IFT 6085
Theoretical principles for deep learning

Winter 2019

Instructor: Ioannis Mitliagkas

Today [overview; not much content]

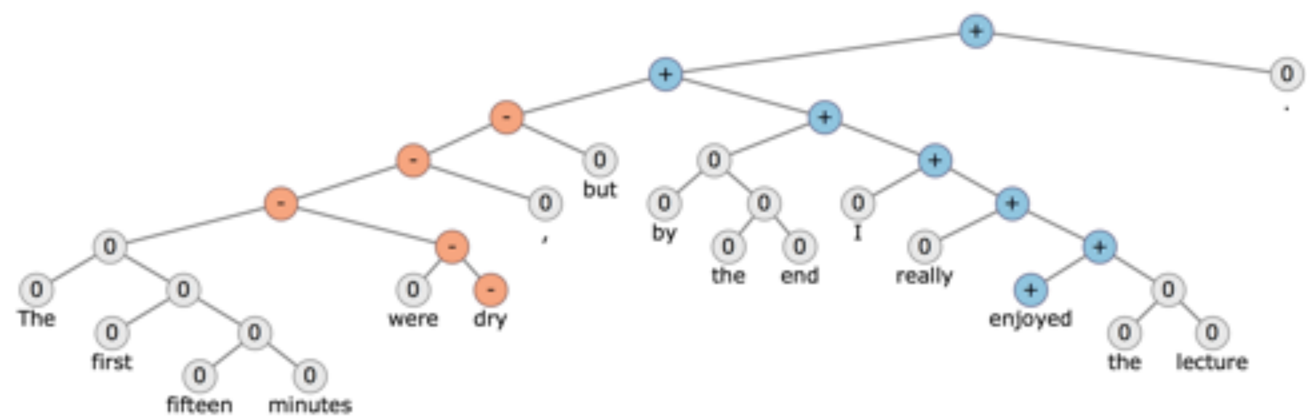
- Why deep learning?
- How do we make it work?
- Why **does** it work? We don’t fully know
- Class goals: learn tools, do research, present well
- Summary of content
- Class logistics
- Short quiz (not graded :))
- Questions

Why deep learning?

DEEP LEARNING IS SO COOL!!

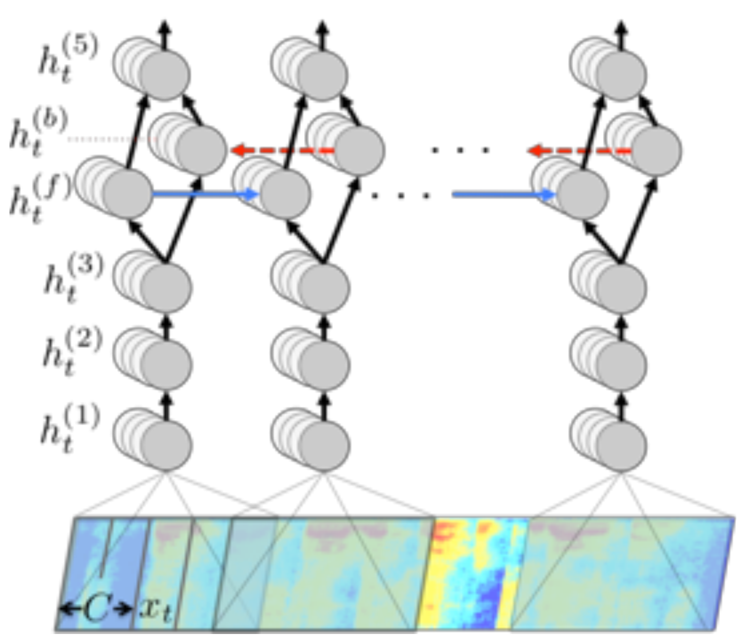
Deep learning drives significant progress

NATURAL LANGUAGE PROCESSING



cs224d.stanford.edu

SPEECH RECOGNITION

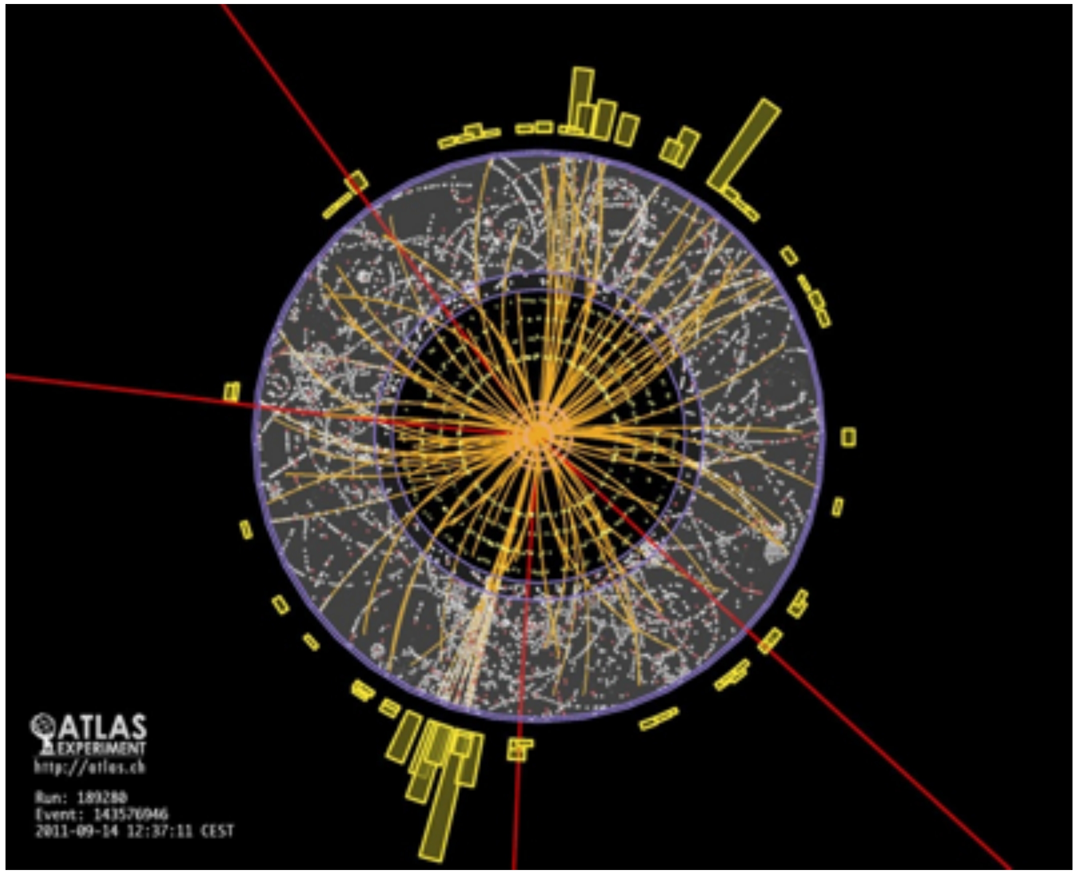


COMPUTER VISION

NVIDIA

LARGE-SCALE DEEP LEARNING FOR SCIENCE

- rapid development
    - fast training times enable rapid prototyping even for large models
- large problem scale
    - scientific datasets can be huge
        - ATLAS: ~5GB/sec
        - LSST: ~15TB raw images/night
    - scientific datasets are feature-rich
- engineering challenge: ~10K nodes

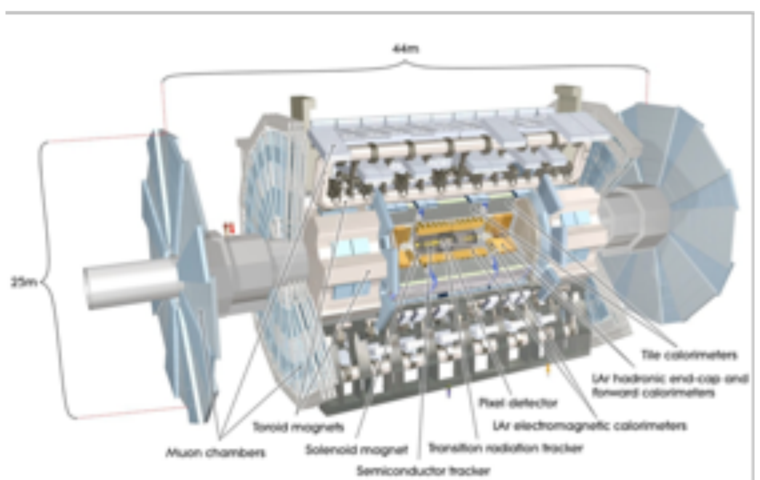


atlas.ch

CORI PHASE II

- 9600+ Knights Landing nodes

HIGH-ENERGY PHYSICS (HEP)



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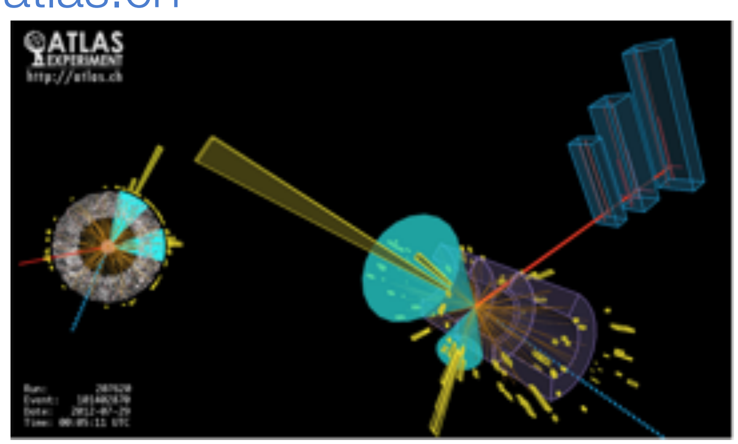
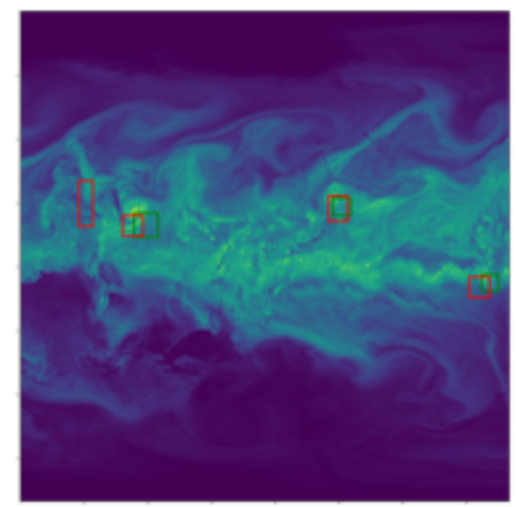
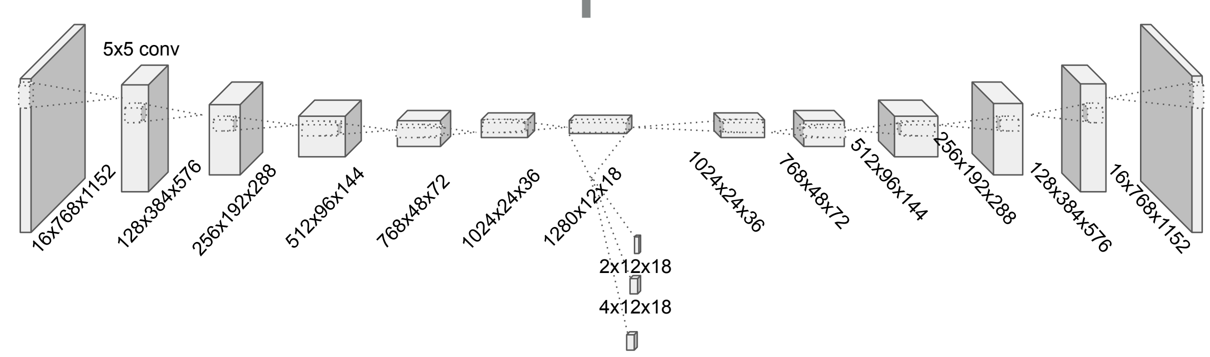


7.4TB data

CLIMATE SCIENCE



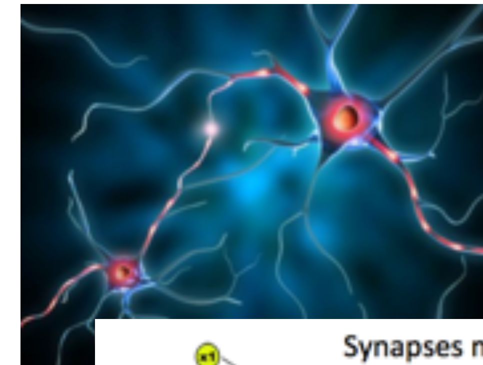
15TB data
semi-supervised

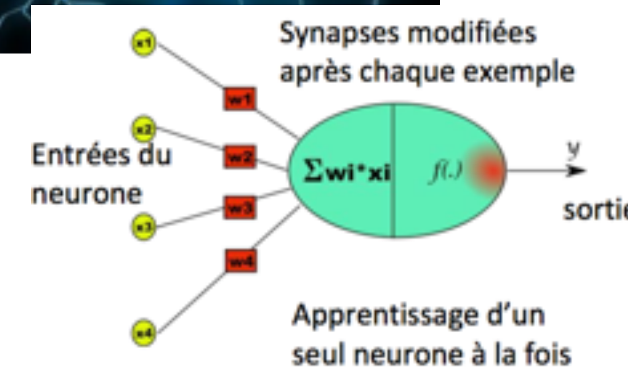


Economy-altering potential

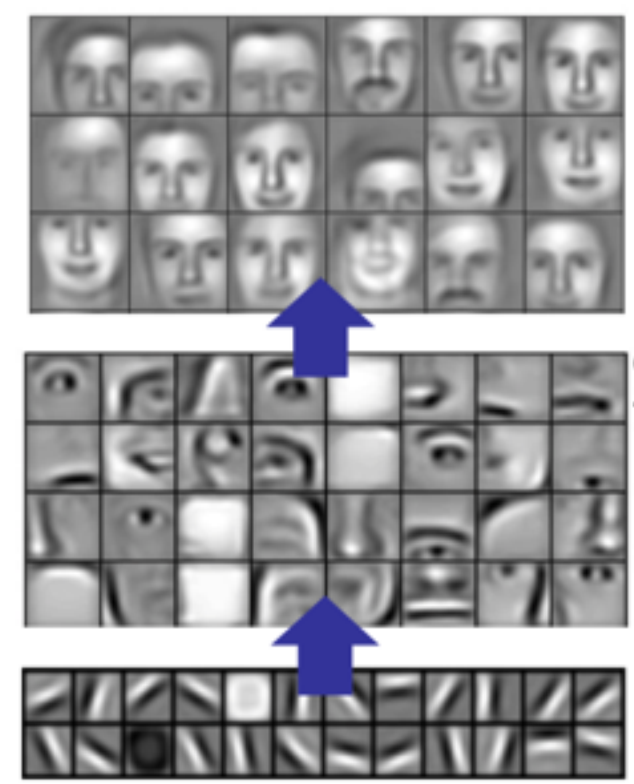
How do we achieve this great performance?

Knowledge from decades of research



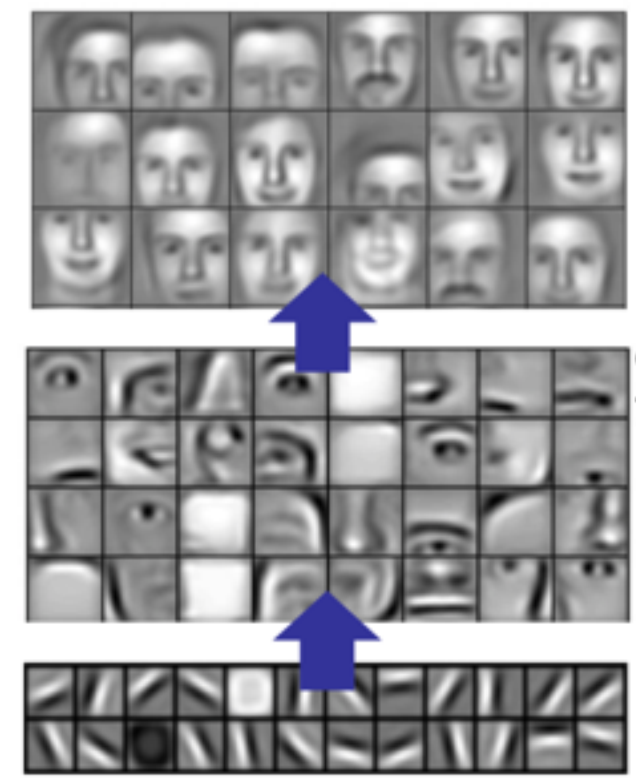


- Perceptron [Rosenblatt, 1957]
- [skipping people here!! not meant as a complete history]
- Progress in the 1980s-1990s
    - Bengio, Hinton, LeCun
    - Schmidhuber
- Took off again (seriously) in the 00's
- CIFAR-funded program gave new life to area



Recent boom

- We have more data
- We have more computational power
- We have improved our techniques (though they're not brand-new)



Making things work

- Good research labs and big companies know how to make deep learning systems work

- MSc/PhD here is great way to pick up skills
—> very valuable in industry

- Important announcement:
Professional MSc in ML:

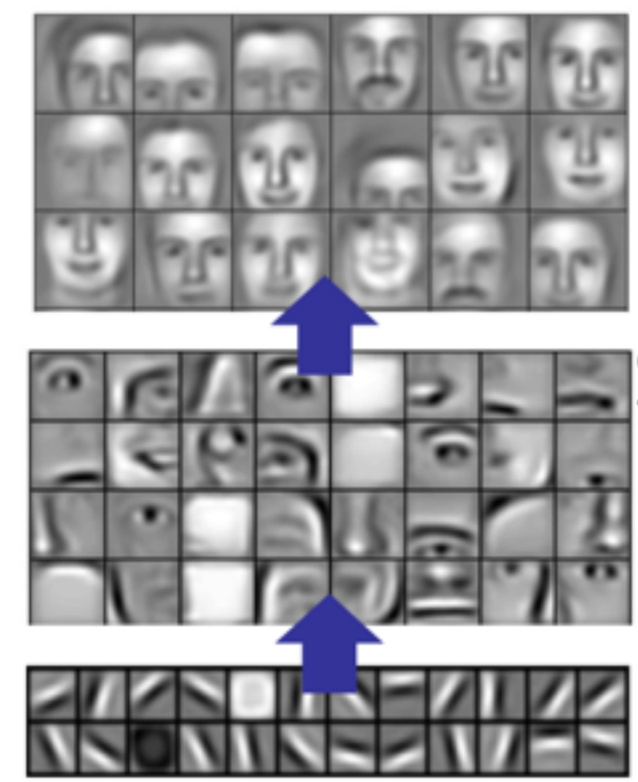
    - 2 extra classes instead of research project

    - MILA staff arranges/oversees internship on final semester

    - Can switch within 1-2 semesters. Email Linda Peinthière (lpeinthiere.umontreal@gmail.com) if interested.

Driven primarily by intuition and empirical success

- Good research and progress based on solid intuition
- **Practice leads** the way
- **Theory lags** dramatically
    - no guarantees
    - little understanding of limitations
    - limited interpretability



- More interestingly, classic theory suggests currently successful DL practices, wouldn't be likely to succeed.

Why does deep learning work?

We do not fully understand

==

Research opportunity

This class

- Seminar-style: we go over recent papers
- We go over recent **theoretically-driven or theoretically-supported advances in deep learning**
- We cover different topics, but try to tie them under common themes
- With every opportunity we study some underlying theoretical tools.
- Students read and present papers, and work on a semester research project

Goals of the class

- Exposure to useful theoretical tools
- Engaging in research
- Practicing good presentation skills

- **ALL THREE ARE VERY IMPORTANT**

Main areas/topics of focus

- Optimization
- Information theory
- Statistics and Generalization
- Generative models
- Expressivity of deep architectures

Who is this class for?

Advanced grad students

- If you are a **first/second-semester MSc** student this class may not be good for you.
- Assumes solid knowledge of machine learning, and understanding of deep learning models
- Heavy focus on mathematics

Prerequisites I

- Linear algebra
  - vector and matrix norms
  - singular value decomposition
  - eigen-decomposition, change of basis
  - spectral radius vs operator norm

Prerequisites II

- Basic probability
  - Probability spaces
  - Basic distributions (Bernoulli, Gaussian, exponential…)
  - Basic statistics: mean, variance, …
  - Basic concentration bounds:
    - union bound, Markov inequality, Chebyshev…
    - [We’ll likely cover Chernoff bounds in class]

Prerequisites III

- Machine learning/deep learning
  - Graduate class in ML/DL
  - the basic workflow of supervised learning (training/validation/test splits, evaluation …)
  - composing and training basic ML models in PyTorch/TensorFlow/Keras…
  - **having read a few ML papers**

“Should I take this class?”

- It’s going to be rewarding: new research!
- If you can’t wait to start doing research do it!
- This class is not necessary if you want to:
  - Be a successful practitioner
  - Do more applied research
- **Surprise quizzes** the first few lectures will help us with assessment
- You can switch within the first couple of weeks to avoid fees (***please double check)

What are we going to achieve?

Calibrating expectations: tiny victories

- Deep learning theory is **hard**
- Researchers are extremely interested in it, but struggling to provide general results
- Many interesting results depend on strong assumptions
  - e.g. ‘for a class of objectives all local minima are global minima **if the data is Gaussian**’ [Ma et al. 2017]
  - or a study of the expressivity of neural networks **with random weights** [Poole et al. 2016]
- Still, even this kind of theory is much-needed progress!

Theory reading group

- Every Tuesday 10:30-11:30pm this room
- Brady Neal, Rémi Le Priol run it
- Similar focus as this class

Logistics

Logistics

- Language of instruction
- Grade breakdown
- Class hours
- Office hours
- Auditing policy

Language of instruction

- International group: many foreign students
- Lectures, notes and quizzes will be in english
- Contact instructor if this is a concern

Grading

- Participation 5%
- Scribing 10%
- Surprise quizzes, midterm 20%
- Paper presentations 25%
- Research project 40%

Participation 5%

- Questions, comments during lectures
- Class project updates
  - scheduled in-class
  - over email

Scribing 10%

- Most lectures will be given by me on the board
- A group of students each time will be responsible for taking notes
- Deliverable: notes in Latex format one week after the lecture
    - 5% penalty for late notes
- Everyone has to scribe once

Quizes/midterm 20%

- Focus on research project
- Low weight for in-class evaluation
- Surprise quizzes (10-15 minutes):
  - At least 4 of them
  - You need to be here for at least half of them to get the full quiz grade
- Short midterm, date TBA
- All material already available

Paper presentations 25%

- 4-5 classes will consist of paper presentations by students
  - they will only start after the fourth week (more later)
- Groups of 2-3 students:
  - read an agreed-upon paper from literature
  - prepare slides
  - present the work in class (20 minute talks)
- Graded based on quality of slides, and clarity of presentation

Research project 40%

- Groups of 2-3 students
- Proposal due in the middle of the semester
- Short, in-class progress report (5 minute talk)
- Poster presentation (date TBD)
- End of semester report (date TBD)

Research project 40%

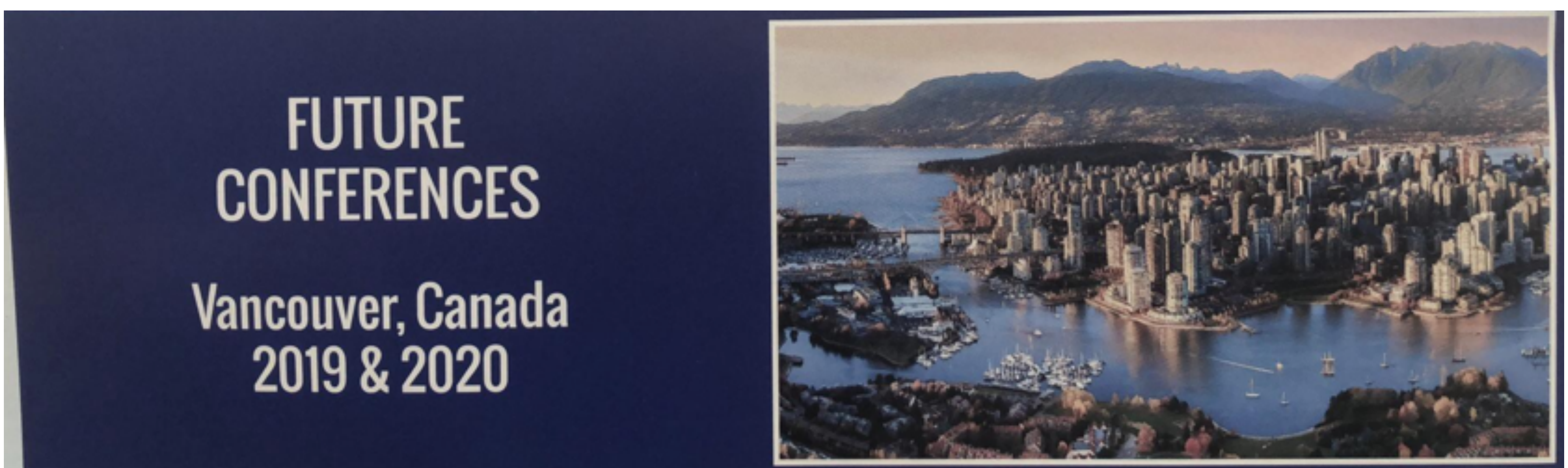
- Topics (I will release list of suggested topics):
  - Optimization
  - Generalization
  - Representation
  - Generative models
- Chosen based on:
  - Your own research interests (as aligned with the class)
  - Lists of papers I will be making available as we're covering the topics

Research project 40%

- Types of projects
    - Comprehensive literature review of selected topic, with careful presentation of relative merits of different methods and ideally performing simple experiments.
    - Application of ideas seen in class on your own research or other problem you find interesting.
    - Focusing on the math/analysis of existing or proposed methods.
    - Demonstrating limitations (via theory/experiments) of existing work
        - proposing solution
        - demonstrating simple prototype of new idea or analysis on a simplified setting (toy model)

Research project 40%

- The ideal project ==> NeurIPS submission
  - ambitious and difficult goal but worth it
  - not required to do well in class!



Class hours

- Wednesday 9:30-11:10
- Thursday **9:00**-10:40

Office hours

- Talk to me after class
- If needed, we’ll amend

Communication

- Email is risky
  - Helps if you clearly label subject: “IFT6085: … “
- Google group
- We won’t use Studium much

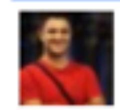
Auditing policy

- You’re free to sit in!
- As long as we have enough seating for registered students
- Interested in working on a project along with the class? Maybe we can accommodate. Come talk to me.
- Google group

Studium

- Mostly for announcements
- All material will be available on my website
- Students who took older version of class with same number IFT-6085, email me if you cannot see IFT-6085 on studium

IFT6085-A-H18 » Forums » Nouvelles » Welcome!



Welcome!
par Ioannis Mitliagkas, mardi 9 janvier 2018, 22:35

Dear students,

we begin this winter semester with our first lecture, tomorrow January 10th in André-Aisenstadt 3195 at 9:30am.

We will spend the lecture on an overview that motivates, introduces the topics and covers the class format, prerequisites and goals.

See you all in the morning!

The instructur,

Ioannis Mitliagkas

Répondre
Voir ce message dans son contexte

A theme:

When ML theory breaks down

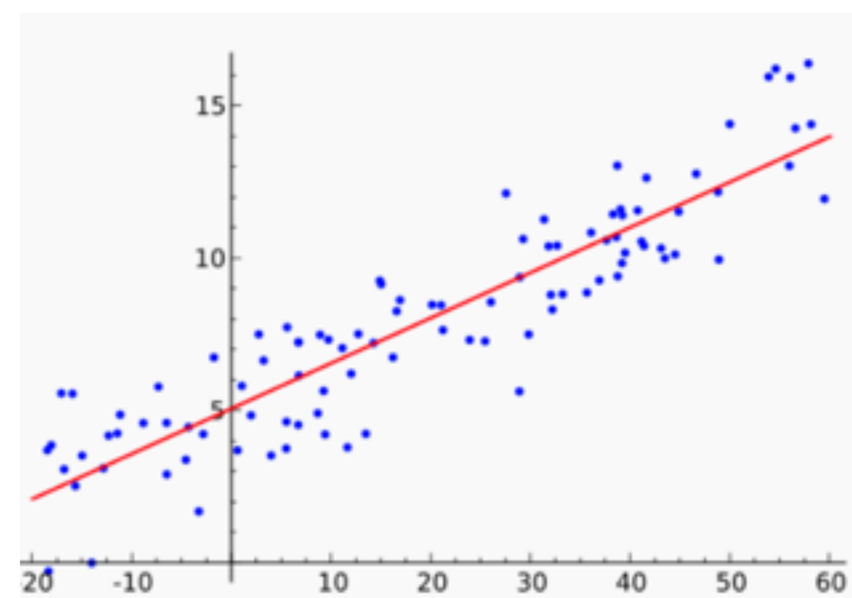
Machine learning is rigorous

Logistic regression

$$J(\theta) = \sum_{i=1}^{m} y^i \left[-\log\left(h_\theta\left(x^i\right)\right)\right] + \left(1 - y^i\right)\left[-\log\left(1 - h_\theta\left(x^i\right)\right)\right] \quad (1)$$

$$where \;\; h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}$$

- Classic and very successful tool from statistics
    - If you're in this class you've at least heard of it
- Used for classification
- IMPORTANT BASELINE

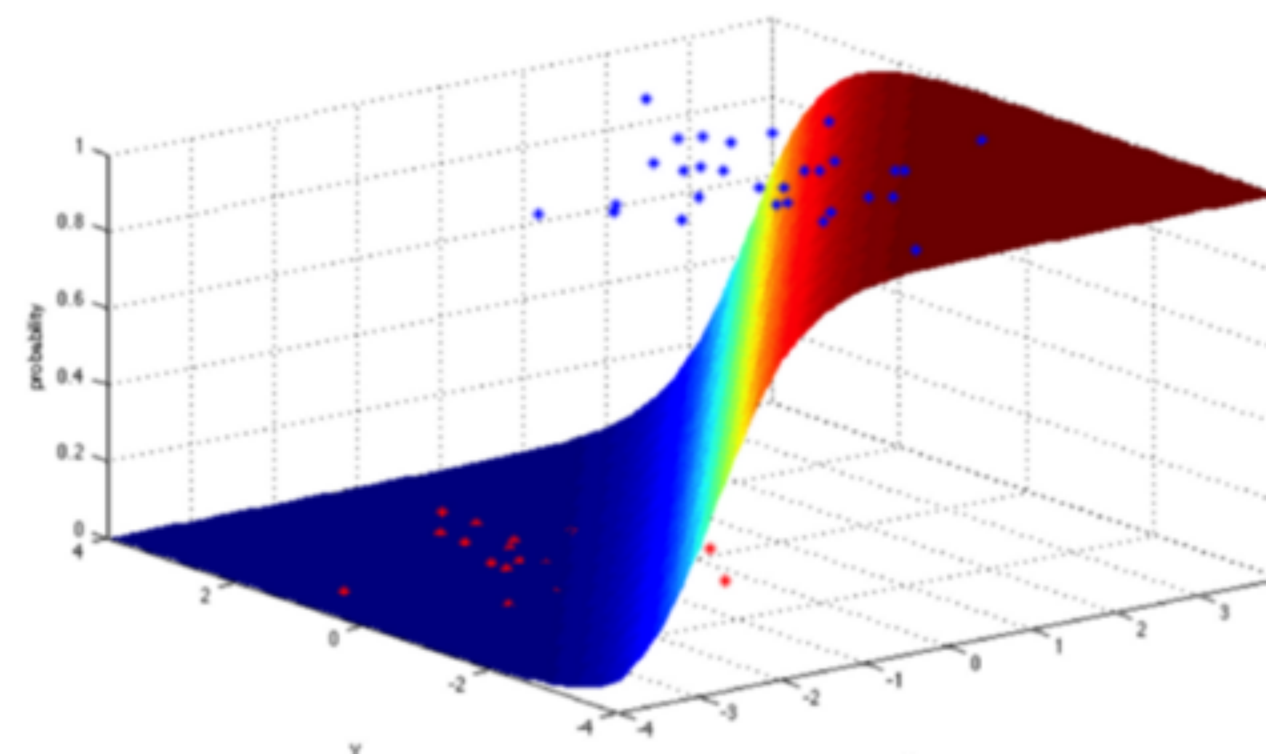


Logistic regression: ‘linear model’

$$J\left(\theta\right)=\sum_{i=1}^{m}y^{i}\left[-\log\left(h_{\theta}\left(x^{i}\right)\right)\right]+\left(1-y^{i}\right)\left[-\log\left(1-h_{\theta}\left(x^{i}\right)\right)\right] \quad (1)$$

$$where \;\; h_{\theta}\left(x\right)=\frac{1}{1+e^{-\theta^{T}x}}$$

- **Hypothesis class**: What kind of functions do we represent when we vary the model parameters, θ?

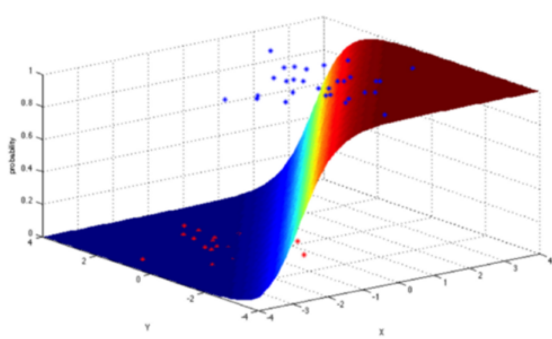


Logistic regression is interpretable

$$J(\theta) = \sum_{i=1}^{m} y^i \left[-\log\left(h_\theta\left(x^i\right)\right)\right] + \left(1 - y^i\right)\left[-\log\left(1 - h_\theta\left(x^i\right)\right)\right] \quad (1)$$

$$where \;\; h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}$$

- Predicted values can be interpreted as probabilities



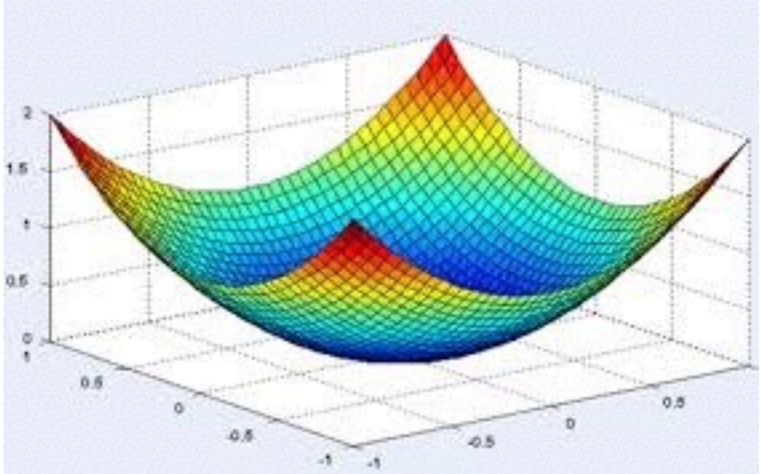
- Learned coefficients have rigorous interpretation through log-odds

Logistic regression: convex objective

$$J(\theta) = \sum_{i=1}^{m} y^i \left[-\log\left(h_\theta\left(x^i\right)\right)\right] + \left(1 - y^i\right)\left[-\log\left(1 - h_\theta\left(x^i\right)\right)\right] \quad (1)$$

$$where\ \ h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}$$

- Convex objective! link to proof. This means
  - It is easy to optimize!
  - (Stochastic) gradient descent works wonderfully
  - We have convergence guarantees



Logistic regression generalizes as expected

$$J(\theta) = \sum_{i=1}^{m} y^i \left[-\log\left(h_\theta\left(x^i\right)\right)\right] + \left(1-y^i\right)\left[-\log\left(1-h_\theta\left(x^i\right)\right)\right] \quad (1)$$

$$where \;\; h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$$

- We fit models on the **training set**
- But in the real world they are used on unseen data
- How well do they do out there? (**Generalization**)
- Classic ML bounds are good at predicting the generalization error for logistic regression

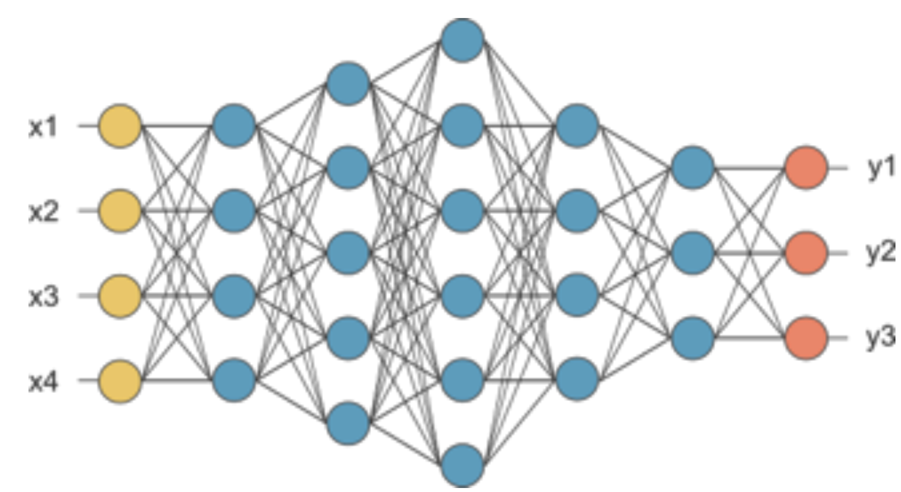
Deep learning: magic?

Deep neural networks

$$J(\theta) = \sum_{i=1}^{m} y^i \left[-\log\left(h_\theta\left(x^i\right)\right)\right] + \left(1-y^i\right)\left[-\log\left(1-h_\theta\left(x^i\right)\right)\right] \quad (1)$$

$$where \;\; h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$$

- Softmax output (related to logistic regression's logit)
- Multiple layers of non-linearities!
- Very powerful
- State of the art



Deep neural networks: hypothesis class?

$$J(\theta) = \sum_{i=1}^{m} y^i \left[-\log\left(h_\theta\left(x^i\right)\right)\right] + \left(1-y^i\right)\left[-\log\left(1-h_\theta\left(x^i\right)\right)\right] \quad (1)$$

$$where \;\; h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$$

- **Hypothesis class**: What kind of functions do we represent when we vary the model parameters, θ?

- **Universal approximation**: single hidden layer with infinite neurons can approximate any function**

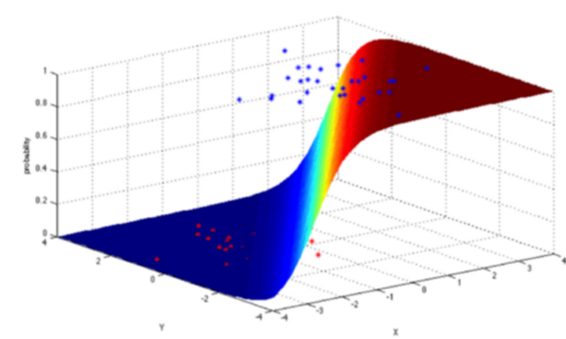
- More generally, we don't exactly know.

Deep neural networks: interpretability

$$J(\theta) = \sum_{i=1}^{m} y^i \left[-\log\left(h_\theta\left(x^i\right)\right)\right] + \left(1 - y^i\right)\left[-\log\left(1 - h_\theta\left(x^i\right)\right)\right] \quad (1)$$

$$where \;\; h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}$$

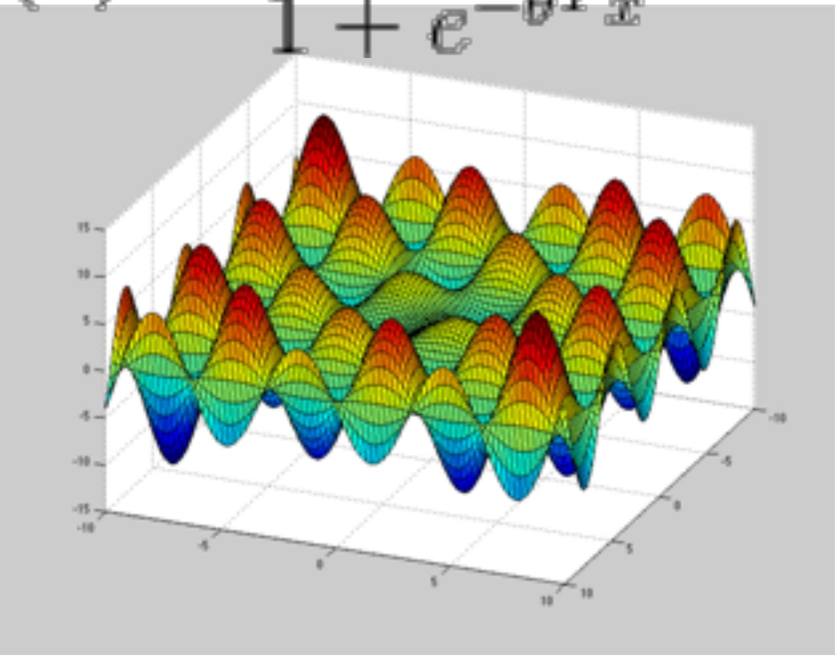
- Why is our deep learning model coming up with this prediction?
  - We don’t exactly know how to attribute outputs to inputs like logistic regression
  - With some notable exceptions
- Active area of research!



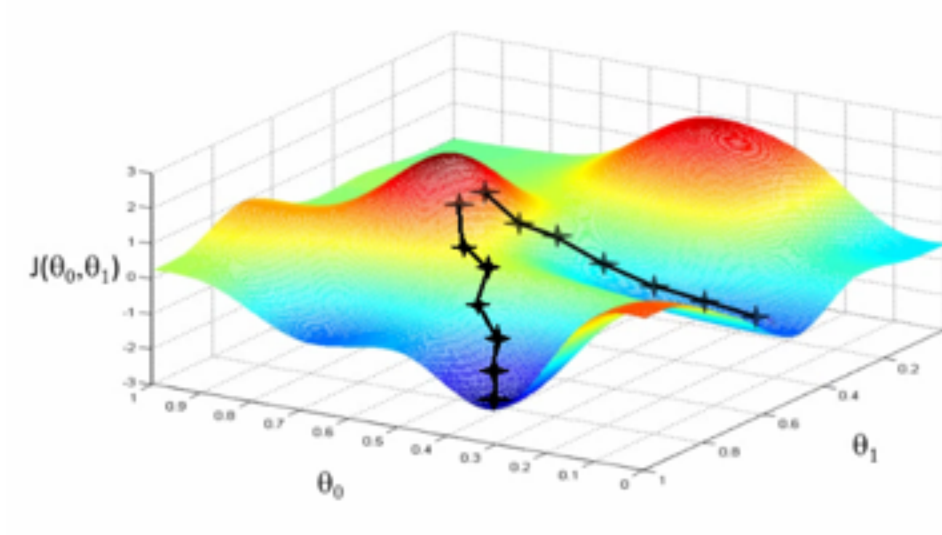
Deep neural networks: non-convex objective

$$J(\theta) = \sum_{i=1}^{m} y^i \left[-\log\left(h_\theta\left(x^i\right)\right)\right] + \left(1-y^i\right)\left[-\log\left(1-h_\theta\left(x^i\right)\right)\right] \quad (1)$$

$$where \;\; h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$$



- Non-convex objective!
  - All bets are off
  - We have no convergence guarantees
  - Different minima from different initializations
- However, gradient descent STILL WORKS!



Deep neural networks: generalize against all odds

$$J(\theta) = \sum_{i=1}^{m} y^i \left[-\log\left(h_\theta\left(x^i\right)\right)\right] + \left(1 - y^i\right)\left[-\log\left(1 - h_\theta\left(x^i\right)\right)\right] \quad (1)$$

$$where \;\; h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}$$

- Classic generalization bounds suggest that to get good generalization in DL, we should be using 10x or 100x the data we are actually using.
- What is going on?
- One of the most interesting questions right now in DL.

First part of course:

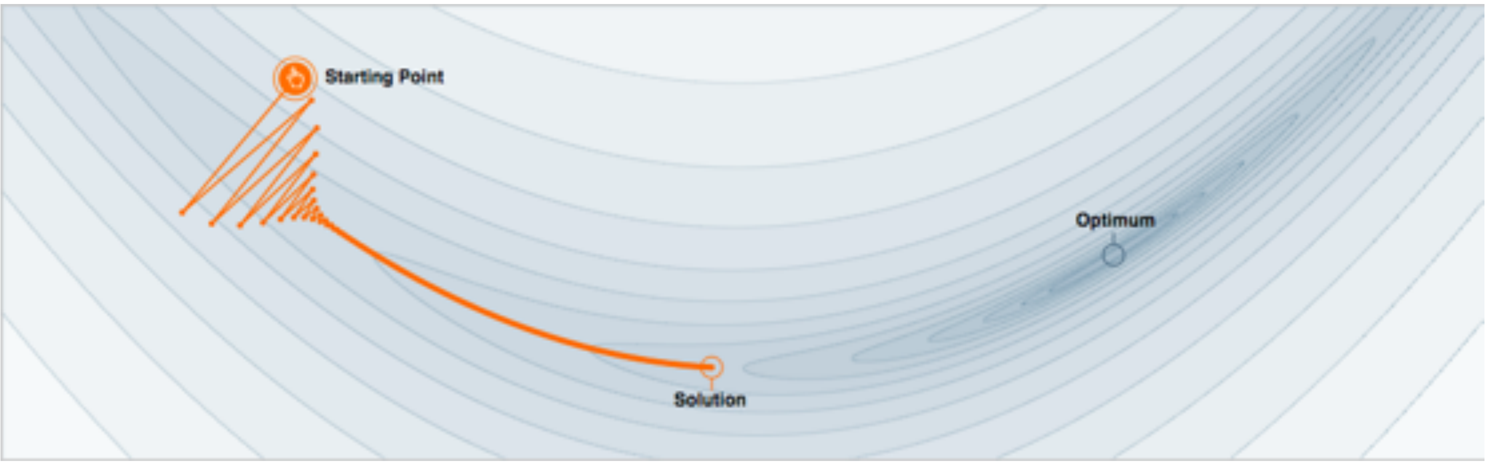
Some classic results

Crash course in optimization

GRADIENT DESCENT AND MOMENTUM ALGORITHMS

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

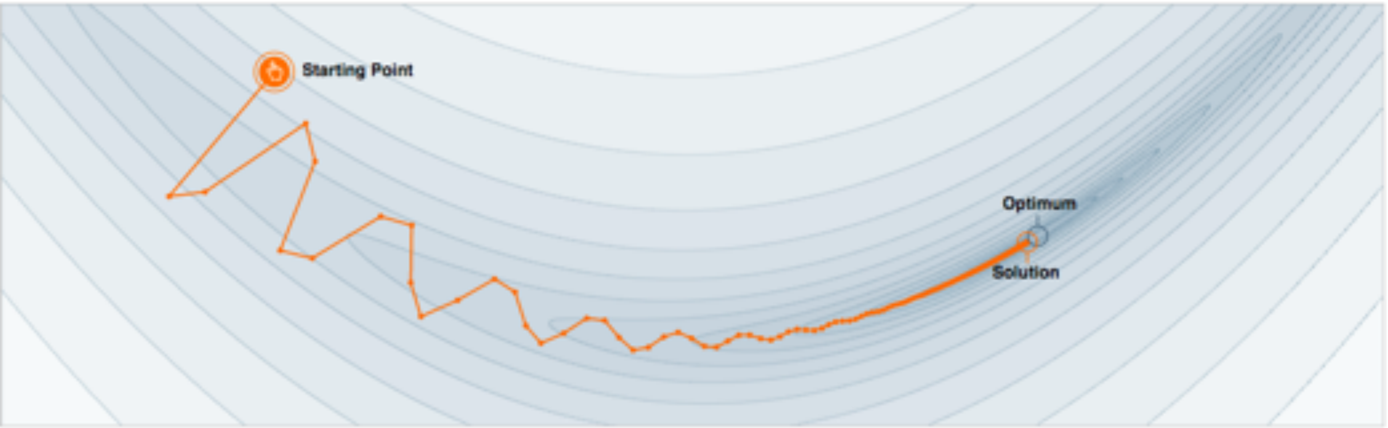
Without momentum



[Polyak, 1964]

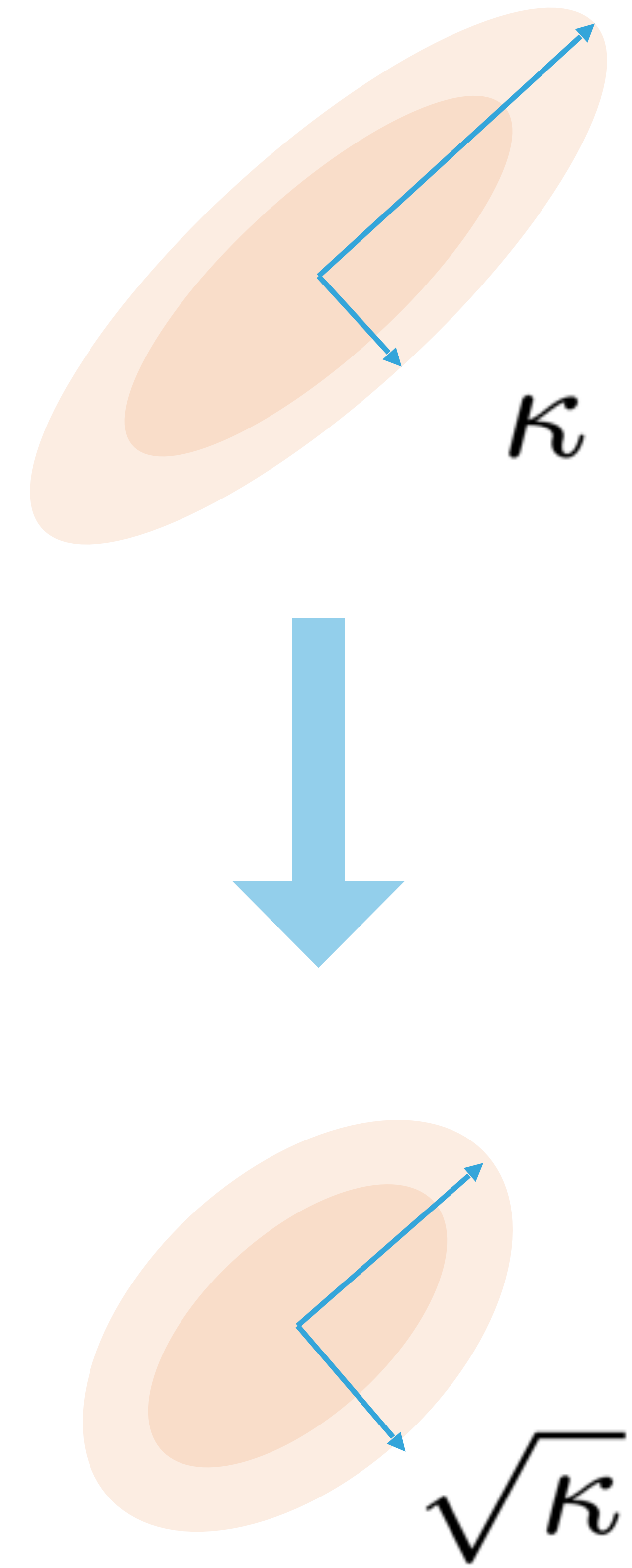
With momentum

[Distill blog]



CONDITION NUMBER

Dynamic range of curvatures, κ



GRADIENT DESCENT ON STRONGLY CONVEX

Convergence rate $O(\frac{\kappa-1}{\kappa+1})$

GRADIENT DESCENT WITH MOMENTUM

Dependence on κ changes

$$O(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1})^*$$

EFFECTIVELY IMPROVES THE CONDITION NUMBER

OBJECTIVE

$$f(w) = \frac{1}{n}\sum_{i=1}^{n} f(w; z_i)$$

z_i : data point/batch

GOAL: MINIMIZE TRAINING LOSS

STOCHASTIC GRADIENT DESCENT

$$w_{t+1} = w_t - \alpha_t \nabla_w f(w_t; z_{i_t})$$

α_t : step size

i_t : batch used for step t

MOMENTUM

$$w_{t+1} - w_t = \mu_L (w_t - w_{t-1}) - \alpha_t \nabla_w f(w_t; z_{i_t})$$

Quick review of basic elements of statistical learning

Statistical learning

- Real quick: supervised learning
- Concentration bounds
  ===> Classic generalization bounds
- VC dimension
- PAC-Bayes bounds

Main part of course:

recent papers

Paper topics

- Generalization: theoretical analysis and practical bounds

- Information theory and its applications in ML (information bottleneck, lower bounds etc.)

- Generative models beyond the pretty pictures: a tool for traversing the data manifold, projections, completion, substitutions etc.

- Taming adversarial objectives: Wasserstein GANs, regularization approaches and controlling the dynamics

- The expressive power of deep networks

Generative models

DISCRIMINATIVE

$$\boxed{p(y|x;\theta)}$$

GENERATIVE

$$\boxed{p(x|y) \qquad p(y)}$$

Bayes rule: $$p(y|x) = \frac{p(x|y)p(y)}{p(x)}$$

MODELING ASSUMPTIONS

DISCRIMINATIVE

$$p(y|x;\theta)$$

Logistic regression $$h_\theta(x) = g(\theta^T x)$$

Sigmoid function

GENERATIVE

$$p(x|y) \qquad p(y)$$

Bayes rule: $$p(y|x) = \frac{p(x|y)p(y)}{p(x)}$$

Gaussian discriminant analysis (GDA)

GAUSSIAN DISCRIMINANT ANALYSIS

$$\begin{aligned} y &\sim \text{Bernoulli}(\phi) \\ x|y=0 &\sim \mathcal{N}(\mu_0, \Sigma) \\ x|y=1 &\sim \mathcal{N}(\mu_1, \Sigma) \end{aligned}$$

CONNECTION TO LOGISTIC REGRESSION

$$p(y=1|x;\phi,\Sigma,\mu_0,\mu_1) = \frac{1}{1+\exp(-\theta^T x)},$$

Same form as logistic regression, though not exact same decision surface.

Converse not true:

Logistic regression form for y|x does not imply Gaussian distribution for x|y

GENERATIVE MODELS MAKE STRONGER ASSUMPTIONS

GENERATIVE MODELS

- Stronger assumptions
- Better/faster fit when assumptions are correct

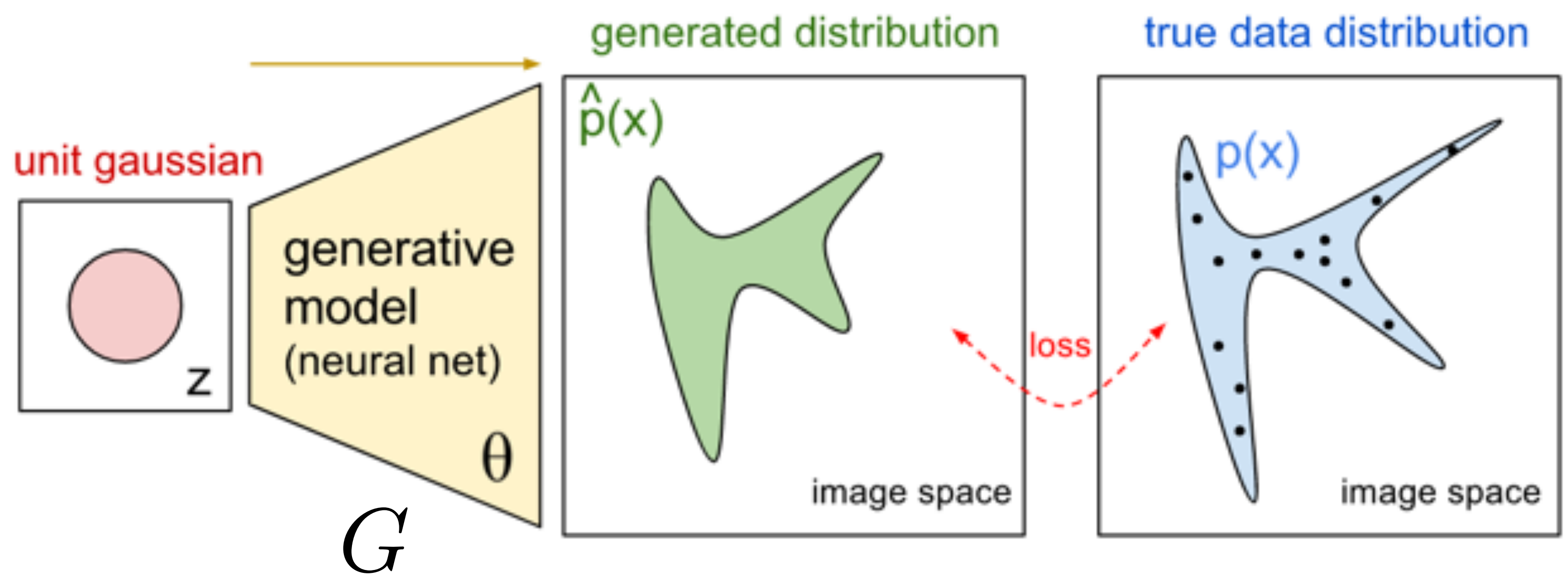
  Asymptotically efficient

- Can perform badly when assumptions are bad

DISCRIMINATIVE

- Weaker assumptions
- More robust!!
- More widely used for classification

NO MODELING DECISIONS (*RATHER, HIGHER LEVEL MODELING)



A FEW APPROACHES TO TRAIN AND REGULARIZE

- Autoregressive models (PixelRNN)
- Variational AutoEncoders
- Generative moment matching networks

GENERATIVE ADVERSARIAL NETWORKS [GOODFELLOW, 2014]

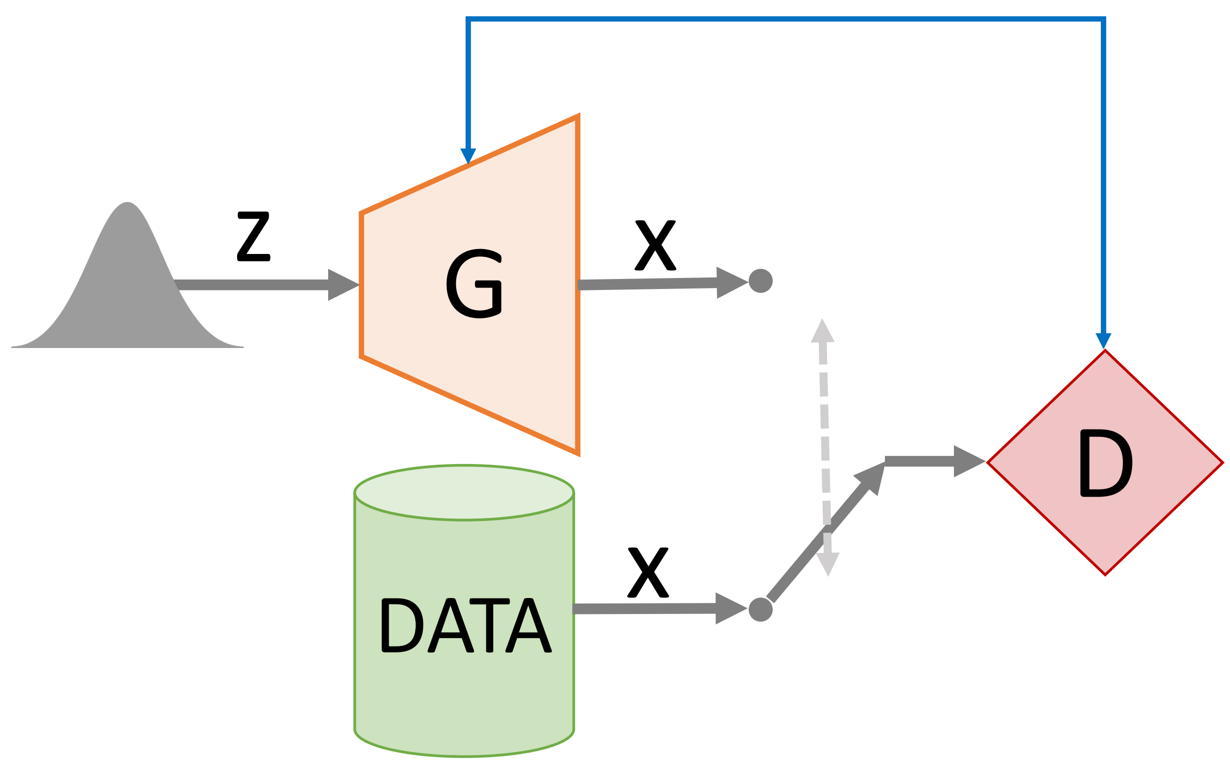
Generator network, G

Given latent code, z, produces sample G(z)

Discriminator network, D

Given sample x or G(z), estimates probability it is real

Both differentiable



GENERATIVE ADVERSARIAL NETWORKS [GOODFELLOW, 2014]

Generator network, G

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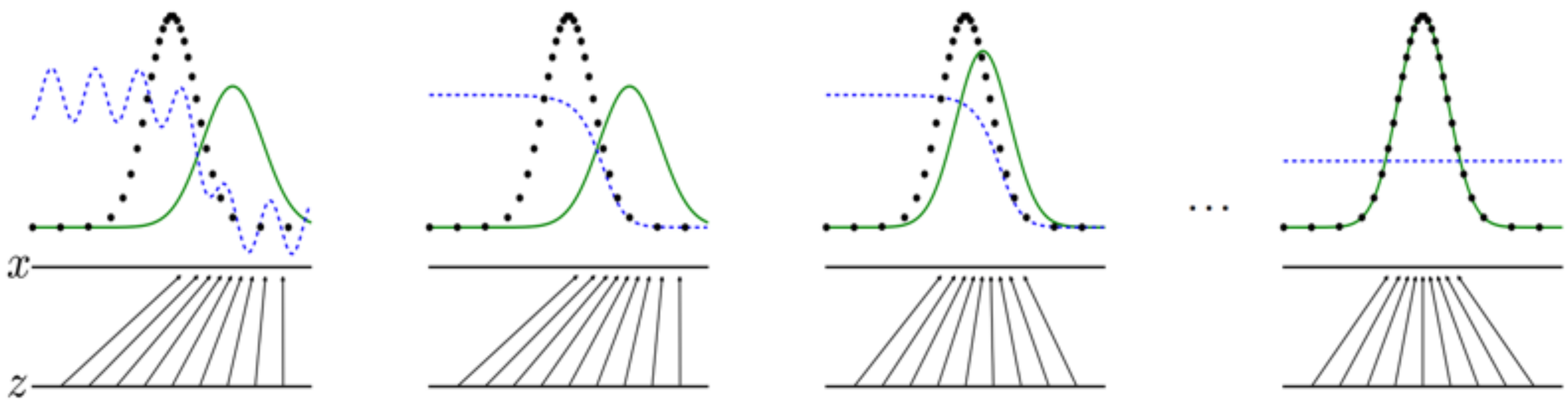
Given sample x or G(z), estimates probability it is real

Both differentiable

$$\min_G \max_D V(D, G) = \mathbb{E}_{\boldsymbol{x} \sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z} \sim p_{\boldsymbol{z}}(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z})))]$$

GENERATIVE ADVERSARIAL NETWORKS [GOODFELLOW, 2014]

$$\min_G \max_D V(D,G) = \mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z}\sim p_{\boldsymbol{z}}(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z})))]$$



BENEFITS

- Easy to implement
- Computational (No approximate inference/no partition function estimation)

DIFFICULT TO TRAIN

SATURATION

Gradients become zero

MODE COLLAPSE

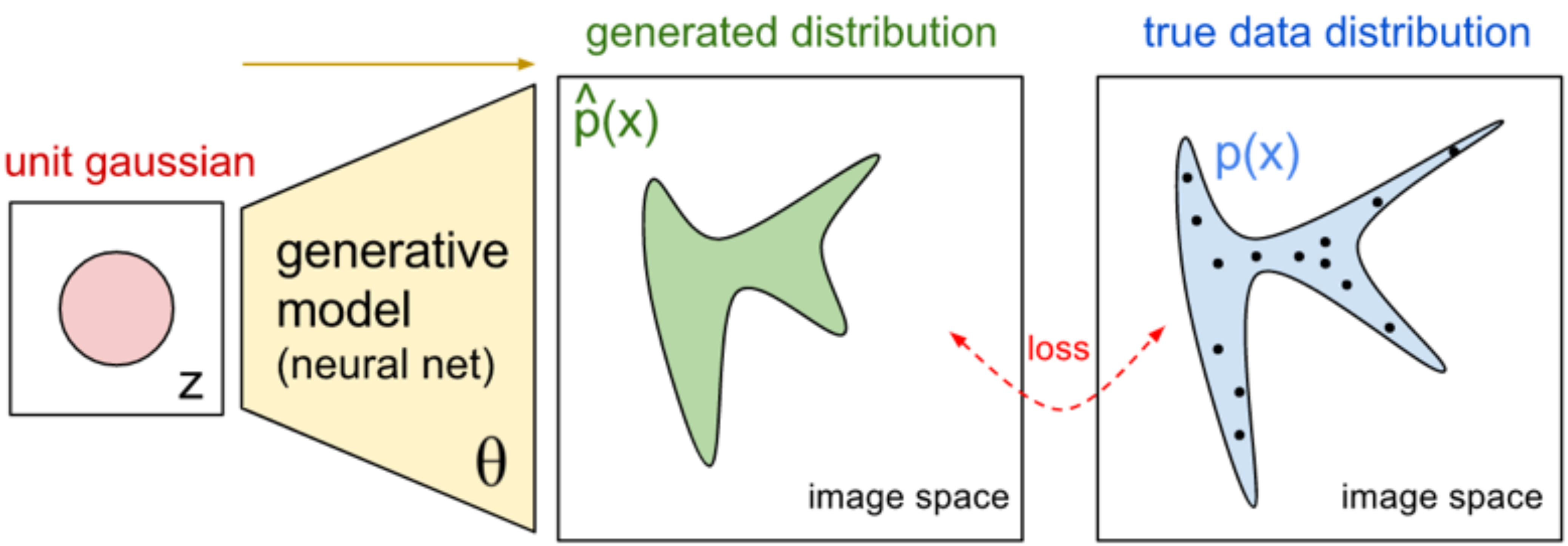
Whole chunks of space can be dropped.

Wasserstein GANs deal with some of those issues

DYNAMICS OF SADDLE POINT OPTIMIZATION!

Momentum dynamics play important role.
Negative momentum can help.

GENERATIVE ADVERSARIAL NETWORKS [GOODFELLOW, 2014]



But why?

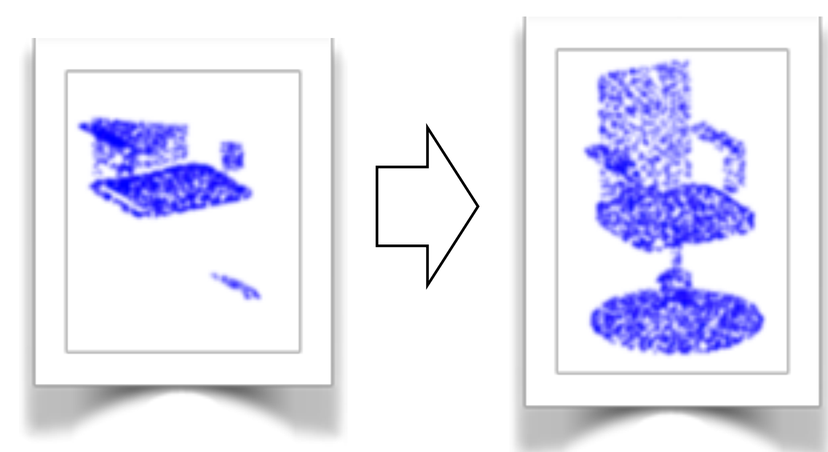
DREAMING UP STUFF?

Generated images

VERY USEFUL COMPONENT!!

- Data augmentation

- Semantic operations/analogies



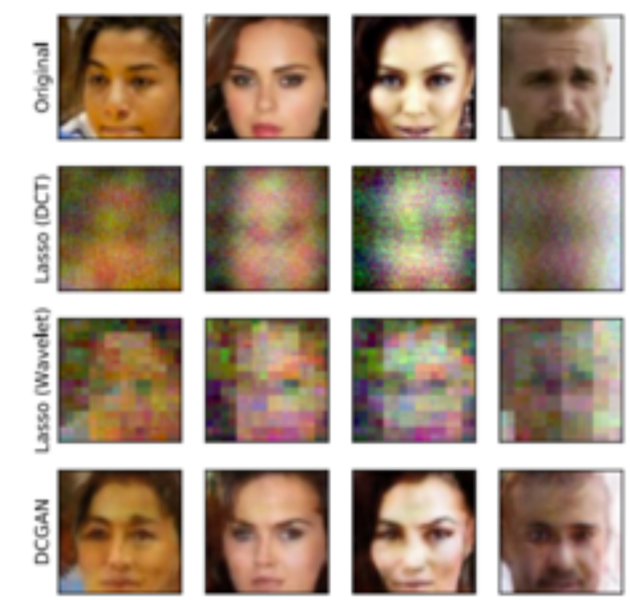
- Completion
- Segmentation…

BEYOND SPARSITY [BORA ET AL., 2017]

Generator G trained on desirable manifold (faces, 3D objects)

Given sample y,

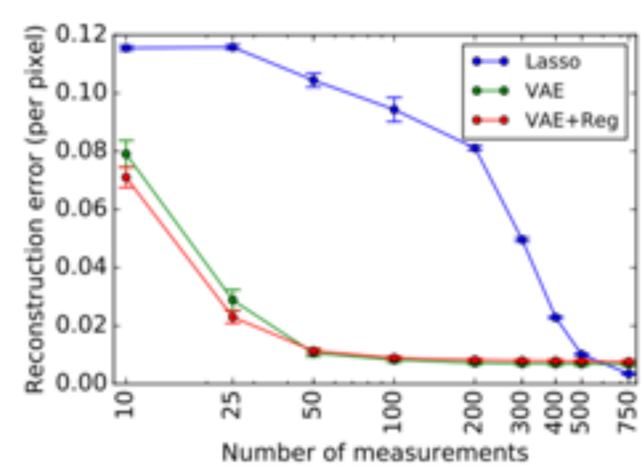
potentially corrupted by function M



We can ‘invert’ the generator

$$min_z \|M(G(z)) - y\|$$

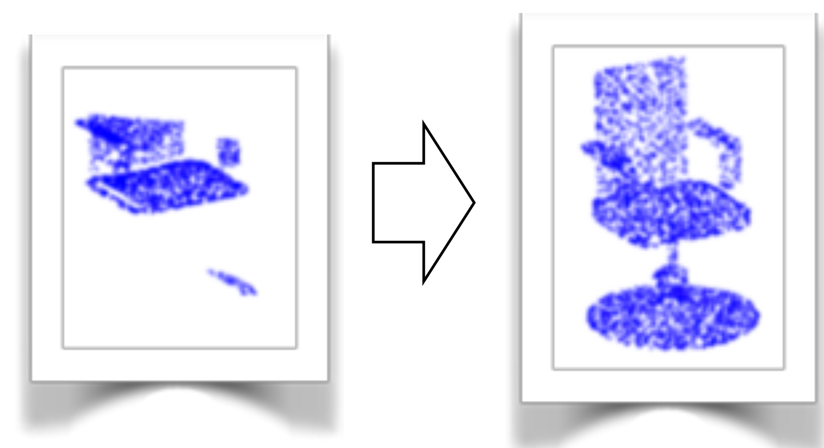
and find a pre-image of y on the manifold



The trained generative model is critical!

INTERESTING QUESTIONS

- How do we use generative models?



- How do we evaluate?
- How do we stabilize adversarial training?

- How do we reduce mode collapse?

Resources on website

mitliagkas.github.io/ift6085-dl-theory-class/

- Currently contains info about 2018, will be updated soon
- Most course material will remain the same
- First two monographs are a **great** sources of classic optimization and ML resource.
- I will be using them a lot throughout (and assigning some readings from there)

Resources

1. Convex Optimization: Algorithms and Complexity, Sebastien Bubeck.
2. Understanding Machine Learning: From Theory to Algorithms, by Shai Shalev-Shwartz and Shai Ben-David.
3. iPython notebook demonstrating basic ideas of gradient descent and stochastic gradient descent, simple and complex models as well as generalization.

Questions

Quiz :)

First quiz

- **Not** part of grade
- Will allow us to assess the background of the class and adjust material accordingly

Self assessment

- Did you feel like you knew what most of the quiz questions were talking about?
- Have you seen some of the “I hope you know this”-topics I mentioned in a previous class?
- Can you follow the code and ideas in the iPython notebook listed #3 under ‘Resources’ in the class website?
- Have you read 3 different machine learning papers?