IFT 6085

Theoretical principles for deep learning

Winter 2021

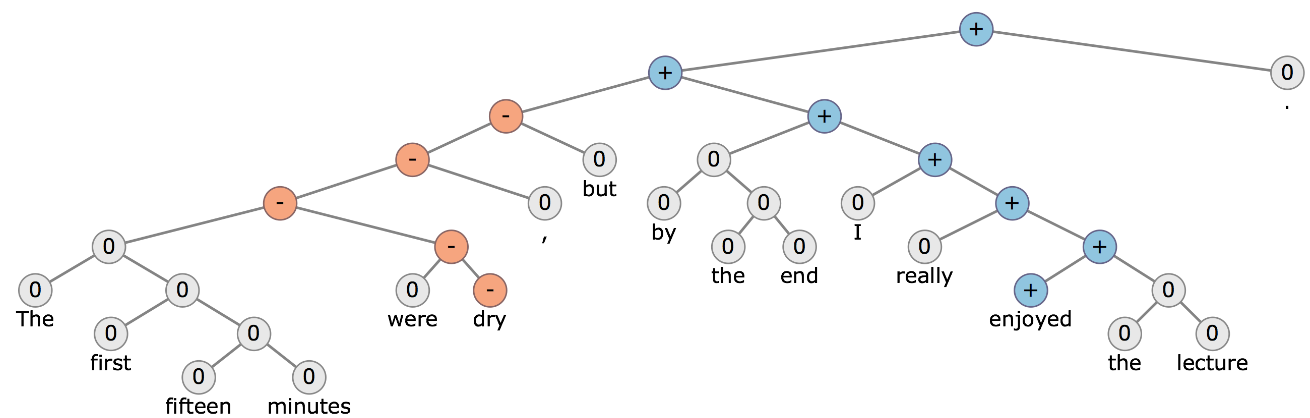
Instructor: Ioannis Mitliagkas

Today [overview mostly]

- 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

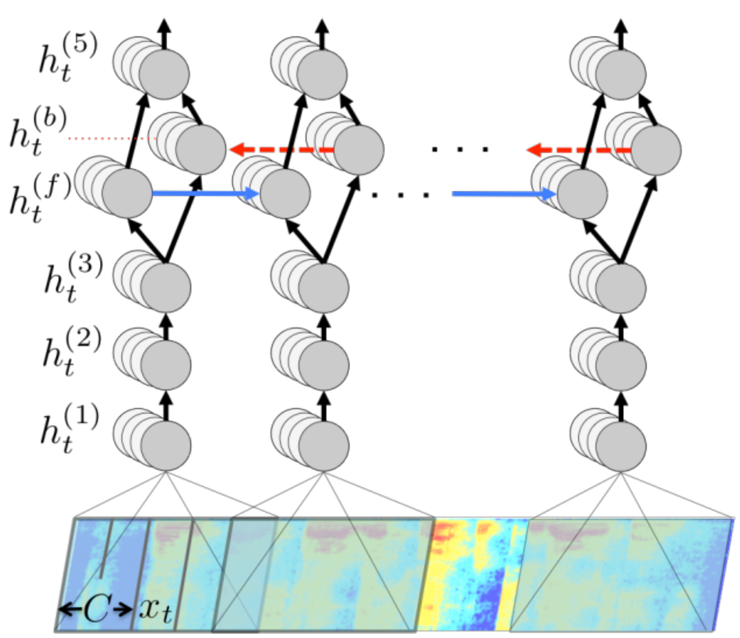
Deep learning drives significant progress in modern ML/AI

NATURAL LANGUAGE PROCESSING



cs224d.stanford.edu

SPEECH RECOGNITION



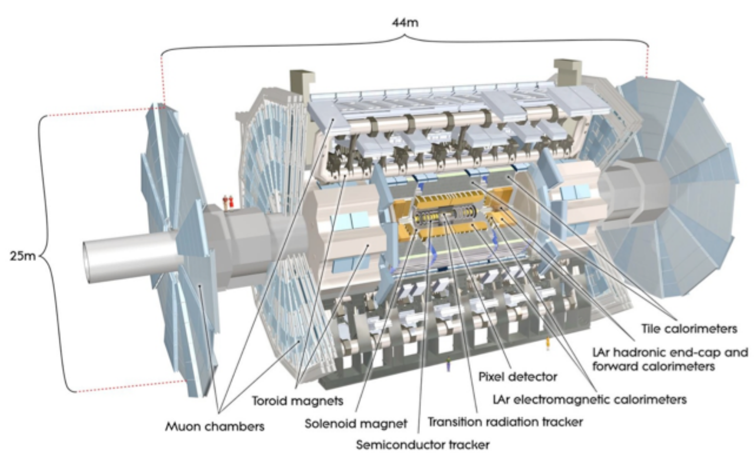
COMPUTER VISION

NVIDIA

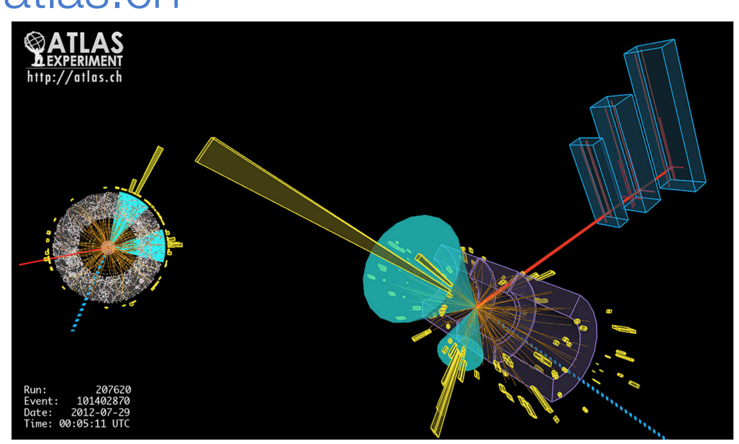
CORI PHASE II

- 9600+ Knights Landing nodes

HIGH-ENERGY PHYSICS (HEP)

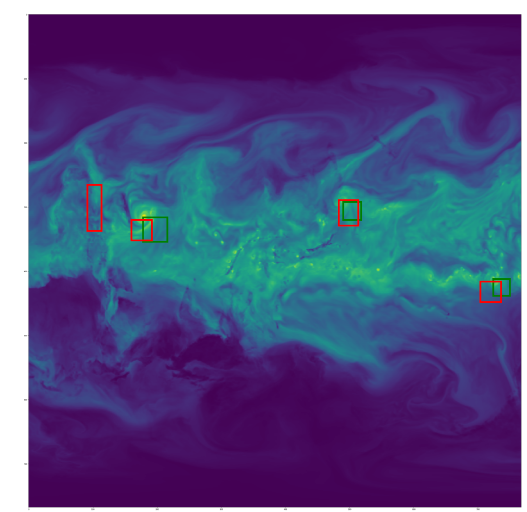


atlas.ch

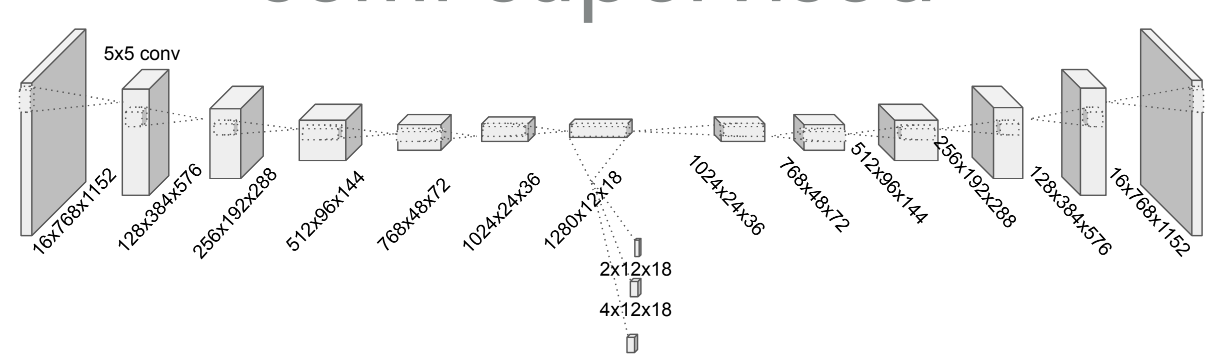


7.4TB data

CLIMATE SCIENCE



15TB data
semi-supervised

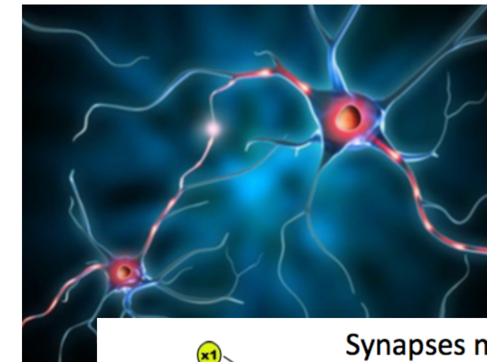


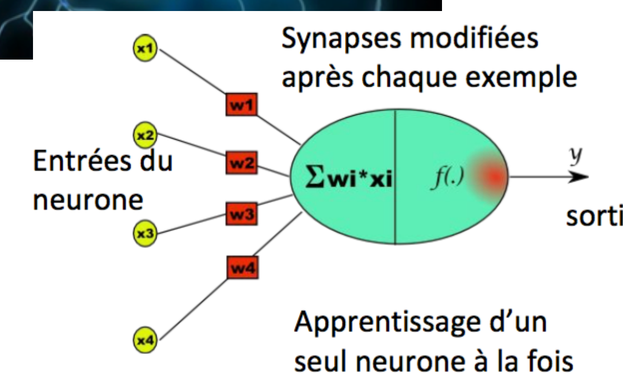
Economy-altering potential

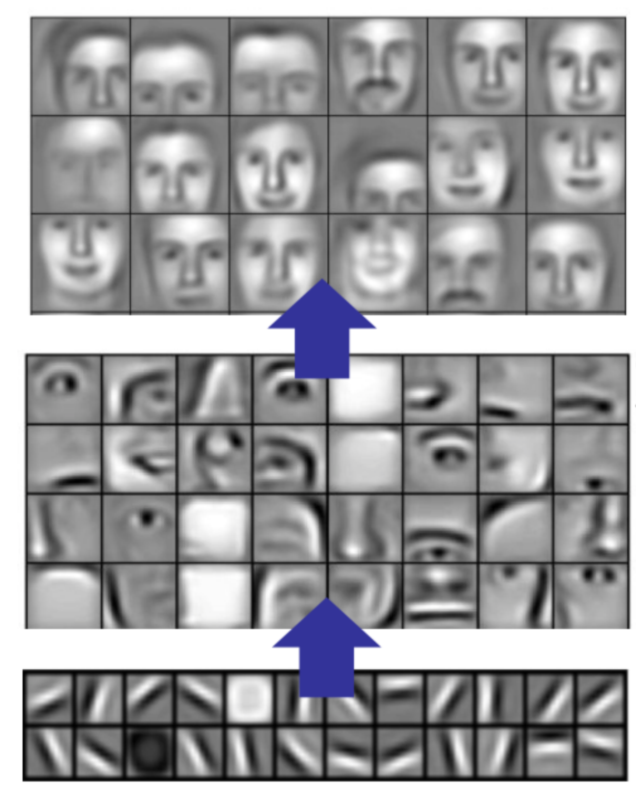
How do we achieve this great performance?

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

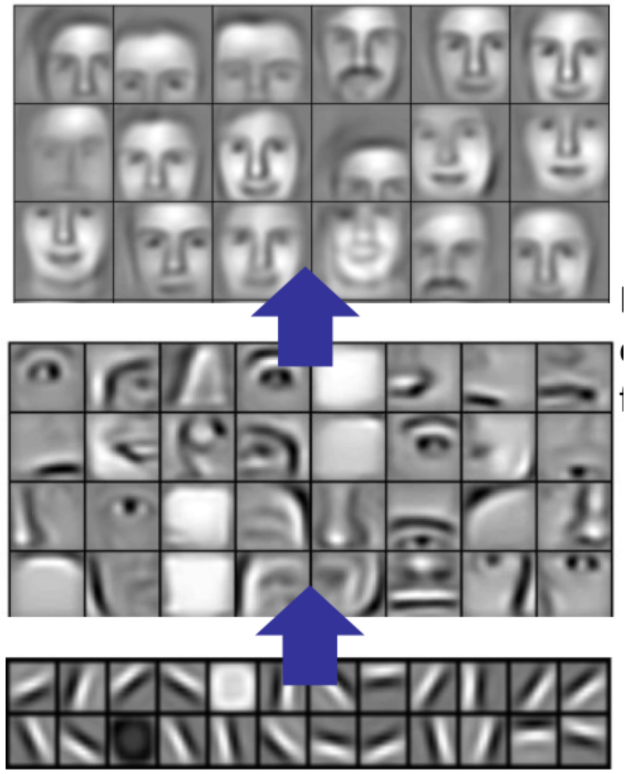






Recent boom

- 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

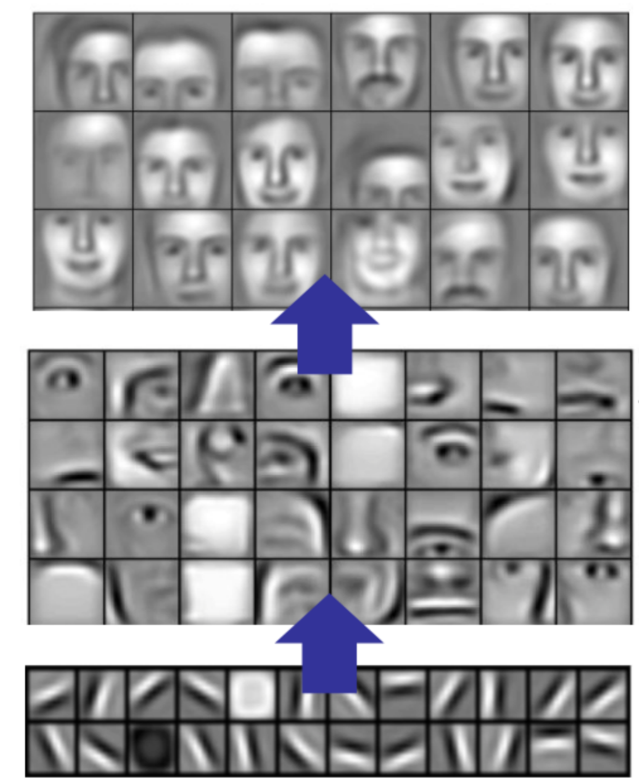
  - Can switch within 1-2 semesters. Email Linda Peinthière (lpeinthiere.umontreal@gmail.com) if interested.

MILA

Université de Montréal

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

This class

- Will not teach you machine learning
  - You must have passed ML class first
- Will not teach you deep learning
  - You might be ok without DL class if you took ML
- Will not teach you math
  - You must have taken math classes before

Goals of the class

- Exposure to useful theoretical tools
- Motivate you to apply your math skills
- Read many papers
- Engage in research
- Practice good presentation skills

- **ALL 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 is not 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?”

- 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
- **Quizzes** on every lecture 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!

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

Grading

- Participation 5%
- Scribing 10%
- **Daily quizzes 15%**
- **Early in-class exam 5%**
- Midterm 15%
- Paper presentations 15%
- Research project 35%

Scribing 10%

- Most lectures will be given by me on the board
- 1-2 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

Daily quizzes 15%

- On the reading material of the day
- 5-10 minutes at beginning of lecture, **on your laptop**
- 14-18 quizzes
- Grade computed as average of 8 best quizzes
- All material already available
- First graded quiz tomorrow morning!

Midterm 15%

- Mostly on crash course material
  - Optimization
  - Statistical learning theory
- DATE TBA (mid-late February)

Paper presentations 15%

- ~4 lectures will consist of paper presentations by students
  - they will only start after the fourth week (more later)
- Groups of 2 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 35%

- Groups of 2 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 35%

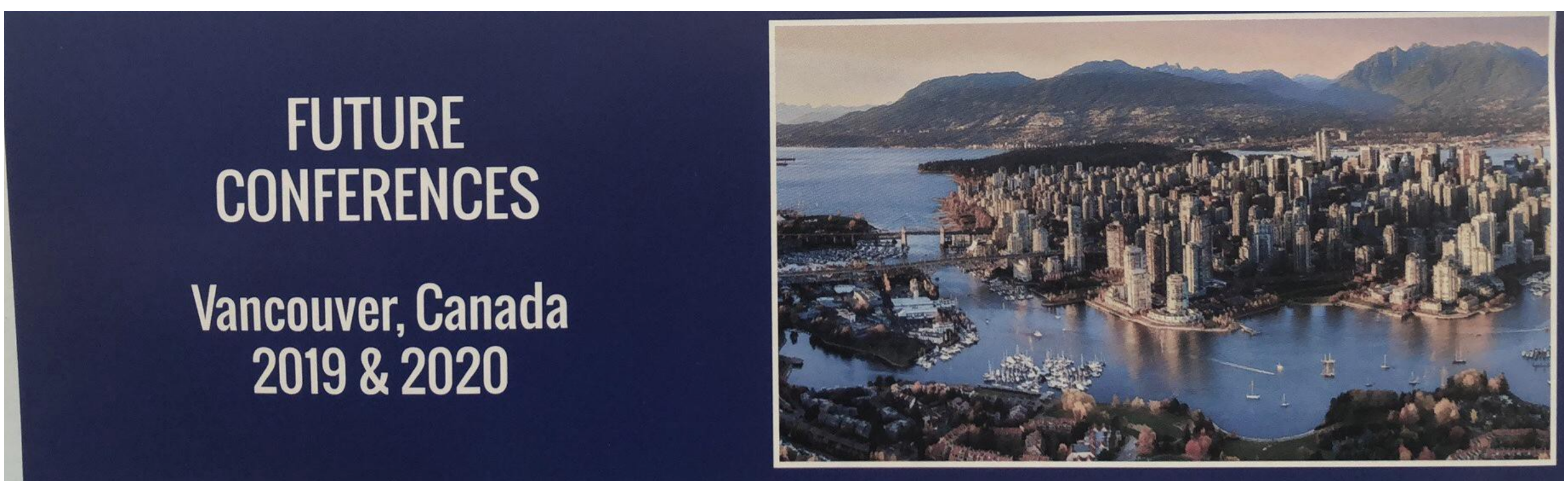
- Topics (I will release list of suggested topics):
    - Optimization
    - Generalization
    - Representation
    - Generative models
- Chosen based on:
    - Your own research interests (as aligned with the class)
    - Lists of papers I will be making available as we're covering the topics

Research project 35%

- 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 35%

- 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 bad idea
  - Helps if you clearly label subject: “IFT6085: … “
- Slack
- Studium for announcements

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.
- Slack

A theme:

When ML theory breaks down

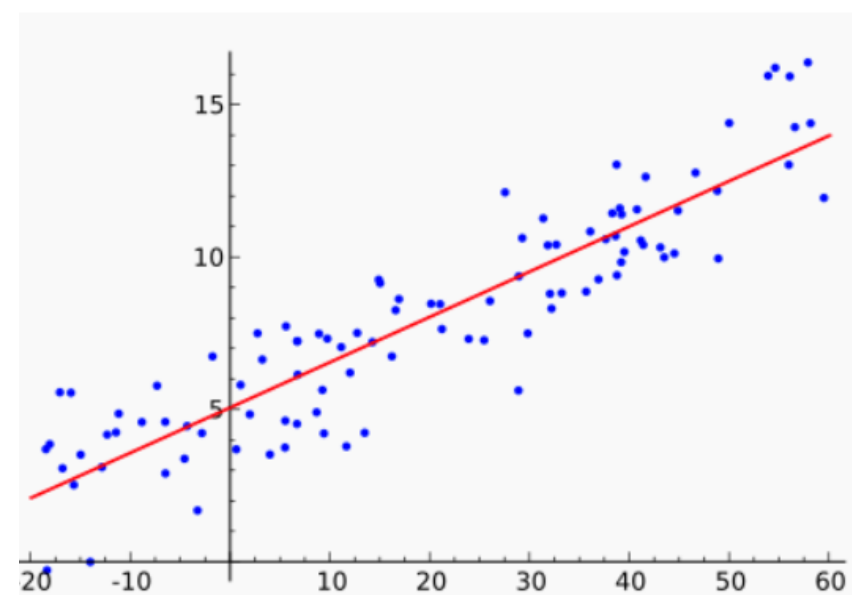
Machine learning is rigorous

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

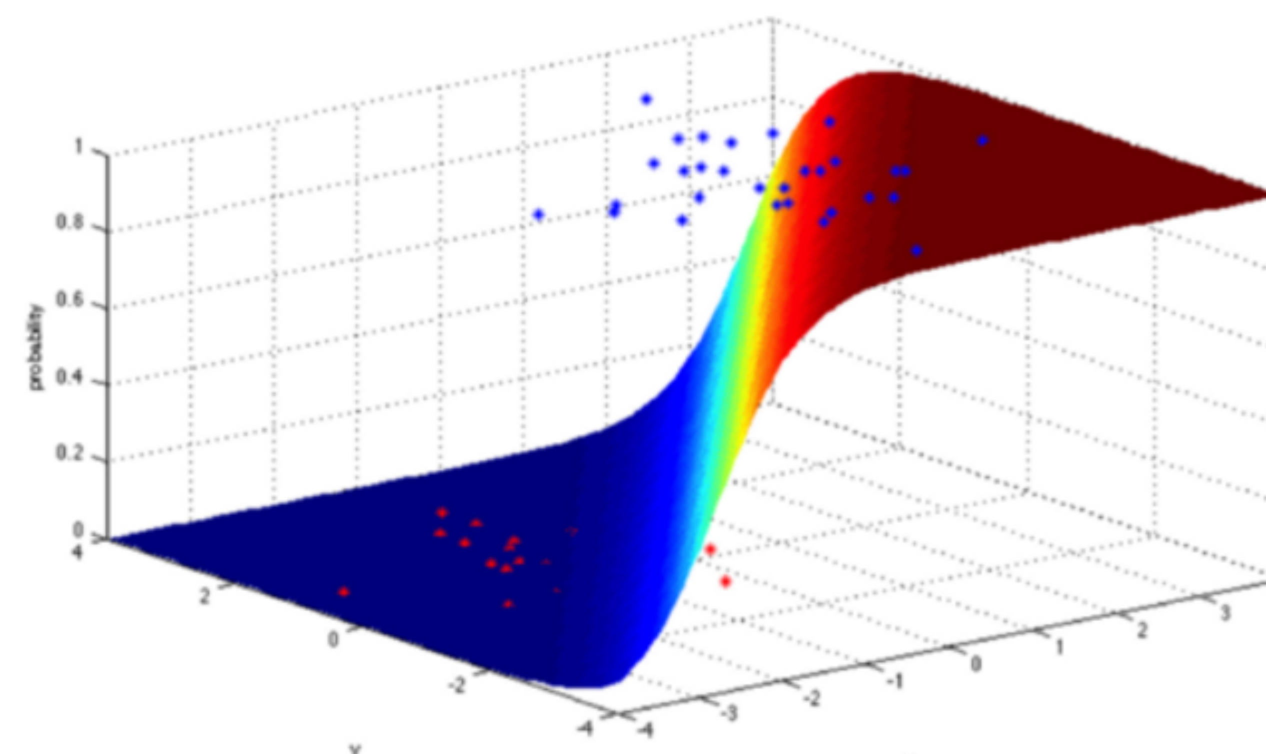


Logistic regression: ‘linear model’

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

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

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

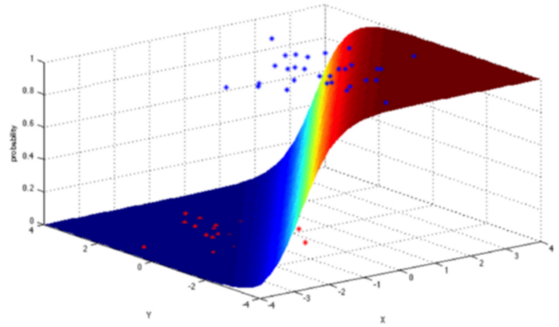


Logistic regression is interpretable

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

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

- Predicted values can be interpreted as probabilities



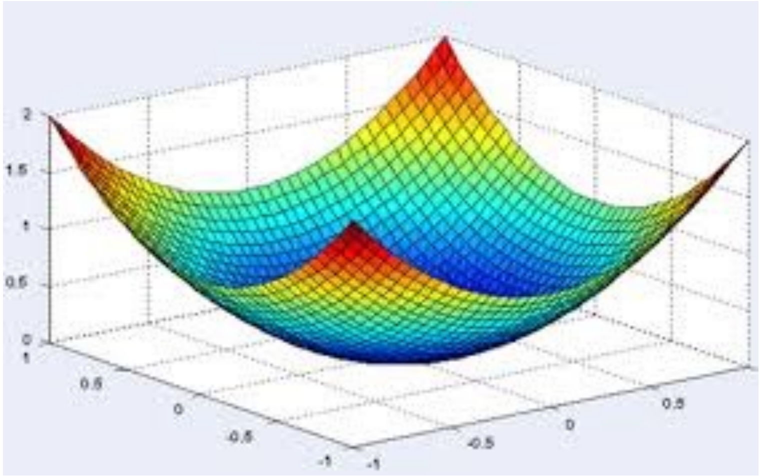
- Learned coefficients have rigorous interpretation through log-odds

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

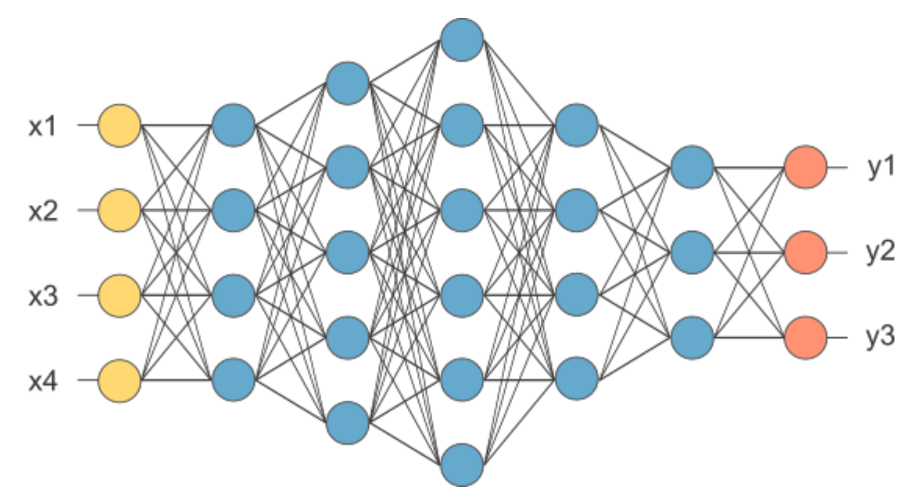
Deep learning: magic?

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?

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

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

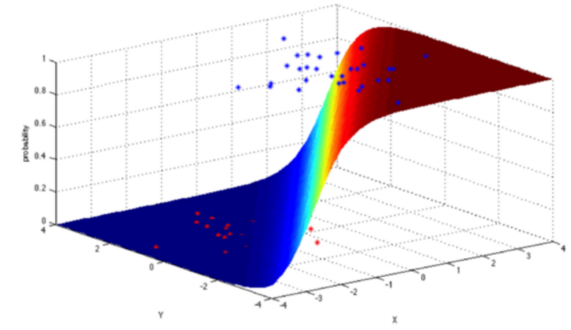
- **Hypothesis class**: What kind of functions do we represent when we vary the model parameters, θ?
- **Universal approximation**: single hidden layer with infinite neurons can approximate any function**
- More generally, we don’t exactly know.

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!

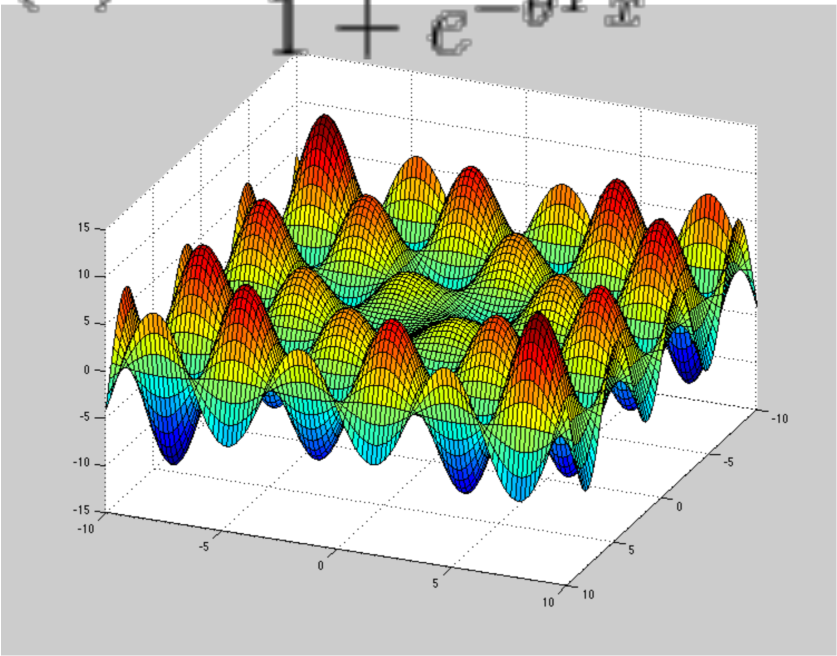


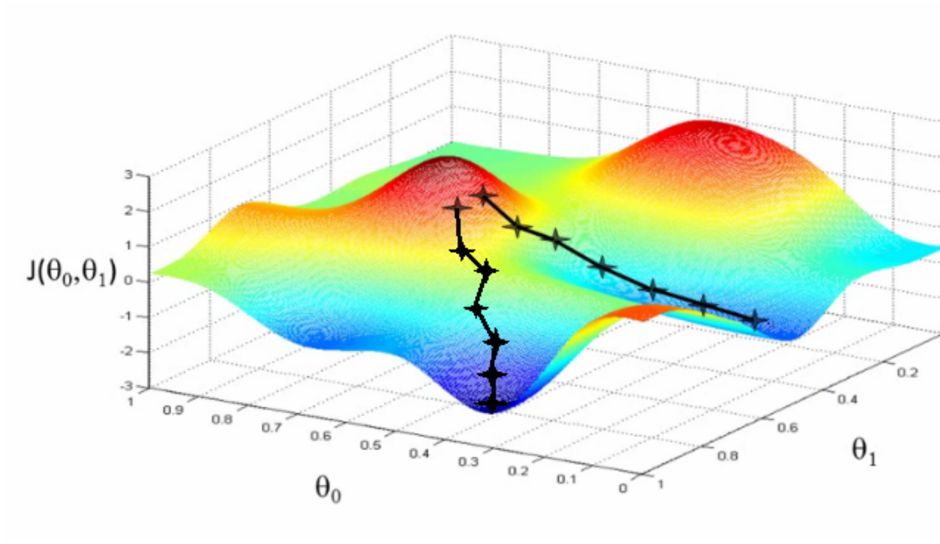
Deep neural networks: non-convex objective

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

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

- 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:

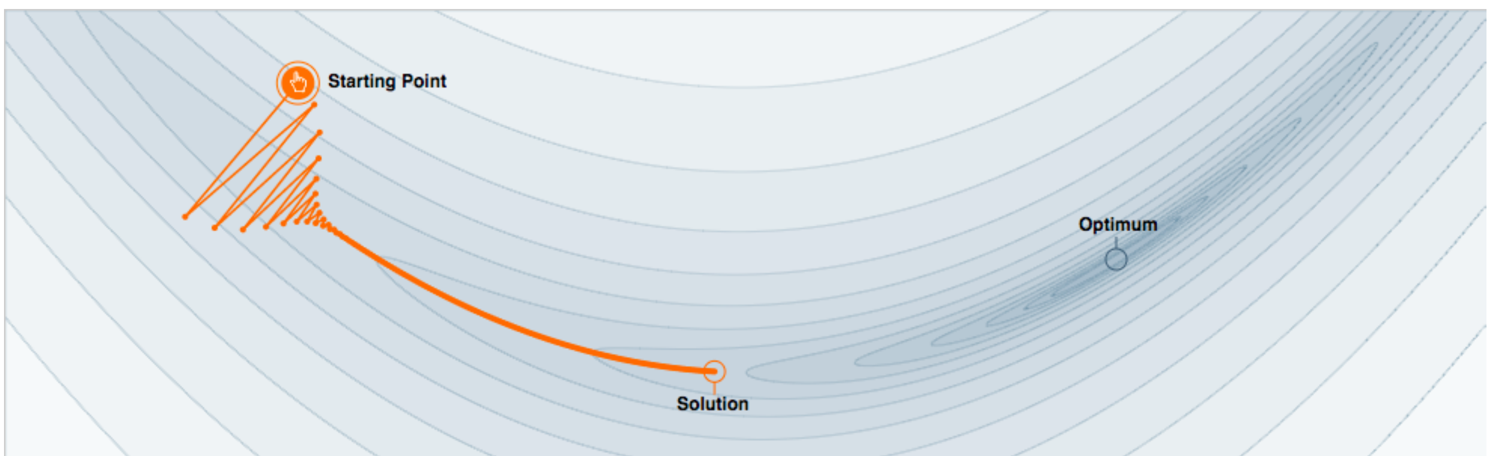
Some classic results

Crash course in optimization

GRADIENT DESCENT AND MOMENTUM ALGORITHMS

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

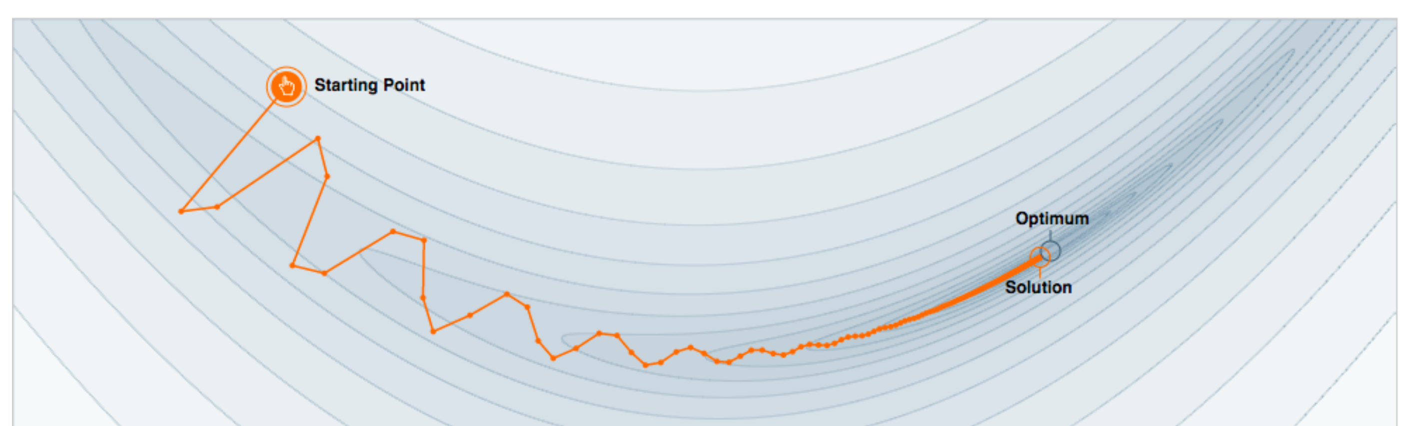
Without momentum



[Polyak, 1964]

With momentum

[Distill blog]



CONDITION NUMBER

Dynamic range of curvatures, κ

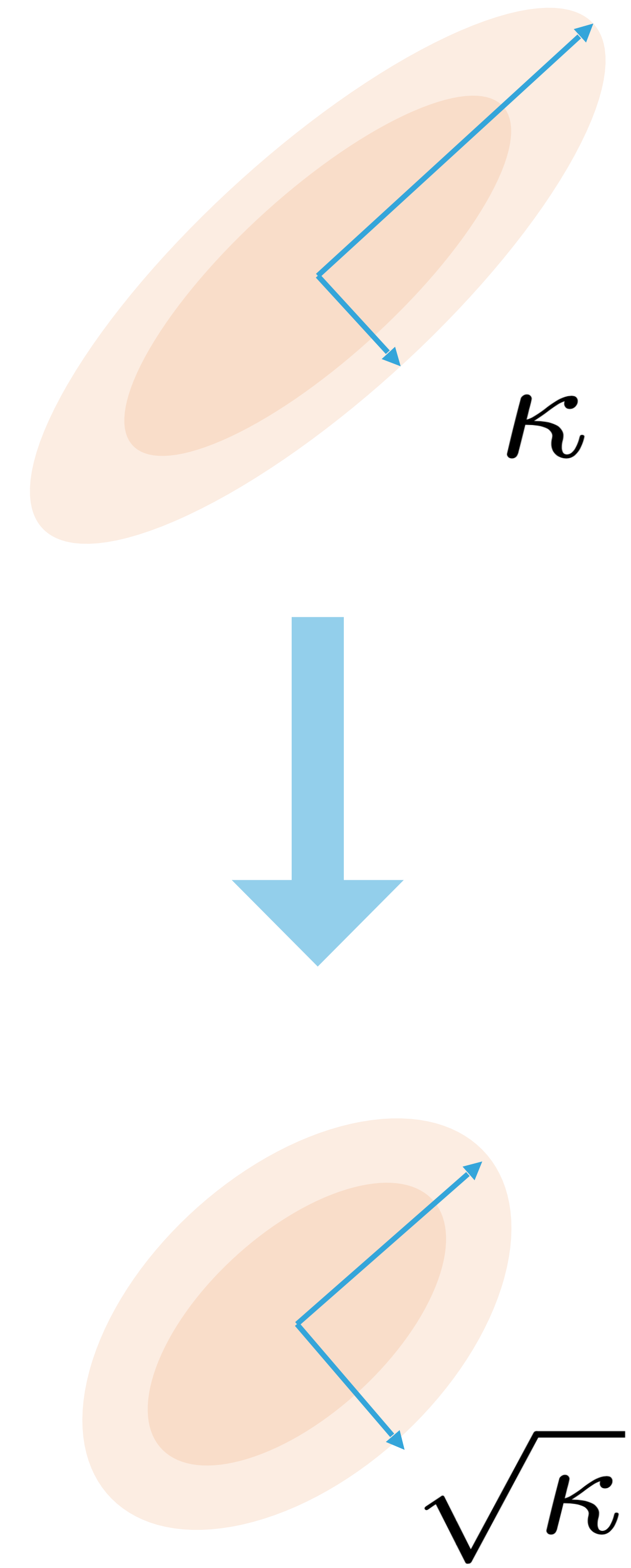
GRADIENT DESCENT ON STRONGLY CONVEX

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

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

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

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

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

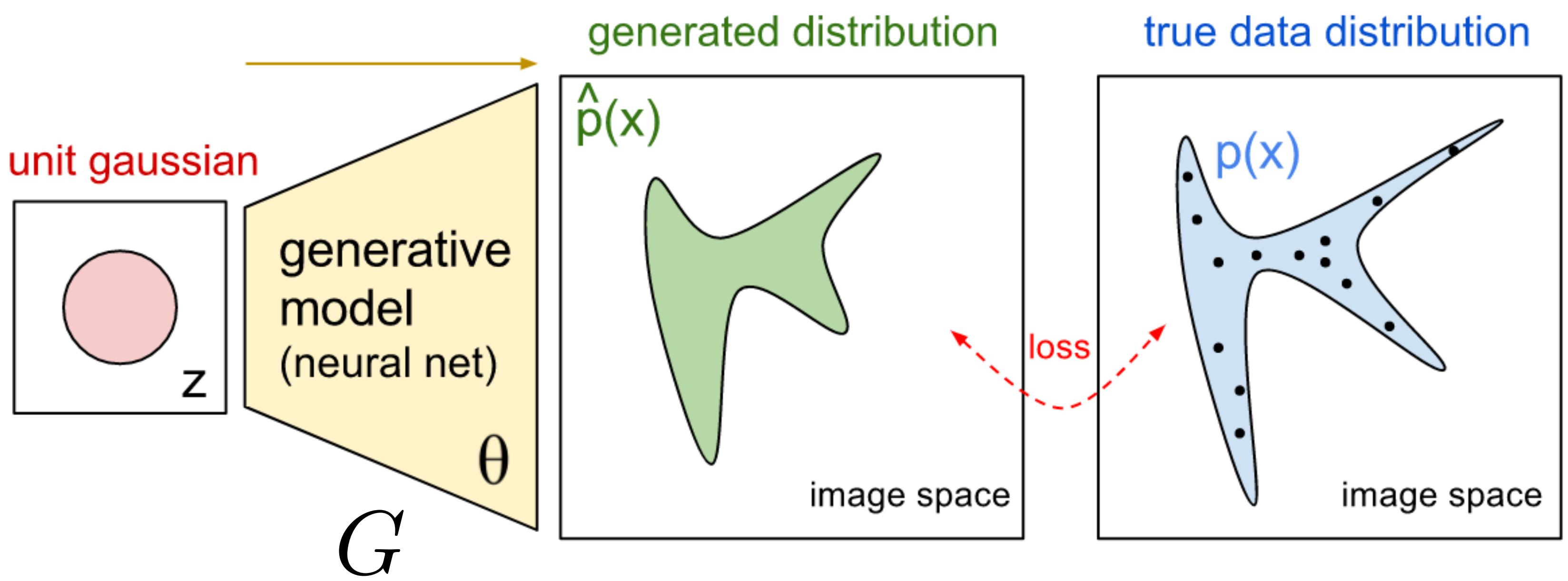
  Asymptotically efficient

- 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]

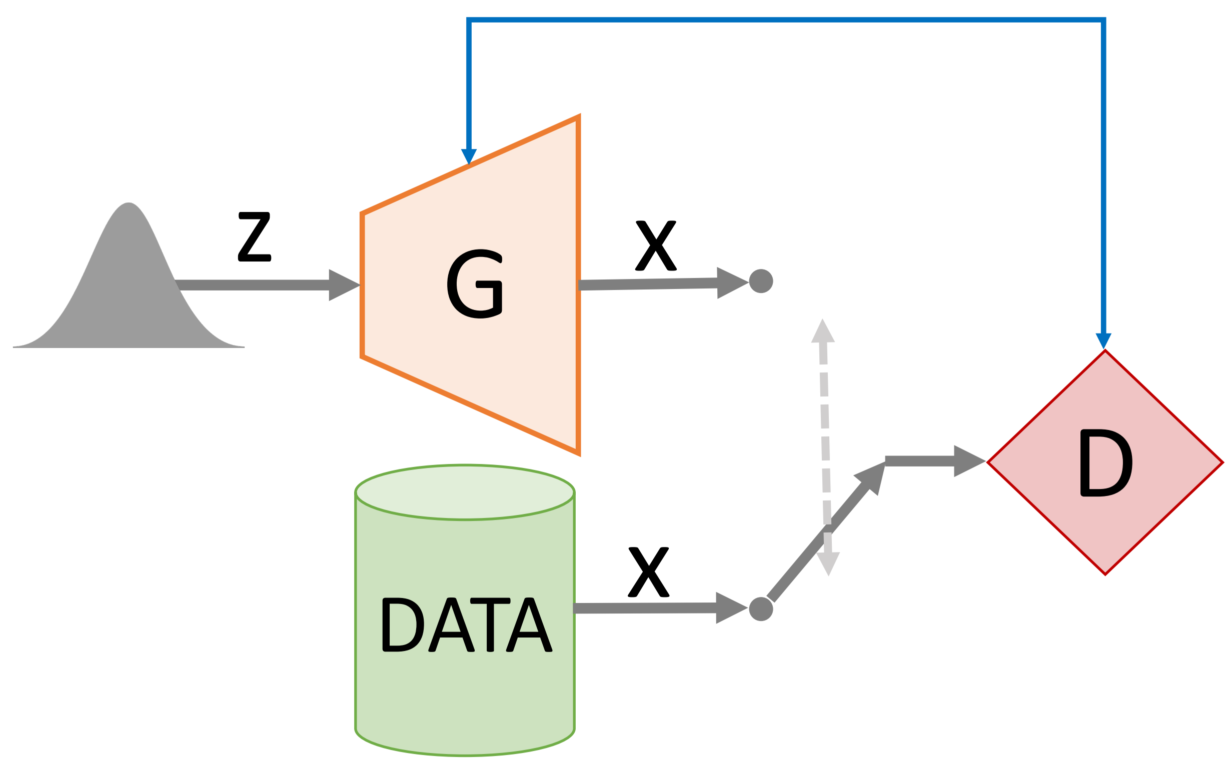
Generator network, G

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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Discriminator network, D

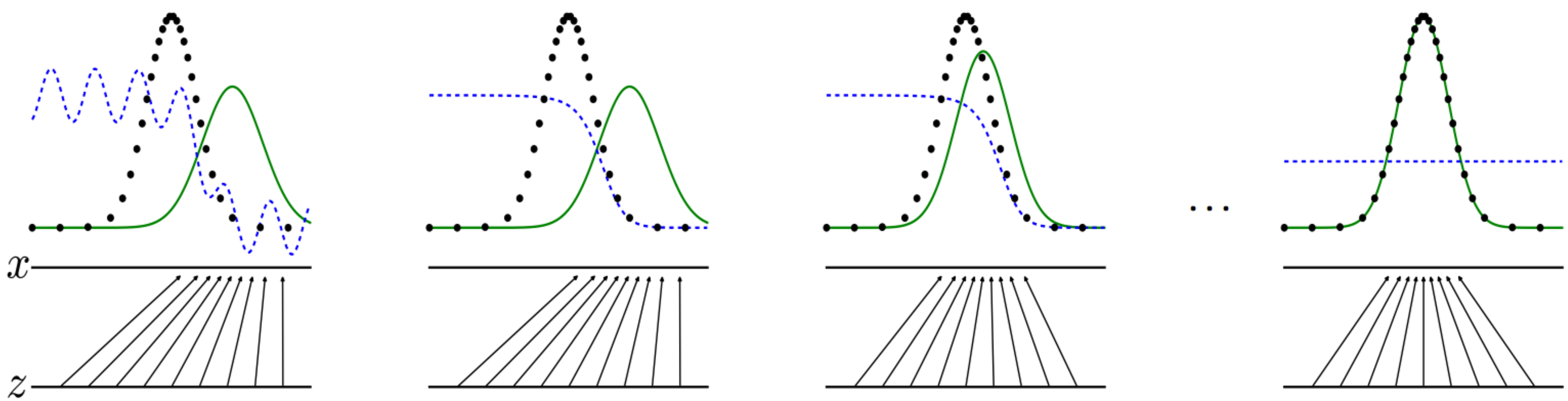
Given sample x or G(z), estimates probability it is real

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

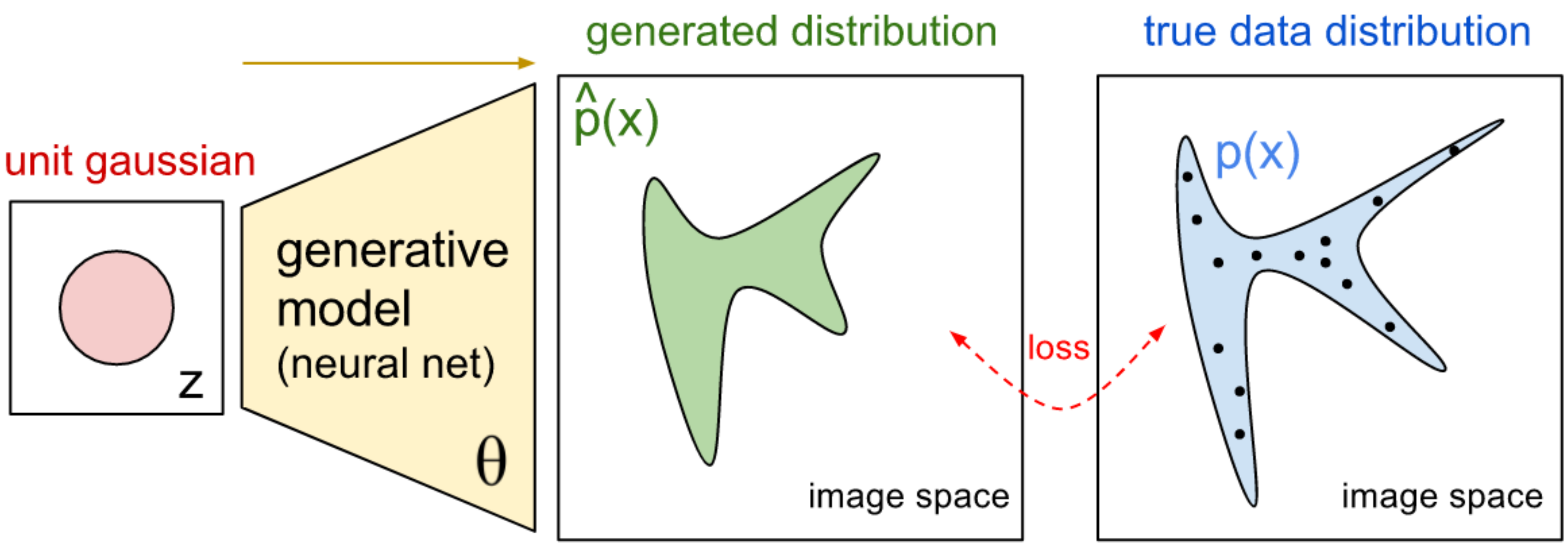
Whole chunks of space can be dropped.

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?

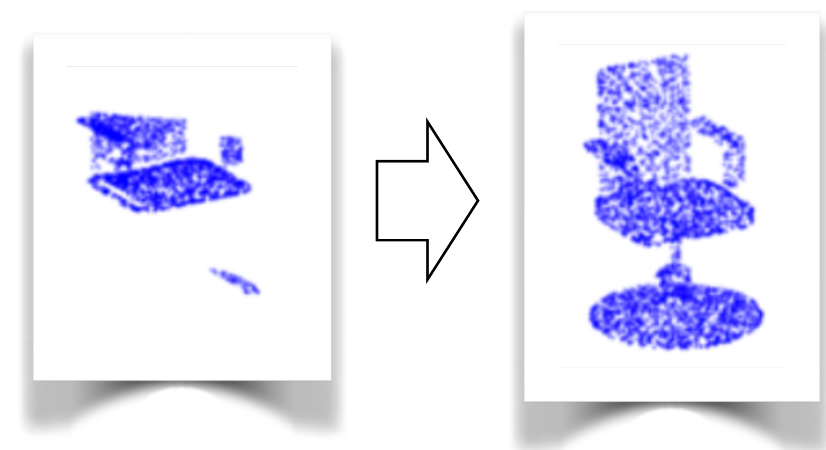
DREAMING UP STUFF?

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,

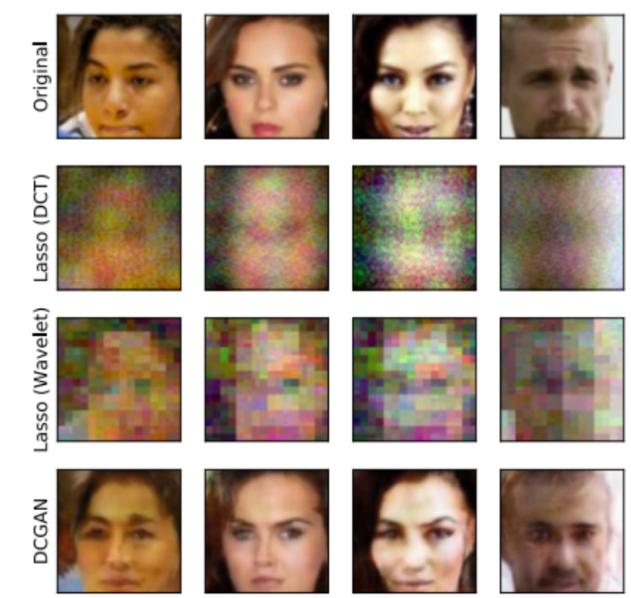
potentially corrupted by function M

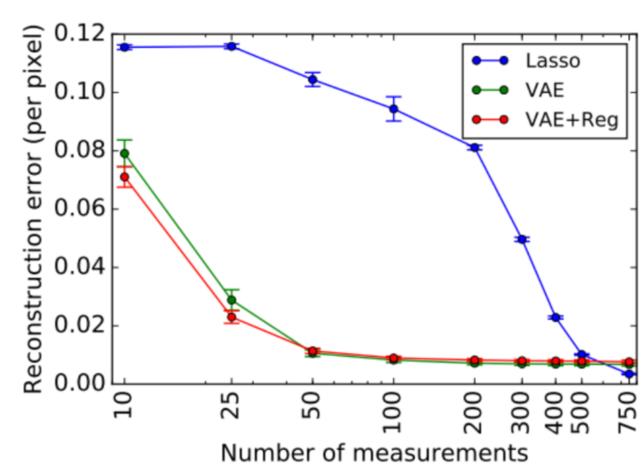
We can 'invert' the generator

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

and find a pre-image of y on the manifold

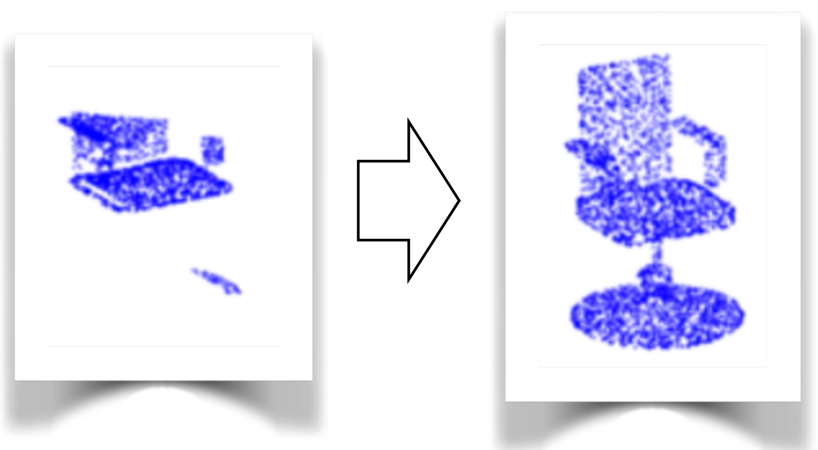
The trained generative model is critical!



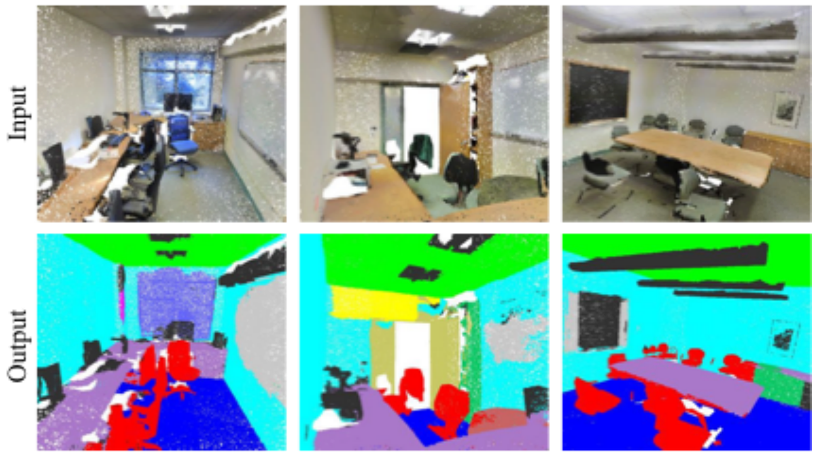


INTERESTING QUESTIONS

- 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 been taught most of the prerequisites mentioned in this slide deck?
- 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?