimensional manifold

PCA Auto encoders

Week 10. Lecture 19.

Sequence models.

$x \in \mathbb{R}^{d \times n}$ ← different per example.

discussion:

- takes sequence as input.

↳ generate sequence output.

○ handle sequence input/output?

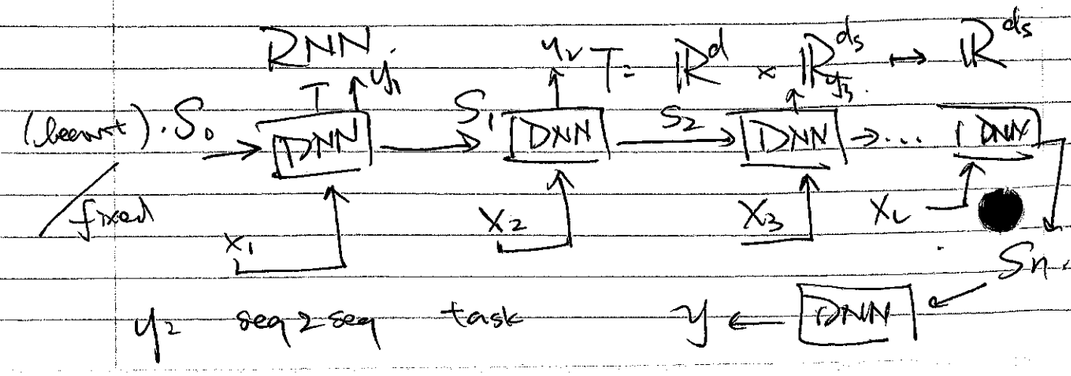
- padding → max length.

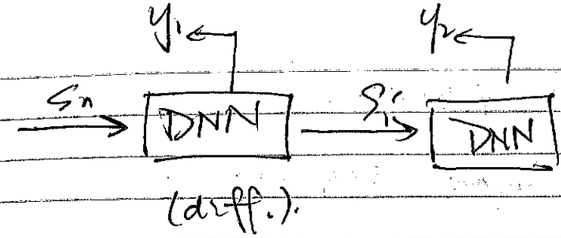
- counts / sum

- RNN ≈ sequential

- Transformers. ≈ parallel

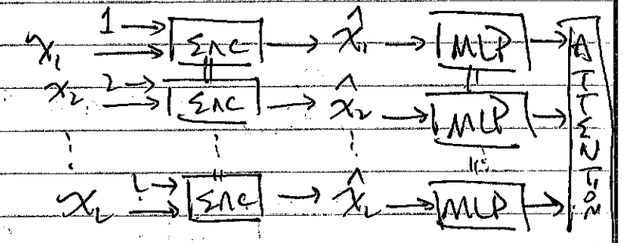
DfA: $S_{next} = T(S_{current}, X_i)$. $\times \mathbb{R}^c \to \mathbb{R}^{d_s}$





- LSTM.

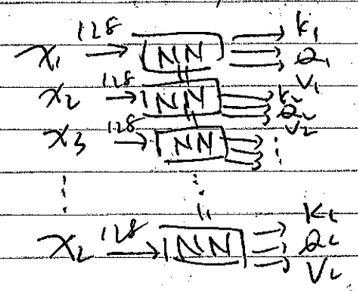
- Transformers.



(input sequence

$x_i = Enc(x_i, \psi)$.

Mathematically attention layer:



$k_i \in \mathbb{R}^{d_k}$

$V_i \in \mathbb{R}^{d_v}$.

$Q_i \in \mathbb{R}^{d_k}$.

$Q, k \in \mathbb{R}^{n \times d_k}$.

$V \in \mathbb{R}^{n \times d_v}$.

$\text{Softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right) \cdot V$

approximate table lookup:

↓

Attention block.

Multihead Attention

Same input sequence.

↓

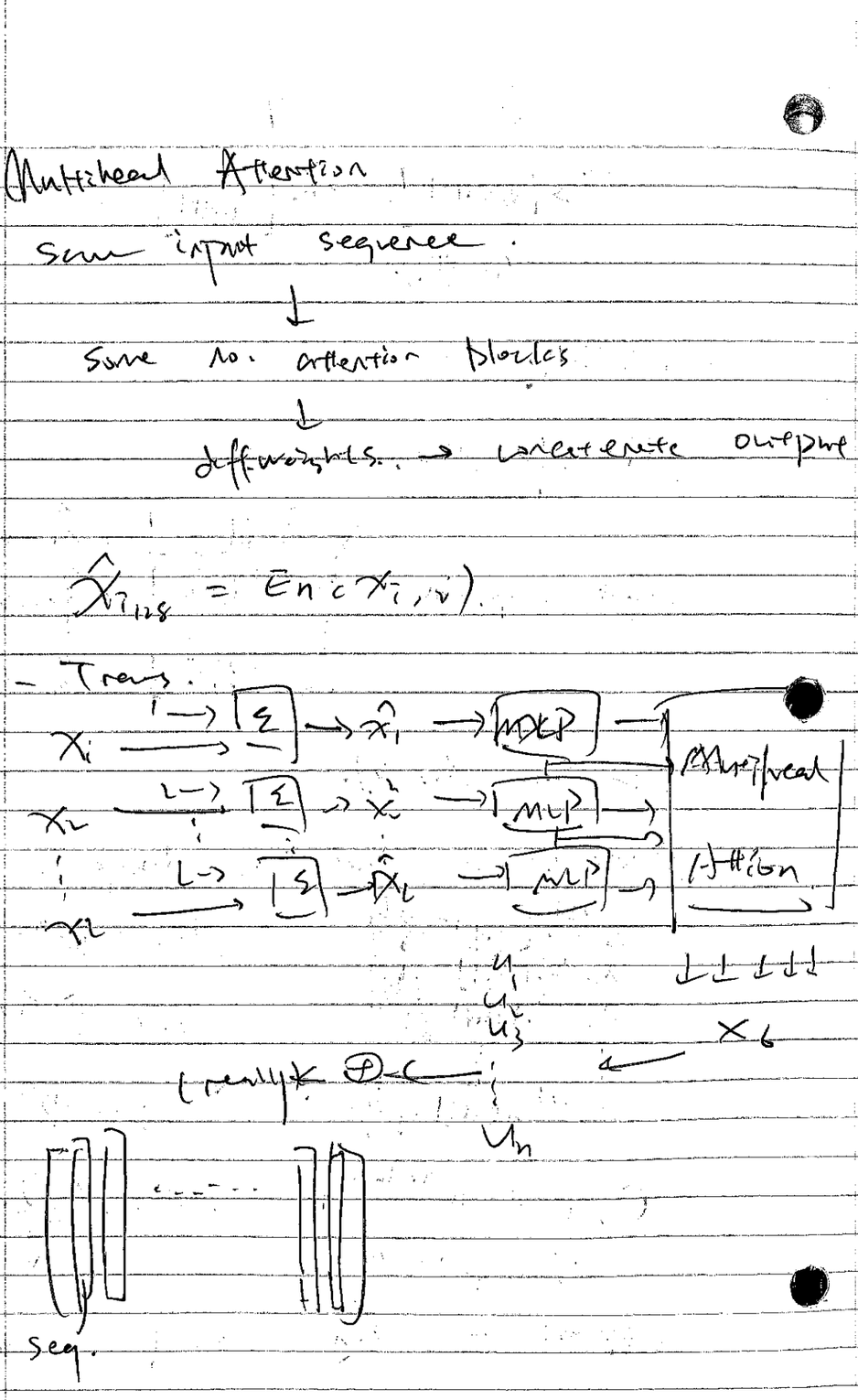
Same no. attention blocks

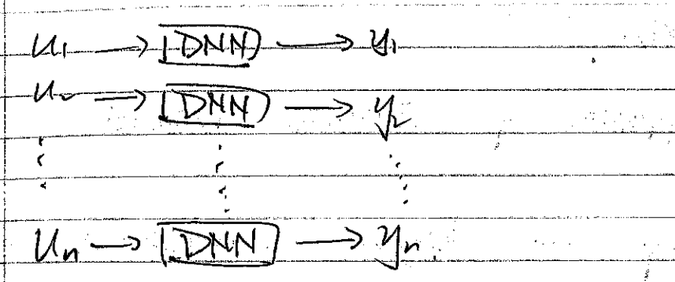
↓

diff weights → concatenate output

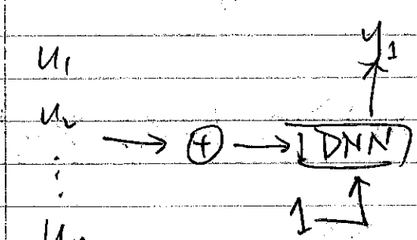
$\hat{X}_{i_{128}} = Enc(X_{i,v})$

- Trans.





instead, we do



Lecture 20.

Kernels.

opposite of dimension reduction.

map into higher dimensional space.

$$\phi(x) = \mathbb{R}^d \mapsto \mathbb{V}$$

$$\langle \phi(x_1), \phi(x_2) \rangle = k(x_1, x_2).$$

$$k: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$$

Examples

- Gaussian Kernels

$$k(x_1, x_2) = \exp(-\gamma \|x_1 - x_2\|^2).$$

a.k.a. RBF kernel

- linear kernel

$$k(x_1, x_2) = x_1^T x_2.$$

- exponential kernel (laplacian)

$$k(x_1, x_2) = \exp(-\gamma \|x_1 - x_2\|)$$

- Polynomial kernels

$$k(x_1, x_2) = (1 + x_1^T x_2)^p.$$

Kernel definition.

$$k: \mathcal{X} \times \mathcal{X} \to \mathbb{R}.$$

$$k(u, v) = k(v, u)$$

→ kernel must be symmetric.

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j k(x_i, x_j) \geq 0.$$

$$\| \sum_{i=1}^{n} c_i \phi(x_i) \|^2 \geq 0$$

if $K_{ij} = k(x_i, x_j) \Rightarrow K$ is positive semidefinite

k is a kernel implies:

$\exists \mathbb{V}$ vector space & ϕ s.t.

$\langle \phi(x_1), \phi(x_2) \rangle = k(x_1, x_2)$

if k_1 & k_2 are kernels. w/ feature maps ϕ_1 & ϕ_2, then $k = k_1 + k_2$

$k(u, v) = k_1(u, v) + k_2(u, v)$.

$\phi(x) = \begin{bmatrix} \phi_1(x) \\ \phi_2(x) \end{bmatrix}$ ← is a kernel.

$k(u,v) = c\,k_1(u,v)$ if $c \geq 0$.

$\phi(x) = \sqrt{c}\,\phi_1(x)$.

$k(u,v) = k_1(u,v)\,k_2(u,v)$.

$\phi(x) = \phi_1(x) \otimes \phi_2(x)$.

$k(u,v) = f_1(u)\,k_1(u,v)\,f_2(v)$.

$\phi(x) = f(x)\,\phi(x)$.

$f : x \to \mathbb{R}$.

component loss ℓ: $f(w, x, y) = \ell(w^T \phi(x), y)$.

$= \ell(\langle w, \phi(x) \rangle, y)$.

$f(w) = \frac{1}{n} \sum_{i=1}^{n} f(w, x_i, y_i)$.

$= \frac{1}{n} \sum_{i=1}^{n} \ell(\langle w, \phi(x_i) \rangle, y_i)$.

$\nabla_w f(w, x, y) = \ell'(w^T \phi(x), y)\,\phi(x)$.

$\Rightarrow$ for GD / SGD.

$w_k \in \text{span}\{\phi(x_1), \phi(x_2), \ldots \phi(x_n)\}$

$w_k = \sum_{i=1}^{n} \alpha_i \phi(x_i)$

$w_k = \sum_{i=1}^{n} a_i \phi(x_i)$.

$F(a, x, y) = \ell(\langle \sum_{i=1}^{n} a_i \phi(x_i), \phi(x) \rangle, y)$.

$= \ell(\sum_{i=1}^{n} a_i \langle \phi(x_i), \phi(x) \rangle, y)$

$= \ell(\sum_{i=1}^{n} a_i k(x_i, x), y)$

$f(a) = \frac{1}{n} \sum_{j=1}^{n} \ell(\sum_{i=1}^{n} a_i k(x_i, x_j), y)$.

let $K_{ij} = k(x_i, x_j)$

$= \frac{1}{n} \cdot \sum_{j=1}^{n} \ell((Ka)_j, y)$.

① compute $\phi(x_i)$ on-the-fly as needed.

② precompute & store $\phi(x_i)$ before training. ✓ train in the transformed space

③ compute k on-the-fly as needed

④ precompute K & store.

Lecture 21.

kernels function $k: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$.

ways to do learning:

(1) Learn in the transformed space, compute ϕ on-the-fly.

(2) learn " " precompute ϕ.

(3) learn in the "kernel" space while computing k on-the-fly.

(4) learn in "kernel trick" space, precompute $K_{ij} = k(x_i, x_j)$

$f_i(w) = \ell(w^T \phi(x_i), y_i)$

$\nabla f_i(w) = \ell'(w^T \phi(x_i), y_i)\, \phi(x_i)$

Suppose n examples, $x_i \in \mathbb{R}^d$, and k takes $\Theta(d)$ to compute.

$\phi(x_i) \in \mathbb{R}^m$.

run for T steps.

cost to compute $\phi \Rightarrow \Theta(md)$.

— Vanilla non-kernel linear model: $\mathbb{R}^d$.

	Compute	Memory
(1)	(H) (Td)	(H) (d) (not inc. train. set)
(2)		
(3)		
(4)		

— learn in the transformed space

	Compute	Memory
(1)	(H) (Tmd). precompute (H) (nm).	"kernel"
(2)	(H) $(Tm + nmd)$.	(H) (nm). (training d.)
(3)	(H) (Tnd).	(H) (n).
(4)	(H) $(Tn + n^2 d)$	(H) (n^2).

$\nabla f_i(w) = \ell'(\sum_{j=1}^{n} u_j k(x_i, x_j), y_i)\, \phi(x_i)$

$\nabla f_i(w) = \ell'(\phi(x_i)^T \sum_{j=1}^{n} u_j \phi(x_j), y_i)\, \phi(x_i)$

an SGD step ⇒ compute $\hat{}$

$$u_i \leftarrow u_i - \alpha \ell'\left(\sum_{j=1}^{n} u_j k(x_i, x_j); y\right)$$

For kernels - subsampling.

$$k(x_i, x_j) \approx \langle \psi(x_i), \psi(x_j) \rangle$$

$$\psi(x) \in \mathbb{R}^D.$$

Approximate feature map.

↳ Random Fourier features.

if kernel : $k(x_i, x_j) = k(x_i - x_j)$.

then $k(x_i, x_j) = \mathbb{E}\left[2\cos(w^T x_i + b), \cos(w^T x_j + b)\right]$.

$b \sim \text{Unif}[0, 2\pi]$

$w \sim \mathcal{F}(k)$ Fourier transform of k.

("Rep" k)

RBF kernel:

$$w \sim \mathcal{N}(0, 2\gamma I),$$

$$b \sim \text{Uniform}([0, 2\pi]).$$

$$\mathbb{E}\left[2\cos(w^T x_1 + b), \cos(w^T x_2 + b)\right]$$

$$= \exp\left(-\gamma \|x_1 - x_2\|^2\right).$$

draw $w_1, w_2, \ldots, w_D \sim \mathcal{N}(0, 2\gamma I)$

$b_1, b_2, \ldots, b_D \sim \text{Unif}([0, 2\pi])$

Set $\psi_i(x) = \frac{1}{\sqrt{D}} \sqrt{2} \cos(w_i^T x + b_i)$

$$\Rightarrow \mathbb{E}\left[\langle \psi(x_i), \psi(x_j) \rangle\right] = \exp\left(-\gamma \|x_i - x_j\|^2\right)$$

; (TBC)

⑤ Learn w/ approx. feature map comp. ψ on-the-fly.

⑥. Learn w/ approx. f. m. compute & cache

Vanilla linear model.

compute. Memory.

(E) (H)(TDd). (H)(D)

(b) (H)(TD) + nDd) (H)(nD).

large D - high "accuracy" in repr. R.

- high compute & memory cost.

Lecture 22.

▷ Hyperparameter optimization

- Step size / lr / α → diverge.

$\alpha \uparrow$ — too large noise ball.

$\alpha \downarrow$ — get "stuck" in non-convex.

- λ for regularization

↓

over/under regularize.

converge too slowly — wrong level of expressivity.

poor generalization.

- β momentum. → if $\beta \notin (0, 1)$.

↓

bad.

- B batch size. → too small can affect noise ball.

too large → much like GD.

performance matching parallel capabilities of HW.

- choice of architecture : DNN

↓

Generalize poorly.

Systems implications.

- Non-DNN -

- tree depth → weak learner

overfit & lots of mem.

- feature vector length for

Random features.

→ poor fidelity,

high compute/memory

cost.

- # of epochs → high loss/error

compute cost.

- dimension → poor accuracy.

high compute cost

- k in kNN & k-means → under/overfit

more compute for larger k.

- the tasks for assigning hp:

→ HPO - Any process assign hps.

Standard: β 0.9 0.99

(β_1, β_2) (0.9, 0.999)

B power of 2, e.g. 256.

- Grid Search

↳ CoD

- Random Search.

less reproducible than GS.

Parallelism.

Early stopping

- droping bad hyperparameters

that perform poor each epoch.

goal: minimize $F(\alpha, \beta, B, k, \lambda)$.

"derivative-free" optimization. (DFO)

Encode our knowledge abt the space & the problem $\rightarrow$ HPO

Bayesian Opt — continued.

Mean / Median $f_0\ f_1\ f_2\ f_3\ f_4\ \ldots$

HPO

$P(f \mid f(x_1)=y_1,\ f(x_2)=y_2)$.

look at: $P(f(x_*) \mid f(x_1)=y_1,\ f(x_2)=y_2, \ldots)$

$f \in \mathbb{R}^d$, $f \sim \mathcal{N}(0, \Sigma_1)$

↓ ↓

mean covariance

↓

{ Set by ~~the~~ according to intuition.

♣ Fact: if (X, Y) are jointly (multivariate) gaussian.

the $X \mid Y = y$ is also Gaussian.

♣ Fact: "$\sim$", then X is Gaussian.

$f(x_*) \mid f(x_1)=y_1,\ f(x_2)=y_2, \ldots$

$\sim \mathcal{N}(\mu, \sigma^2)$

How to pick the next point?

$$x_{next} = \arg\min_{x^*} a(\mu(x^*), \sigma^2(x^*))$$

$a(\mu, \sigma) = \mu - k\sigma$.

(lower confidence bound)

a = acquisition function.

$a(\mu, \sigma) = P(f(x^*) \le f_{best})$.

$\hookrightarrow$ P ~ ...

(Probability of Improvement).

$f(x^*) \sim N(\mu, \sigma^2)$

$= \Phi\left(\frac{f_{best} - \mu}{\sigma}\right)$

Φ

accumulated distribution function.

$\hookrightarrow \Phi(u) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{u} e^{-\frac{z^2}{2}} dz$

$P(f(x^*) \le f_{best} | obs) = P(Z \le f_{best})$

for $Z \sim N(\mu, \sigma^2)$

$= P(\sigma u + \mu \le f_{best})$

for $u \sim N(0, 1)$

$= P(u \le \frac{f_{best} - \mu}{\sigma}) = \int_{-\infty}^{(f_{best}-\mu)/\sigma} P(u)\,du$

$a(\mu, \sigma) = \mathbb{E}[\underbrace{f(x_*) - f_{best}}_{\min(f(x_*), f_{best}) | obs}]$.

Expected Improvement.

by convention:

$= \mathbb{E}[\min(f(x_*) - f_{best}, 0) | obs]$

Thm 3: (Strong max/min principle for heat eqn.)

Assume u is C_C^2 in space & C^1 in time, all within U_T & it is continuous on $\bar{U}_T$, & it satisfies the heat eqn. in U_T.

Then (1) $\max_{\bar{U}_T} u = \max_{\partial U_T} u$.

(2) if Ω is connected, & there exists $\exists (x_0, t_0) \in U_T$, s.t. $u(x_0 t_0) = \max_{\bar{U}_T} u$

then u is constant in $\bar{U}_{t_0}$.

If u attains a max/min @ an interior pt. within U_T, then u must have been constant for all earlier times.

$\Rightarrow$ If u satisfies $u_t - \Delta u = 0$. in U_T.

B.C. $u = 0$, on $\partial\Omega \times [0, T)$.

I.C. $u = g$. on $\Omega \times \{0\}$.

where $g \geq 0$, then $u(x,t) > 0$. if $g(x) > 0$. for some $x \in \Omega$:

another example of infinite propagation speed of info. within ht. eqn.

Thm 5. (uniqueness in Poisson's Eqn.)

If $g \in C^1(\partial\Omega)$ & $f \in C^1(\Omega)$, then $\exists!$ soln $u \in C^2(\Omega) \cap C^1(\bar{\Omega})$.

to

$$-\Delta u = f \quad \text{in } \Omega$$

$$u = g \quad \text{on } \partial\Omega$$

Thm 6. (Regularity in Laplaces Eqn)

If $u \in C^2(\Omega)$ & also satisfies $\fint_{\partial B_r(x)} u\,ds = \int_{B_r(x)} u\,dy$ for any ball $B_r(x) \subset \Omega$ then $u \in C^\infty(\Omega)$

↑ guarantees nth about what happens on $\partial\Omega$

Thm 7 (Harnacks inequality)

Let $V \subset\subset \Omega$ be compact, connected set, &

$\forall v \subset V$, $\exists$ a positive constant, c, for each such v. where $\sup_v u \leq c \cdot \inf_v u$

holds for all non-negative harmonic functions v, defined on Ω.

$\Rightarrow$ The values of a non-negative harmonic function, within an arbitrary V, can't be that different from one another: Laplace's equation smooths things out away from the boundary $\partial\Omega$.

The point of all these thms. is to illustrate that, once we have a mathematical model, we can analyze it to understand its properties, & the properties of its solution ... and potentially this transfers back to the real world & its properties.

Also, we need to understand the properties of our continuous solutions before we can properly discretize things for the computer.

$\not\Rightarrow$ good for code debugging.

Let's go back to Poisson eqn.

Lecture 21

Let's recall Poisson eqn. $\Delta u(x) = f(x)$ & use it to come up with a general viewpoint for thinking about classical solutions to Linear PDE

- The Green's function (GF)

$$G(x, \tilde{x})$$

The whole idea comes down to finding a solution for a special instance of, eg. the Poisson eqn.:

$$\Delta G(x, \tilde{x}) = \delta(x, \tilde{x})$$

Dirac Delta

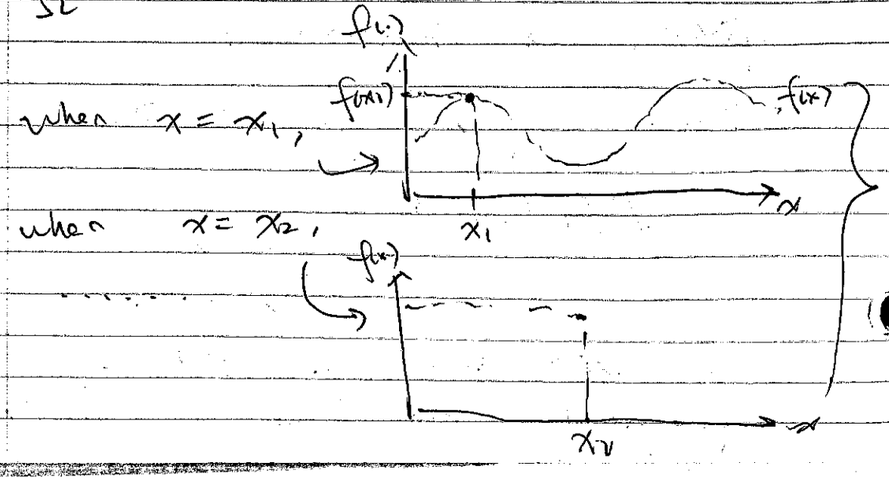
The Dirac Delta is kind of linear functional, known as a distribution.

This means δ likes to operate on some smooth function to produce a real number. The "operation" involves an integral.

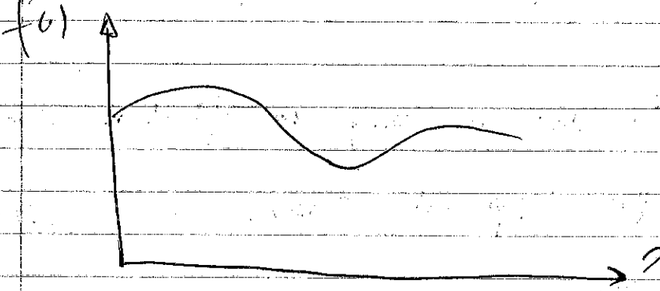
$$\delta(x) = \begin{cases} \infty & x = 0 \\ 0 & x \neq 0 \end{cases} \qquad \text{s.t.} \int_{-\infty}^{\infty} \delta(x)\,dx = 1$$

We can use these interesting properties of δ to "break up" our source term, $f(x)$, into "impulses" meaning

$$\int_{\Omega} \delta(x, \tilde{x}) f(\tilde{x})\, d\tilde{x} = f(x) \qquad (+)$$



"taking" an infinity of such pts, we get a smooth curve"



but we also know that if we substitute a Green's function in $\Delta(\cdot)$. we get the Dirac Delta: $\Delta(G(x,\tilde{x})) = \delta(x,\tilde{x})$ so we rewrite (+): $\int_{\Omega} \Delta(G(x,\tilde{x})) f(\tilde{x})\, d\tilde{x} = f(x)$

Integration is a linear differential operator Ω is fixed.

$$\Delta\left(\int_{\Omega} G(x,\tilde{x}) f(\tilde{x})\, d\tilde{x}\right) = f(x).$$

is a soln to PS, since it satisfies the PDE $\Delta(u(x)) = f(x)$

thus $u(x) = \int_\Omega G(x,\tilde{x}) f(\tilde{x})\, d\tilde{x}$

"Ω is fixed & f is nice".

G.f. not so easy to find ... available only for special cases. w/ simple geometries.

Eg. The Green's function for Poisson's eqn. on the unit disk w/ homogeneous Dirichlet B.C.s. i.e. $(u(x)=0, \forall x \in \partial\Omega)$. is

$$G(x,\tilde{x}) = \frac{1}{2\pi}\left(\ln|x-\tilde{x}| - \ln|x^*-\tilde{x}^*| - \ln|\tilde{x}|\right)$$

Heat Eqn. (Diffusion).

$$u_t - \Delta u = 0$$

if there is a source term within the domain, eq. becomes $u_t - \Delta u = f$.

where $t \geq 0$ & $x \in \Omega \subset \mathbb{R}^n$. The solution $u(x,t)$ is the function satisfying the PDE & I.C. & B.C. such that $u: \bar{\Omega} \times [0,\infty) \to \mathbb{R}$, i.e. our soln is a scalar field over $\bar{\Omega}$.

But where did this PDE come from?

Let's begin from the case with heat flowing: First we need some terminology.

Thermal Energy ≡ instantaneous molecular kinetic Energy.

Heat ≡ Thermal Energy in transit.

Temperature ≡ Average of thermal Energy

Physics Theory = Conservation of Energy

Rate of change in Thermal Energy = Heat Generated by sources within Ω + flow of heat into Ω from outside

taking arbitrary subd. $\Omega' \subset \Omega$

Note: Thermal Energy contained in a body is tied to "heat capacity", C.

$C \equiv$ amount of heat generated per unit mass, per rise in temp, μ.

$\rho \equiv$ mass density.

The total thermal energy with Ω" @ a given temp. t is:

$$\int_{\Omega} C(x)\,\rho(x)\,\underbrace{\mu(x,t)}_{\text{Temp. field}}\,dx$$

if $f(x,t)$ is our heat source, specified per unit volume, per unit time, then the total heat generated by the source within Ω' is: $\int_{\Omega'} f(x,t)\,dx$

Lastly, heat flux thru $\partial\Omega'$ is $q_\theta(x,t)$; thus the total heat flux into the body @ time "t", is given by:

$$\int_{\partial\Omega'} q_\theta \cdot \underbrace{\nu}_{\text{unit outward normal to } \partial\Omega'}\,dS.$$

Rate of change in thermal Energy within Ω = Heat generated in Ω + flow of heat into domain

considering arbitrary sub-domain Ω'

$$-\int_{\partial\Omega'} q_\theta \cdot \nu \cdot ds$$

$$\frac{d}{dt}\int_{\Omega'} C(x)\,\rho(x)\,\mu(x,t)\,dx \qquad \downarrow \text{divergence thm}$$

$$= \int_{\Omega'} f(x,t)\,dx - \int_{\Omega'} \nabla \cdot q_\theta\,dx.$$

$$\int_{\Omega'} \underbrace{\left[C(x)\,\rho(x)\,\frac{\partial \mu(x,t)}{\partial t} - f(x,t) + \nabla \cdot q_\theta\right]}_{=0} dx = 0$$

not the same.

$$\Rightarrow c\rho \frac{\partial \mu}{\partial t} + \nabla \cdot q = f \quad (\#)$$ we now need

a constitutive model (Fourier's law) relating

heat flux w/ gradients in temp.

$$q_q = -k \nabla \mu \quad (*)$$

(k: thermal conductivity)

$(*) \rightarrow (\#)$

$$\frac{\partial \mu}{\partial t} - \left(\frac{k}{c\rho}\right) \nabla \cdot \nabla \mu = f$$

$$\frac{\partial \mu}{\partial t} - \chi \nabla^2 \mu = f$$

(χ: thermal diffusivity)

(RHS=0)

The fundamental sol'n for homogeneous heat eqn.

$$\phi(x,t) := \begin{cases} \frac{1}{(4\pi t)^{n/2}} e^{-\frac{|x|^2}{4t}} & (x \in \mathbb{R}^n, t>0) \\ 0 & (x \in \mathbb{R}^n, t<0) \end{cases}$$

Note singularity @ pt. $(0,0)$.

$|x| = (x_1^2 + x_2^2 + \dots + x_n^2)^{1/2}$

(another radial sol'n)

sol'n is normalized s.t.

$$\int_{\mathbb{R}^n} \phi(x,t)\, dx = 1.$$

Let's consider IVP heat equation.

$$\mu_t - \Delta \mu = 0 \quad \text{in } \mathbb{R}^n \times (0,\infty)$$

$$\mu = g \quad \text{on } \mathbb{R}^n \times \{t=0\}.$$

We note that the fundamental sol'n, ϕ, solves the homogeneous heat eqn. away from the singularity @ $(0,0)$, as it does for any shift in spatial coordinate, as in $\phi(x-y,t)$ for each fixed $y \in \mathbb{R}^n$. As a result, the following convolution is a solution to our IVP.

Thm 1: (Initial value heat eqn.)

Assume $g \in C(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n)$, and define "$\mu$" as, $\mu(x,t) = \int_{\mathbb{R}^n} \phi(x-y,t)\, g(y)\, dy$

$$= \frac{1}{(4\pi t)^{n/2}} \int_{\mathbb{R}^n} e^{-\frac{|x-y|^2}{4t}} g(y)\, dy.$$

$(x \in \mathbb{R}^n,\ t > 0)$

then,

1) $u \in C^\infty(\mathbb{R}^n \times (0,\infty))$ ← soln ↑ smooth

2) $u_t(x,t) - \nabla^2 u(x,t) = 0, \quad x \in \mathbb{R}^n,\ t > 0.$

&

3) $\lim u(x,t) = g(x^0)$ for each $x^0 \in \mathbb{R}^n$.
$(x,t) \to (x^0, 0)$

Since g is bounded & continuous, if we also make it possitive semi definite, then $u(x,t)$ is postive for all Pts $x \in \mathbb{R}^n$ & times $t > 0$.

implies prop. speed for info. regarding I.C.

$u_t - \Delta u = f$ in $\mathbb{R}^n \times (0,\infty)$

$u = 0$ on $\mathbb{R}^n \times \{0\}$.

Thm 2: (forced heat eqn.)

Let $u(x,t)$ be of the form

$$u(x,t) = \int_0^t \int_{\mathbb{R}^n} \phi(x-y, t-s) f(y,s)\, dy\, ds.$$

$$= \int_0^t \underbrace{\frac{1}{(4\pi(t-s))^{n/2}} \int_{\mathbb{R}^n} e^{-\frac{|x-y|^2}{4(t-s)}} f(y,s)\, dy\, ds}_{\text{treating our forcing as I.C. @ "s"}}$$

then ① $u \in C_c^2(\mathbb{R}^n),\ C_c'([0,\infty))$.

② $u_t - \Delta u = f \quad (x \in \mathbb{R}^n,\ t > 0)$.

and

③ $\lim_{(x,t) \to (x^0, 0)}$

↳ $u(x,t) = 0$ for each $x^0 \in \mathbb{R}^n$

Combining Thms 1 & 2, we can solve

$$u_t - \Delta u = f \quad \text{in} \quad \mathbb{R}^n \times (0, \infty)$$

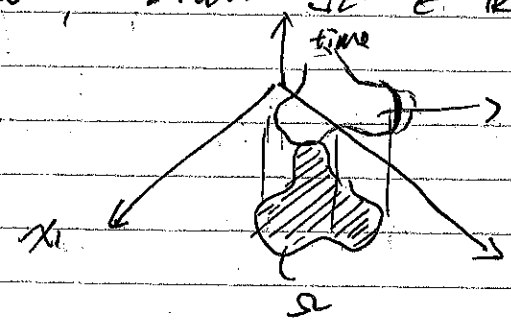
$$u = g \quad \text{on} \quad \mathbb{R}^n \times \{0\}.$$

with $$u(x,t) = \int_{\mathbb{R}^n} \phi(x-y, t)\, g(y)\, dy$$

$$+ \int_0^t \int_{\mathbb{R}^n} \phi(x-y, t-s)\, f(y,s)\, dy\, ds$$

moving away from all $\mathbb{R}^n$, now, let's define an open region of space serving as our spatial domain: $\Omega \in \subset \mathbb{R}^n$.

For now, draw $\Omega \in \mathbb{R}^2$ & time for 3').



$U_T := \Omega \times (0, T]$

↑ open set. | open | final time included

$\partial U_T := \bar{U}_T - U_T$.