Course material at:

https://github.com/lyeskhalil/mlbootcamp2022/

Advanced Topics

Friday

FASE ML Bootcamp

Based on material from various sources:
Data augmentation, Hyperparameter tuning, CNN understanding, Attention, GANs:
http://cs231n.stanford.edu/schedule.html
Uncertainty in Deep Learning: https://www.gatsby.ucl.ac.uk/~balaji/balaji-uncertainty-talk-cifar-dlrl.pdf
Graph Neural Networks: http://tkipf.github.io/misc/SlidesCambridge.pdf
Reinforcement Learning: https://www.davidsilver.uk/wp-content/uploads/2020/03/deep_rl_tutorial_small_compressed.pdf

2022 Free PDF book on all of ML by Kevin Murphy (Google): https://probml.github.io/pml-book/book1.html

Google AI
Brain Team

Introduction to Uncertainty in Deep Learning

Balaji Lakshminarayanan
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Based on NeurIPS tutorial with Dustin Tran & Jasper Snoek



Motivation

What do we mean by Uncertainty?

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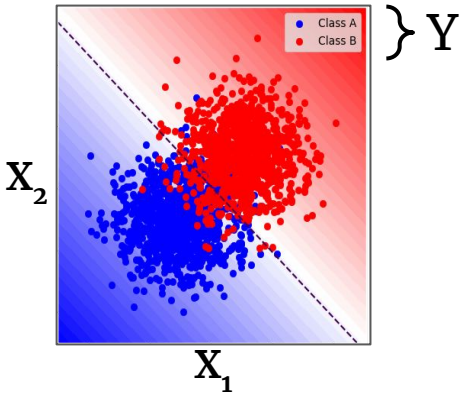
Return a distribution over predictions rather than a single prediction.

- ***Classification***: Output label along with its confidence.
- ***Regression***: Output mean along with its variance.

Good uncertainty estimates quantify ***when we can trust the model's predictions***.



$$p(\mathbf{y}|\mathbf{x})$$

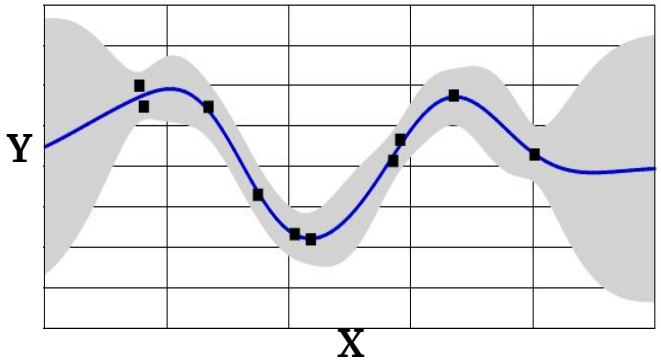


Image credit: Eric Nalisnick

What do we mean by Out-of-Distribution Robustness?

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I.I.D.

(*Independent and Identically Distributed*)

$$p_{TEST}(y,x) = p_{TRAIN}(y,x)$$

O.O.D.

$$p_{TEST}(y,x) \neq p_{TRAIN}(y,x)$$

Examples of dataset shift:

- ***Covariate shift.*** Distribution of features p(x) changes and p(y|x) is fixed.
- ***Open-set recognition.*** New classes may appear at test time.
- ***Subpopulation shift.*** Frequencies of data subpopulations changes.
- ***Label shift.*** Distribution of labels p(y) changes and p(x|y) is fixed.

ImageNet-C: Varying Intensity for Dataset Shift

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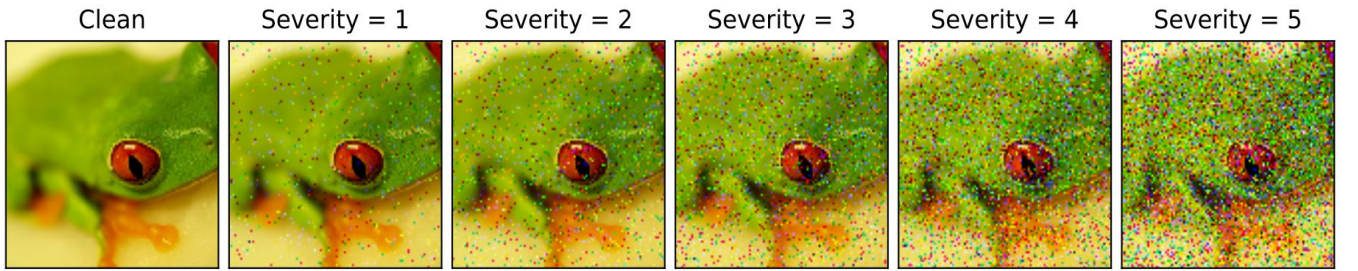

I.I.D test set

“Distance” between $p_{TEST}(y,x)$ and $p_{TRAIN}(y,x)$ increases

Image source: Benchmarking Neural Network Robustness to Common Corruptions and Perturbations, Hendrycks & Dietterich, 2019.

Neural networks do not generalize under covariate shift

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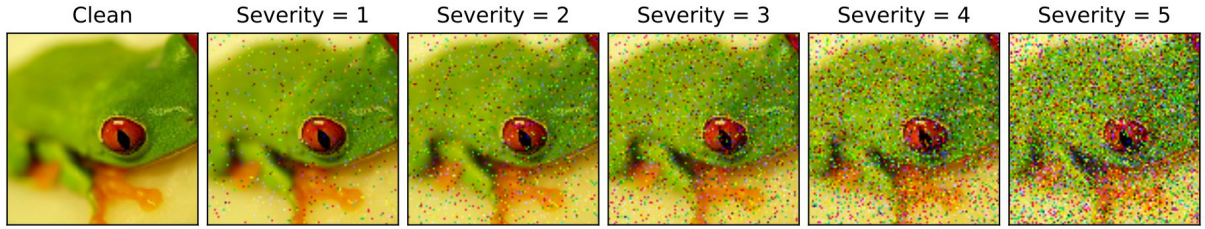
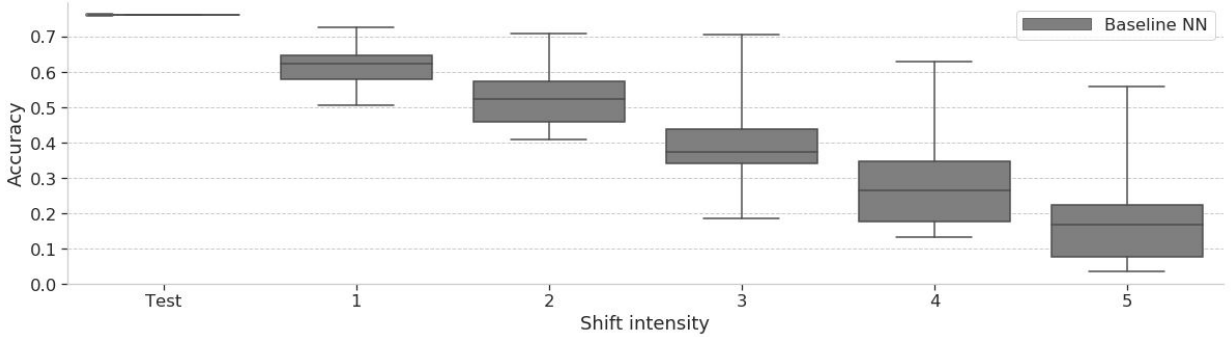


- **Accuracy drops** with increasing shift on Imagenet-C



- But do the models know that they are less accurate?

Can You Trust Your Model's Uncertainty? Evaluating Predictive Uncertainty Under Dataset Shift?, Ovadia et al. 2019

Neural networks *do not know when they don't know*

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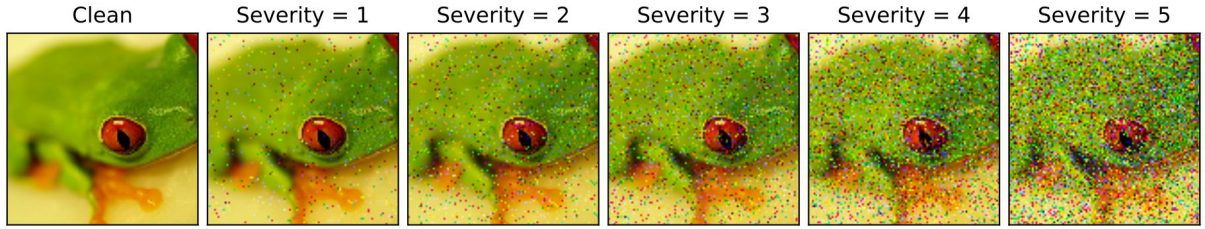

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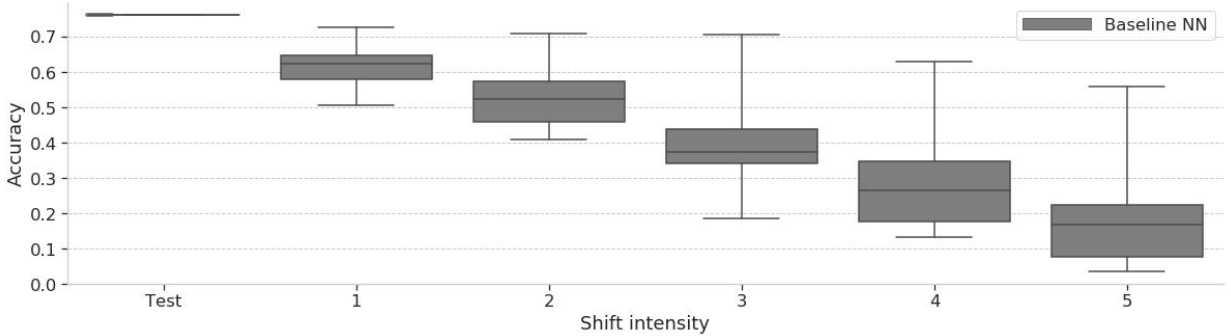
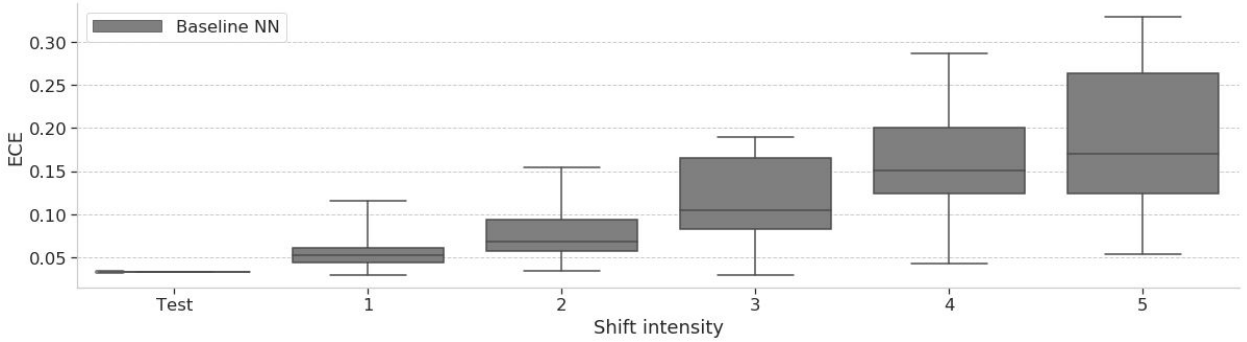


- **Quality of uncertainty degrades with shift** -> "overconfident mistakes"



Models assign high confidence predictions to OOD inputs

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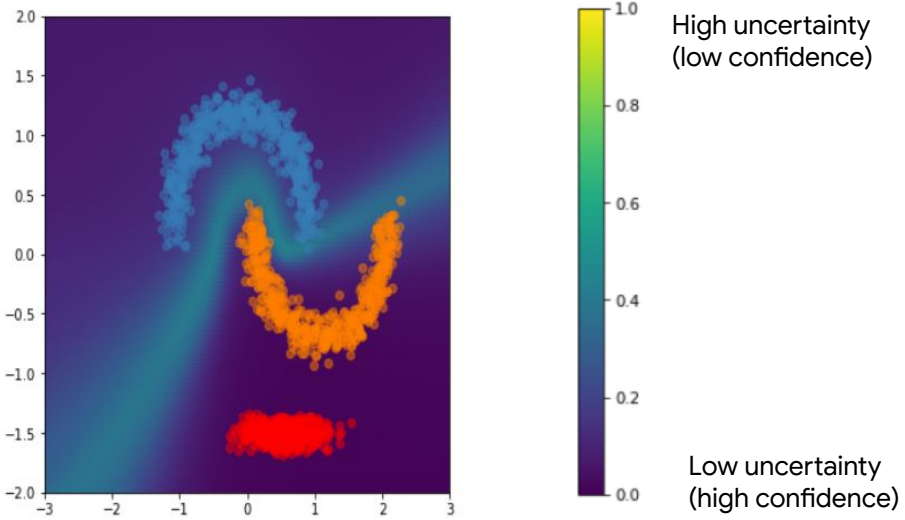

Image source: “Simple and Principled Uncertainty Estimation with Deterministic Deep Learning via Distance Awareness” Liu et al. 2020

Models assign high confidence predictions to OOD inputs

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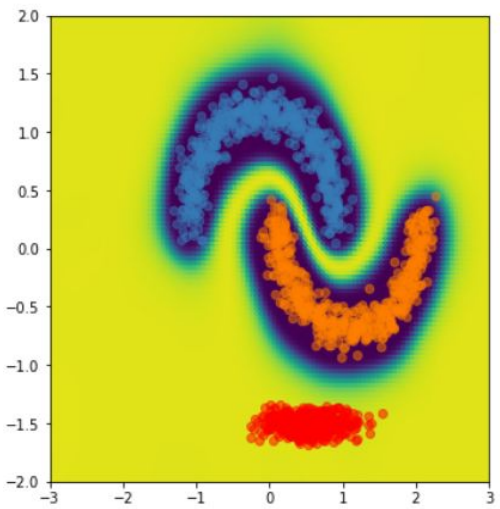
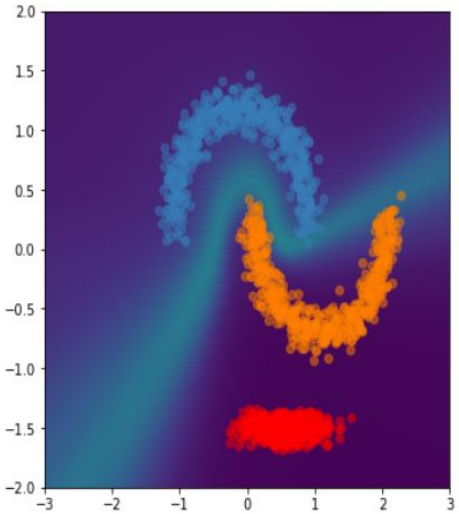


Ideal behavior



Deep neural networks

High uncertainty
(low confidence)

Low uncertainty
(high confidence)

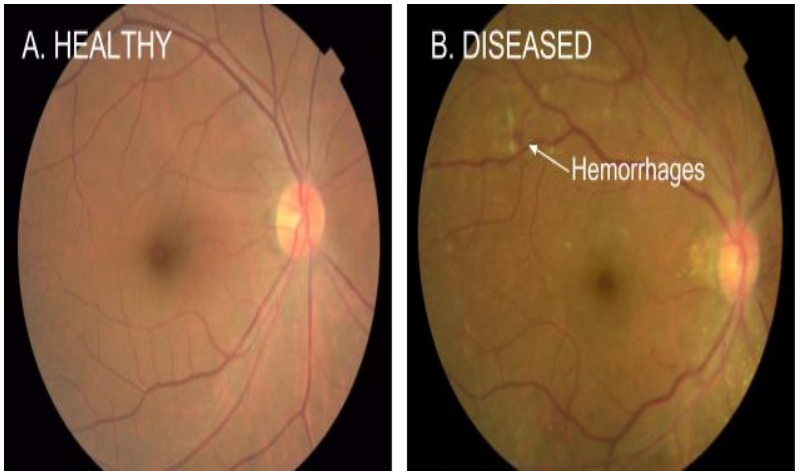
Trust model when x* is close to $p_{TRAIN}(x,y)$

Image source: “Simple and Principled Uncertainty Estimation with Deterministic Deep Learning via Distance Awareness” Liu et al. 2020

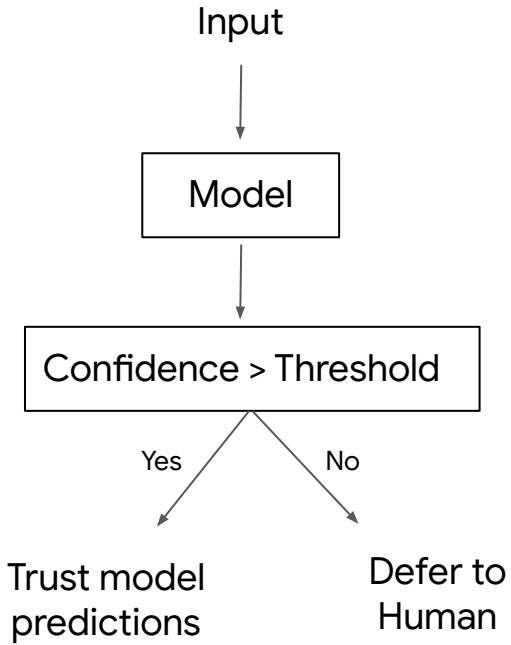
Applications

Healthcare

- Use model uncertainty to decide when to trust the model or to defer to a human.
- Cost-sensitive decision making



Diabetic retinopathy detection from fundus images
Gulshan et al, 2016



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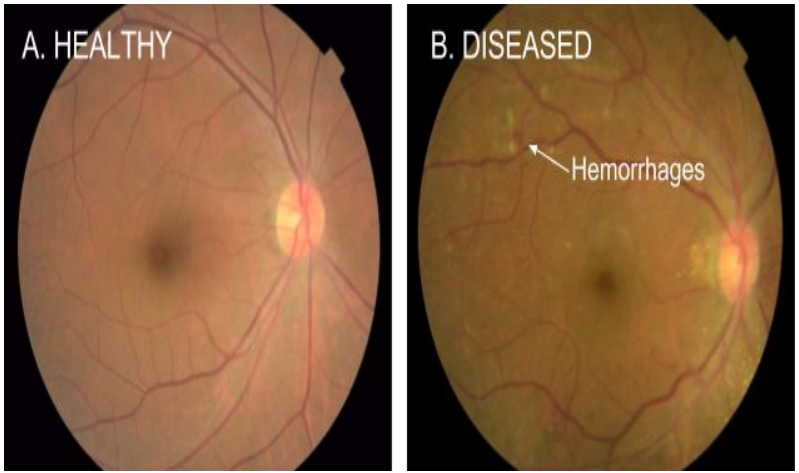

Diabetic retinopathy detection from fundus images
Gulshan et al, 2016

True label

Action		Healthy	Diseased
	Predict Healthy	0	10
	Predict Diseased	1	0
	Abstain "I don't know"	0.5	0.5

Self-driving cars

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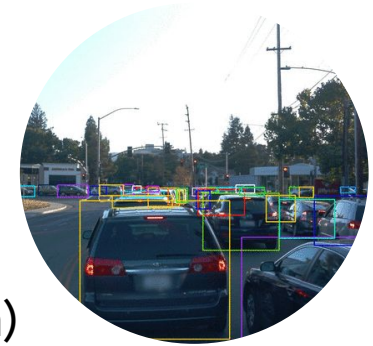
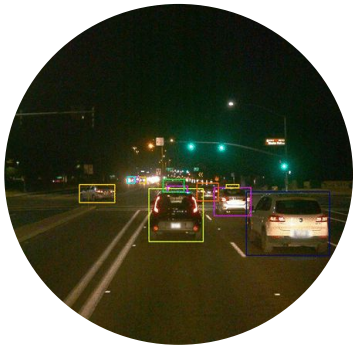
Dataset shift:

- Time of day / Lighting
- Geographical location (City vs suburban)
- Changing conditions (Weather / Construction)



Daylight



Night

Weather

Construction

Downtown

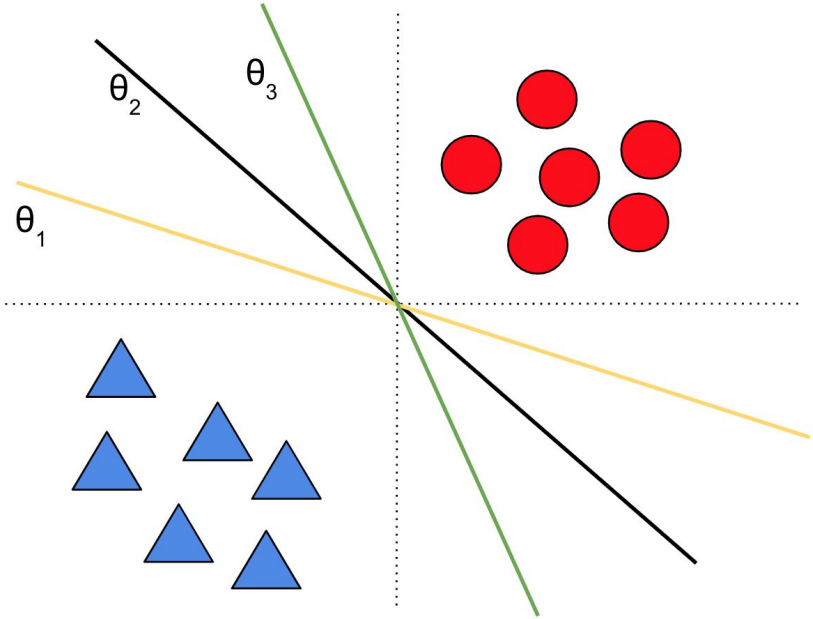
Suburban

Image credit: Sun et al, Waymo Open Dataset

Primer on Uncertainty & Robustness

Sources of uncertainty: *Model uncertainty*

- Many models can fit the training data well
- Also known as ***epistemic uncertainty***
- Model uncertainty is "**reducible**"
  - Vanishes in the limit of infinite data (subject to model identifiability)



Sources of uncertainty: *Model uncertainty*

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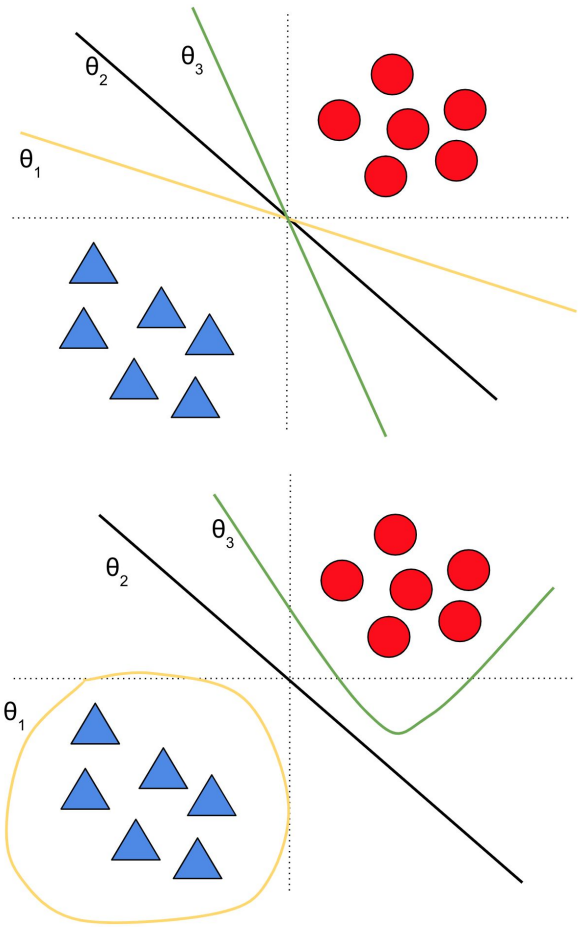
- Many models can fit the training data well
- Also known as ***epistemic uncertainty***
- Model uncertainty is "**reducible**"
  - Vanishes in the limit of infinite data (subject to model identifiability)
- Models can be from same hypotheses class (e.g. linear classifiers in top figure) or belong to different hypotheses classes (bottom figure).



Sources of uncertainty: *Data uncertainty*

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- Labeling noise (ex: human disagreement)

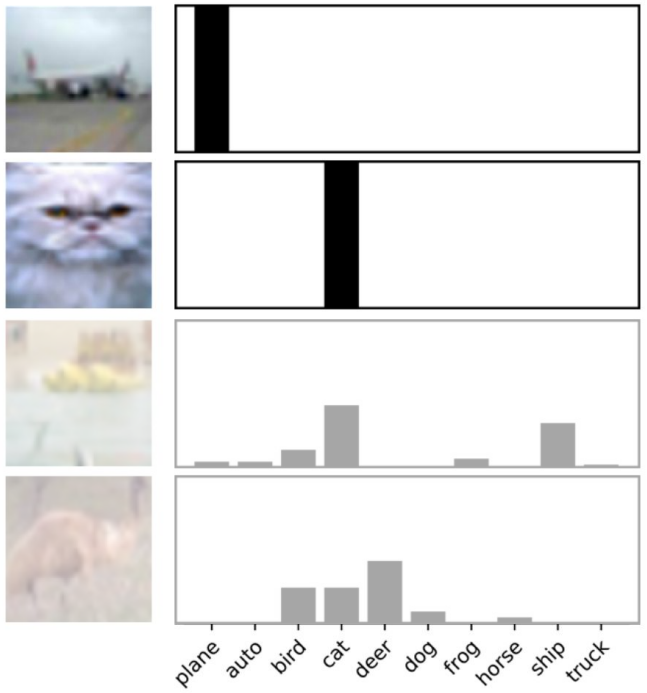

Image source: Battleday et al. 2019 “Improving machine classification using human uncertainty measurements”

Sources of uncertainty: *Data uncertainty*

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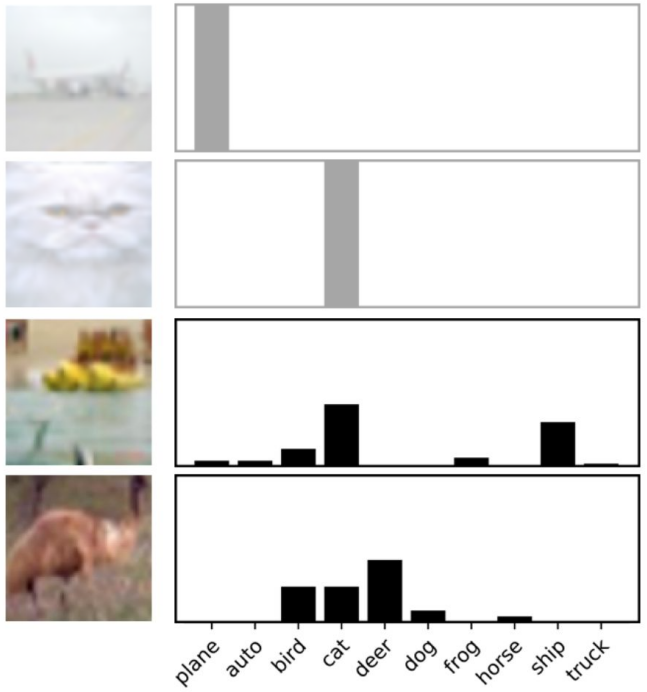


Image source: Battleday et al. 2019 “Improving machine classification using human uncertainty measurements”

Sources of uncertainty: *Data uncertainty*

- Labeling noise (ex: human disagreement)
- Measurement noise (ex: imprecise tools)
- *Missing* data (ex: partially observed features, unobserved confounders)
- Also known as ***aleatoric uncertainty***
- Data uncertainty is "**irreducible***"
  - Persists even in the limit of infinite data
  - *Could be reduced with additional features/views

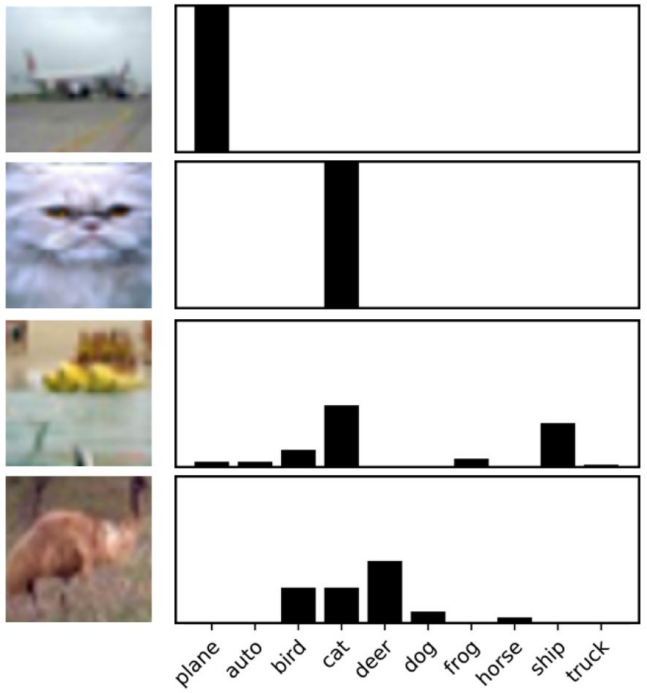


Image source: Battleday et al. 2019 "Improving machine classification using human uncertainty measurements"

How do we measure the quality of uncertainty?

$$\text{Calibration Error} = |\text{Confidence} - \text{Accuracy}|$$

predicted probability of correctness

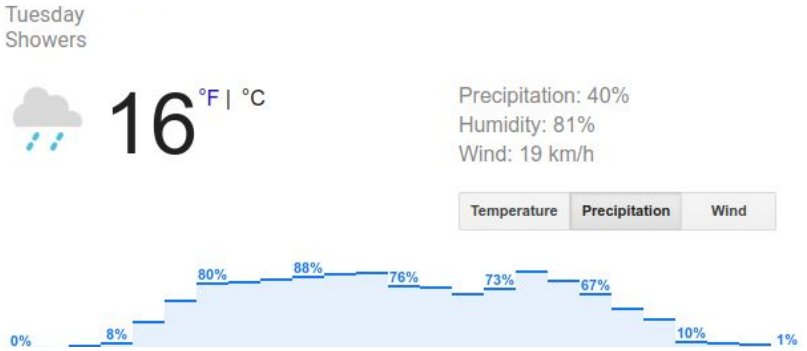
observed frequency of correctness

How do we measure the quality of uncertainty?

$$\text{Calibration Error} = |\text{Confidence} - \text{Accuracy}|$$

Of all the days where the model predicted rain with 80% probability, what fraction did we observe rain?

- 80% implies perfect calibration
- Less than 80% implies model is overconfident
- Greater than 80% implies model is under-confident



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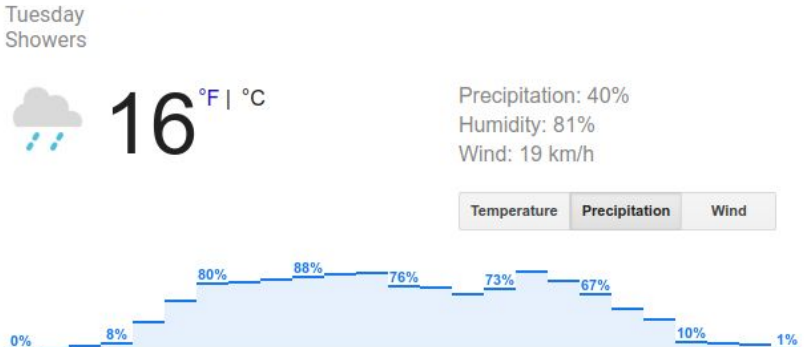


Intuition: For regression, calibration corresponds to coverage in a confidence interval.

How do we measure the quality of uncertainty?

Expected Calibration Error [Naeini+ 2015]:

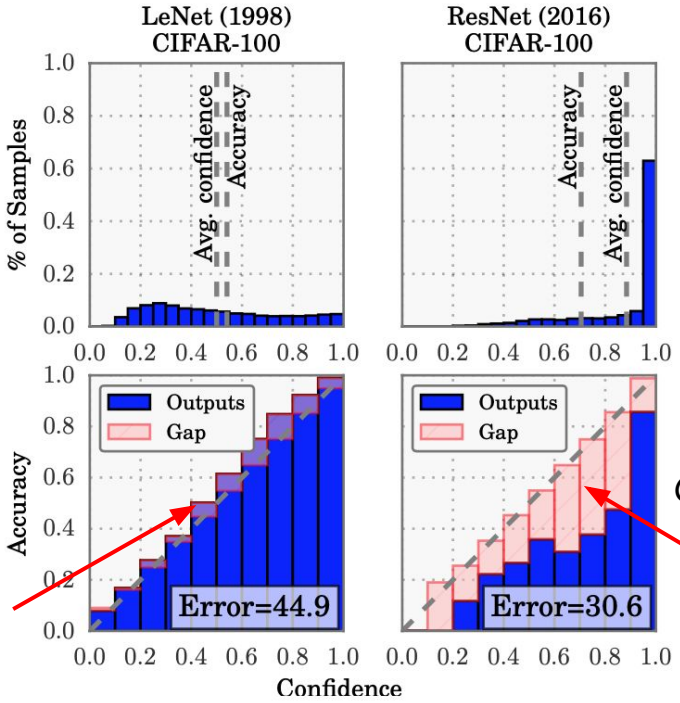
$$\mathrm{ECE} = \sum_{b=1}^{B} \frac{n_b}{N} \left|\mathrm{acc}(b) - \mathrm{conf}(b)\right|$$

- Bin the probabilities into B bins.
- Compute the within-bin accuracy and within-bin predicted confidence.
- Average the calibration error across bins (weighted by number of points in each bin).

How do we measure the quality of uncertainty?

Expected Calibration Error [Naeini+ 2015]:

$$\mathrm{ECE} = \sum_{b=1}^{B} \frac{n_b}{N} \left|\mathrm{acc}(b) - \mathrm{conf}(b)\right|$$



Confidence < Accuracy

=> Underconfident

Confidence > Accuracy

=> Overconfident

Image source: Guo+ 2017 “On calibration of modern neural networks”

Fundamentals to Uncertainty & Robustness Methods

Neural Networks with SGD

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$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\boldsymbol{\theta} \mid \mathbf{x}, \mathbf{y})$$

Problem: results in just one prediction per example
No model uncertainty

How do we get uncertainty?

- Probabilistic approach
  - Estimate a full distribution for $p(\boldsymbol{\theta} \mid \mathbf{x}, \mathbf{y})$
- Intuitive approach: Ensembling
  - Obtain multiple good settings for $\boldsymbol{\theta}^*$

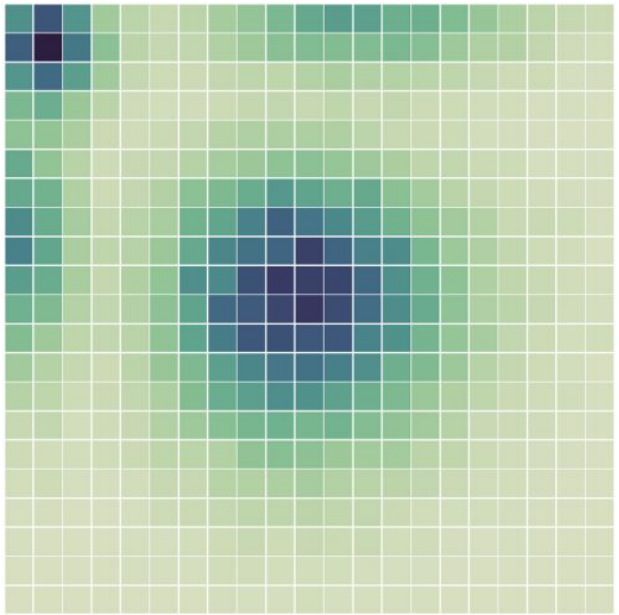


Image source: Ranganath+ 2016

Ensemble Learning

- A prior distribution often involves the complication of approximate inference.
- *Ensemble learning* offers an alternative strategy to aggregate the predictions over a collection of models.
- Often winner of competitions!
- There are two considerations: the collection of models to ensemble; and the aggregation strategy.

Popular approach is to average predictions of independently trained models, forming a mixture distribution.

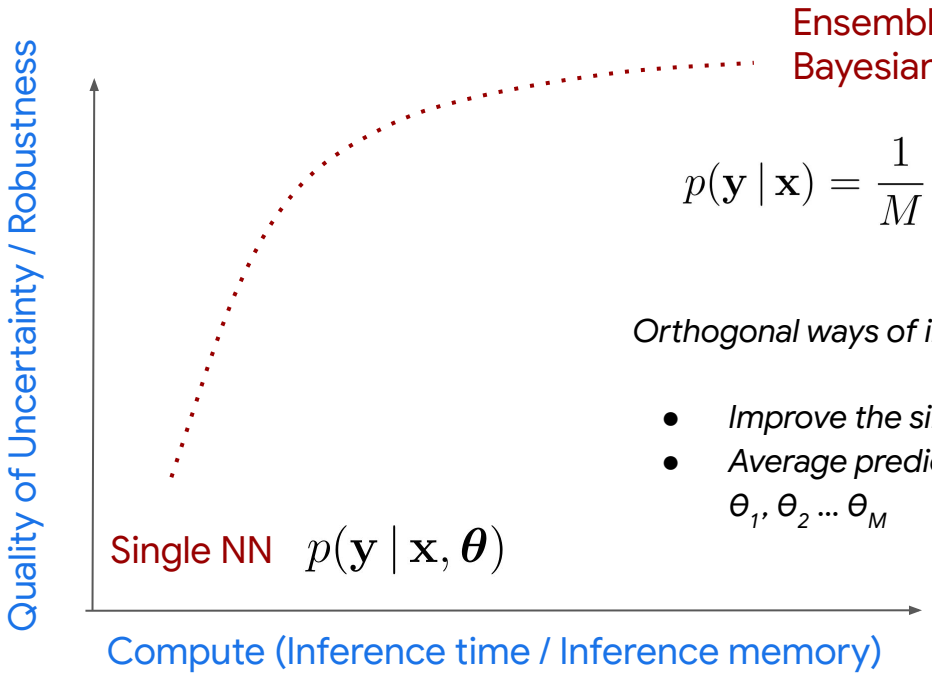
$$p(\mathbf{y} \mid \mathbf{x}) = \frac{1}{K} \sum_{k=1}^{K} p(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta}_k)$$

Many approaches exist: bagging, boosting, decision trees, stacking.

[Dietterich 2000]

Overview of Methods

Cartoon: Uncertainty/Robustness vs Compute frontier

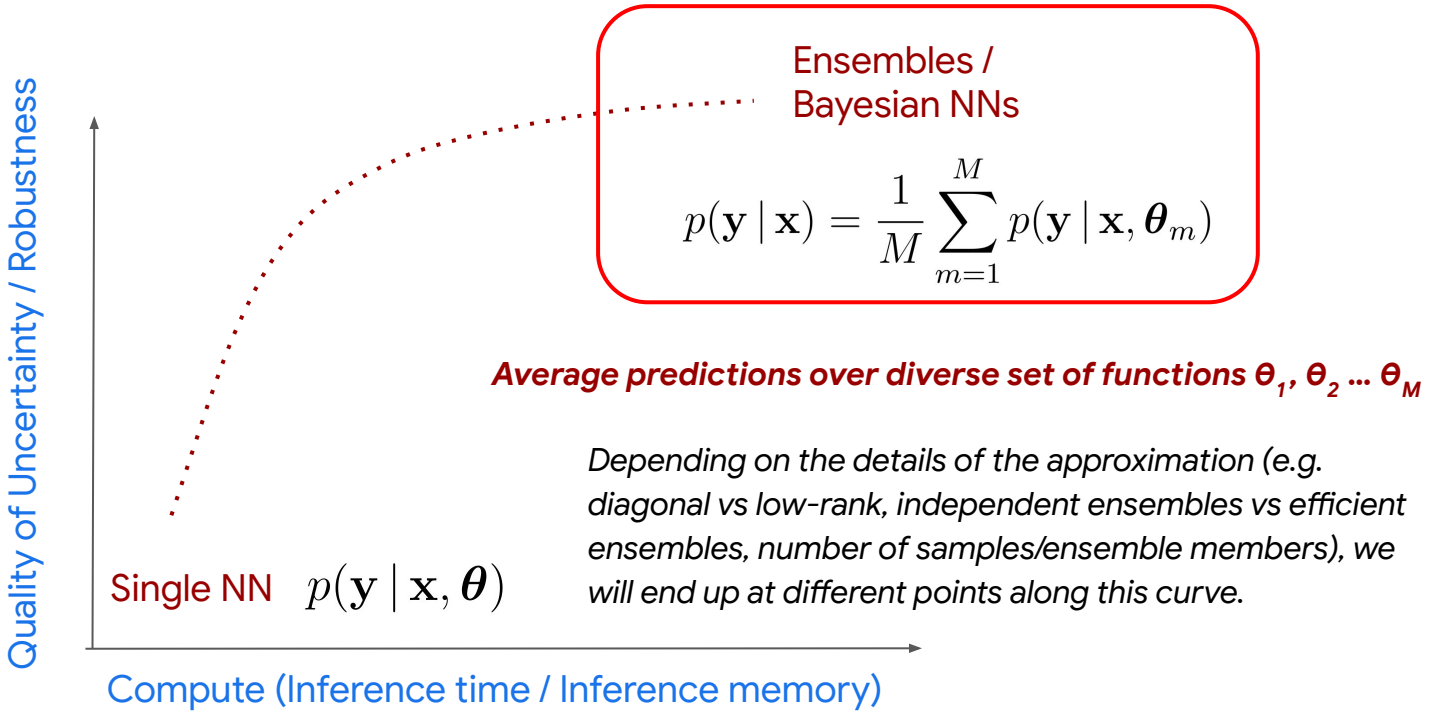


$$p(\mathbf{y} \mid \mathbf{x}) = \frac{1}{M} \sum_{m=1}^{M} p(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta}_m)$$

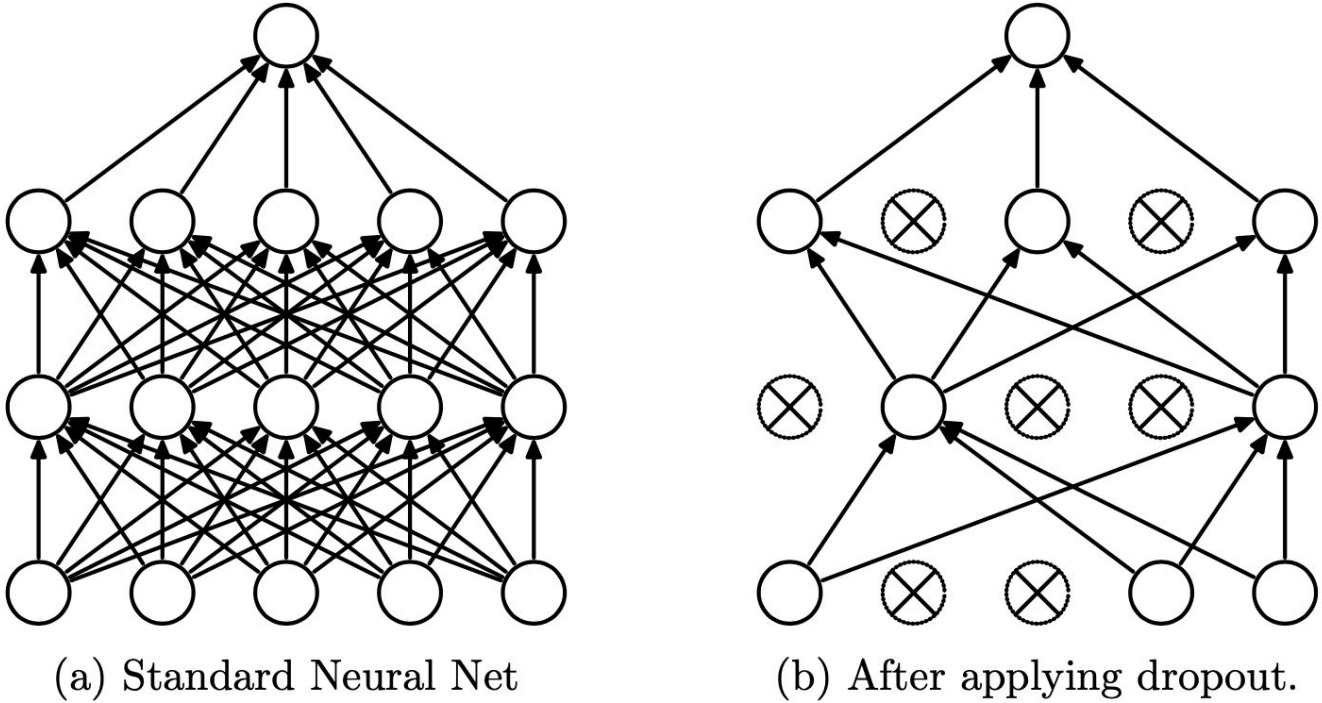
Orthogonal ways of improving performance

- *Improve the single model p(y|x,θ)*
- *Average predictions over diverse set of functions* $\theta_1, \theta_2 \ldots \theta_M$

Improving the quality of model uncertainty



Simple Baseline: Monte Carlo Dropout



(a) Standard Neural Net

(b) After applying dropout.

Image source: Dropout: A Simple Way to Prevent Neural Networks from Overfitting

[Gal+ 2015]

Simple Baseline: Deep Ensembles

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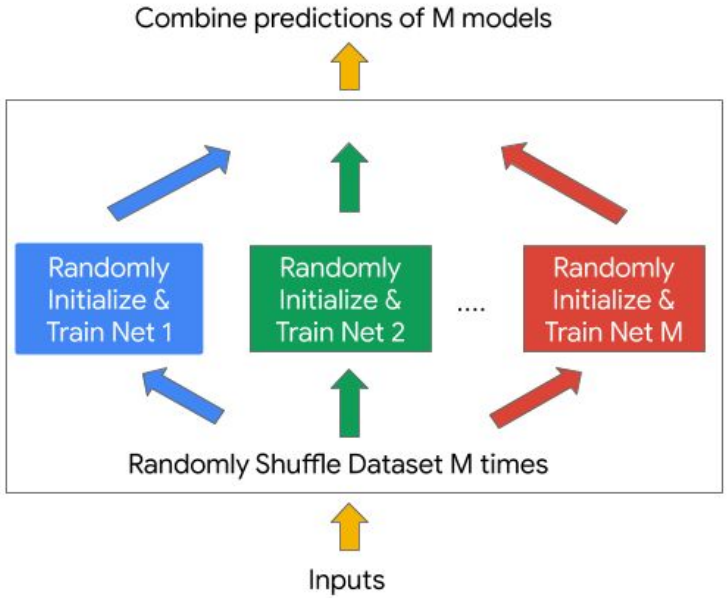
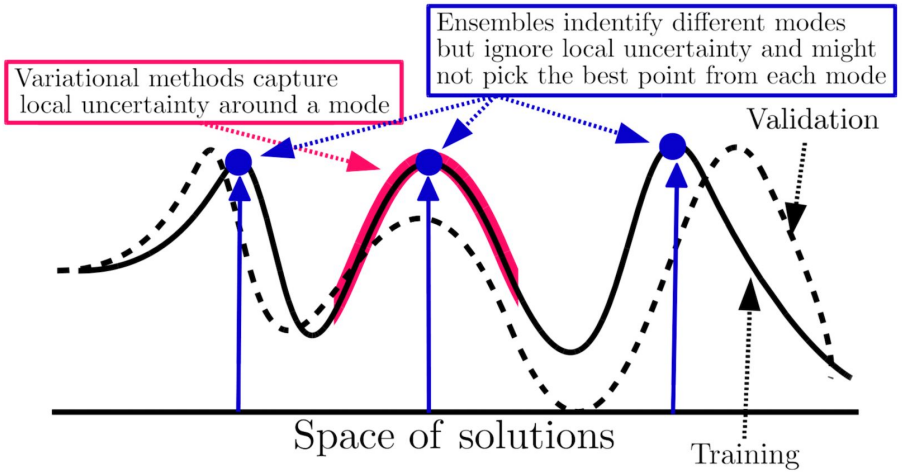
Idea: Just re-run standard SGD training but with different random seeds and average the predictions.

Deep ensembles can capture different modes in function space.

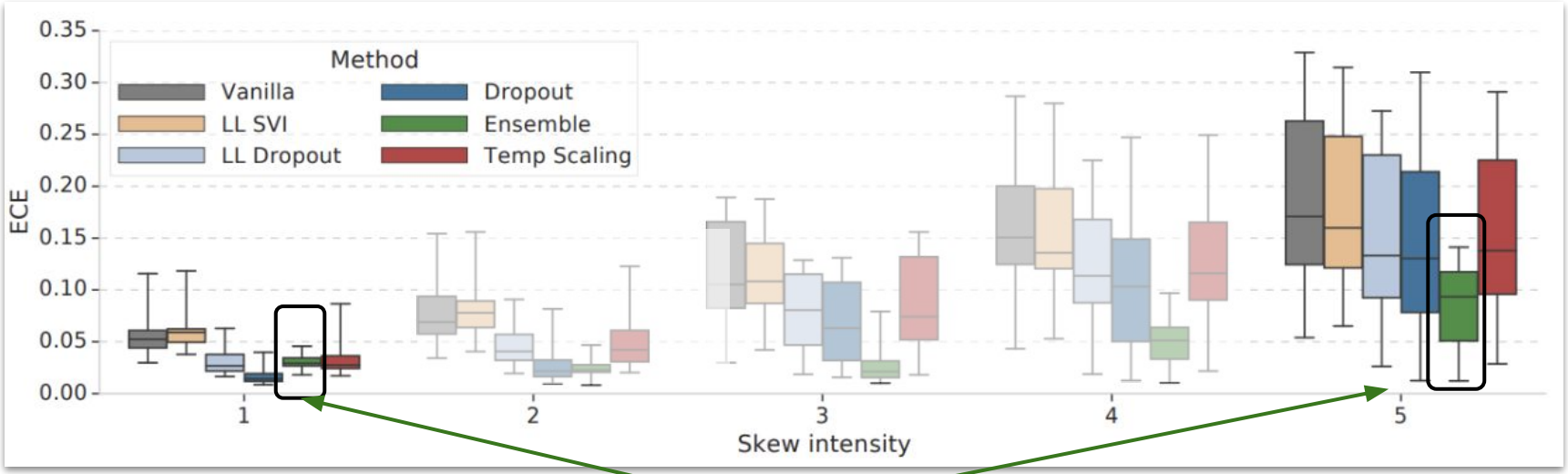


[Lakshminarayanan+ 2016]



[Fort+ 2019]

Deep Ensembles work surprisingly well in practice



Deep Ensembles are consistently among the best performing methods, especially under dataset shift

Can you trust your model's uncertainty? Evaluating predictive uncertainty under dataset shift [Ovadia+ 2019]

Lecture 13: Generative Models

Supervised vs Unsupervised Learning

Supervised Learning

Data: (x, y)
x is data, y is label

Goal: Learn a *function* to map x -> y

Examples: Classification, regression, object detection, semantic segmentation, image captioning, etc.

Supervised vs Unsupervised Learning

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Cat

Classification

Supervised vs Unsupervised Learning

Supervised Learning

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Examples: Classification, regression, object detection, semantic segmentation, image captioning, etc.

A cat sitting on a suitcase on the floor

Image captioning

Supervised vs Unsupervised Learning

Supervised Learning

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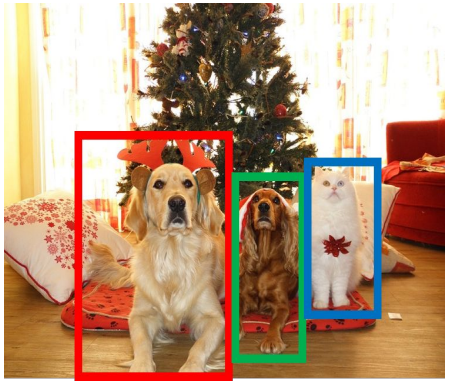
Goal: Learn a *function* to map x -> y

Examples: Classification, regression, object detection, semantic segmentation, image captioning, etc.



DOG, **DOG**, **CAT**

Object Detection

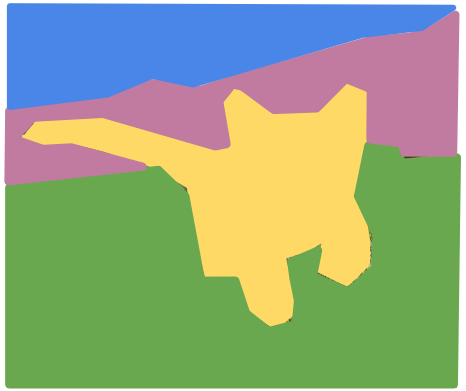
Supervised vs Unsupervised Learning

Supervised Learning

Data: (x, y)
x is data, y is label

Goal: Learn a *function* to map x -> y

Examples: Classification, regression, object detection, semantic segmentation, image captioning, etc.



GRASS, CAT,
TREE, SKY

Semantic Segmentation

Supervised vs Unsupervised Learning

Unsupervised Learning

Data: x
Just data, **no labels!**

Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, feature learning, density estimation, etc.

Supervised vs Unsupervised Learning

Unsupervised Learning

Data: x
Just data, no labels!

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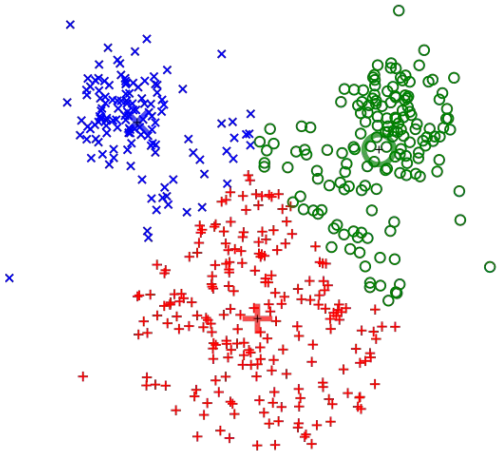
Examples: Clustering, dimensionality reduction, density estimation, etc.



K-means clustering

Supervised vs Unsupervised Learning

Unsupervised Learning

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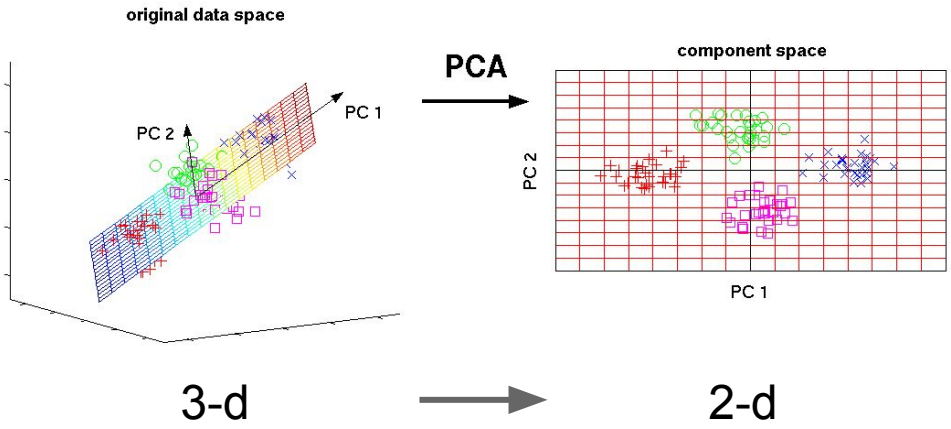
Examples: Clustering, dimensionality reduction, density estimation, etc.



Principal Component Analysis
(Dimensionality reduction)

Supervised vs Unsupervised Learning

Unsupervised Learning

Data: x
Just data, no labels!

Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, density estimation, etc.

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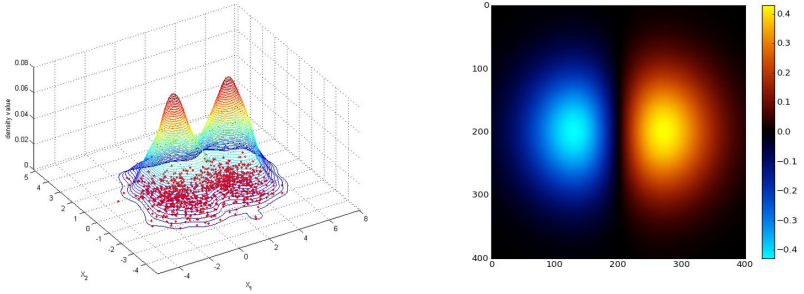
1-d density estimation



2-d density estimation

Modeling p(x)

2-d density images left and right are CC0 public domain

Supervised vs Unsupervised Learning

Supervised Learning

Data: (x, y)
x is data, y is label

Goal: Learn a *function* to map x -> y

Examples: Classification, regression, object detection, semantic segmentation, image captioning, etc.

Unsupervised Learning

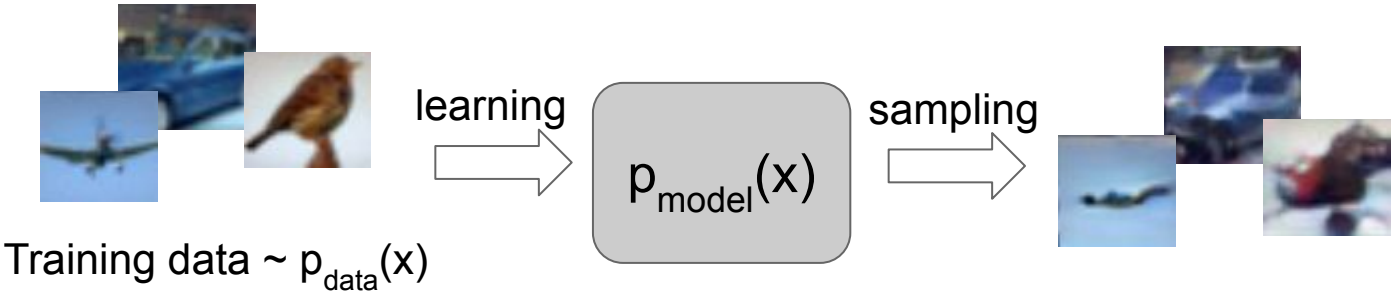
Data: x
Just data, no labels!

Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, density estimation, etc.

Generative Modeling

Given training data, generate new samples from same distribution

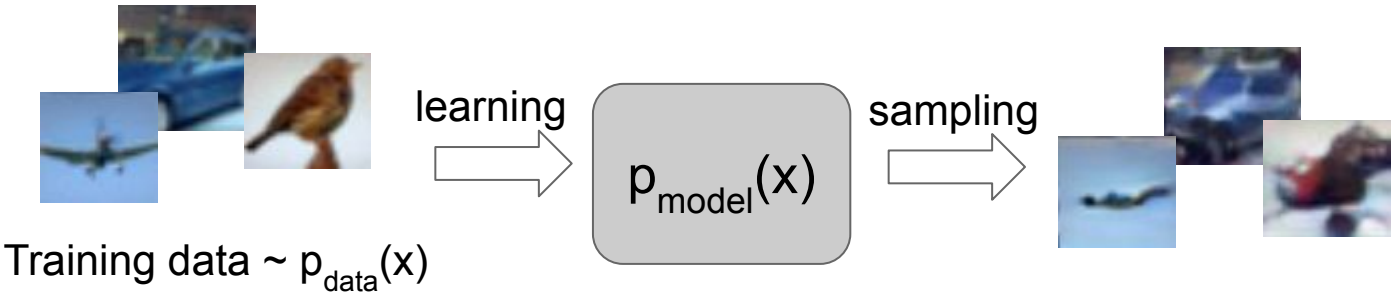


Objectives:

1. Learn $p_{model}(x)$ that approximates $p_{data}(x)$
2. **Sampling new x from $p_{model}(x)$**

Generative Modeling

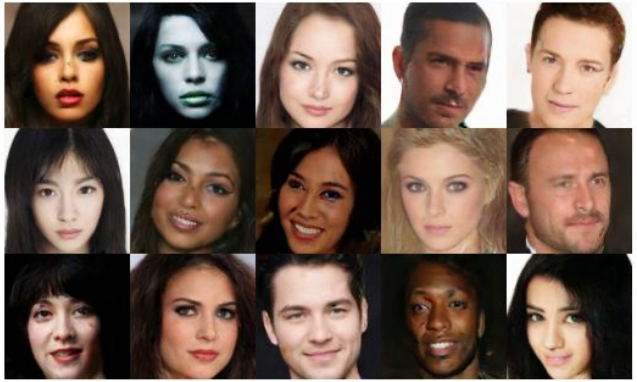
Given training data, generate new samples from same distribution



Formulate as density estimation problems**:**

- **Explicit density estimation**: explicitly define and solve for $p_{model}(x)$
- **Implicit density estimation**: learn model that can sample from $p_{model}(x)$ **without explicitly defining it.**

Why Generative Models?


- Realistic samples for artwork, super-resolution, colorization, etc.
- Learn useful features for downstream tasks such as classification.
- Getting insights from high-dimensional data (physics, medical imaging, etc.)
- Modeling physical world for simulation and planning (robotics and reinforcement learning applications)
- Many more ...

PixelRNN and PixelCNN

(A very brief overview)

Fully visible belief network (FVBN)

Explicit density model

$$p(x) = p(x_1, x_2, \ldots, x_n)$$

Likelihood of image x

Joint likelihood of each pixel in the image

Fully visible belief network (FVBN)

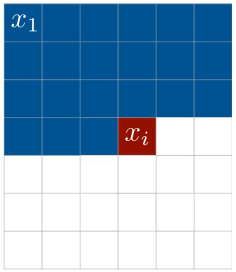
Explicit density model

Use chain rule to decompose likelihood of an image x into product of 1-d distributions:

$$p(x) = \prod_{i=1}^{n} p(x_i | x_1, \ldots, x_{i-1})$$

Likelihood of image x

Probability of i'th pixel value given all previous pixels



Then maximize likelihood of training data

Fully visible belief network (FVBN)

Explicit density model

Use chain rule to decompose likelihood of an image x into product of 1-d distributions:

$$p(x) = \prod_{i=1}^{n} p(x_i | x_1, \ldots, x_{i-1})$$

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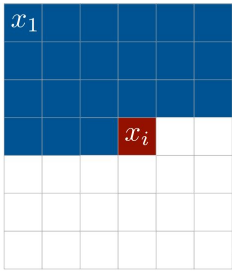
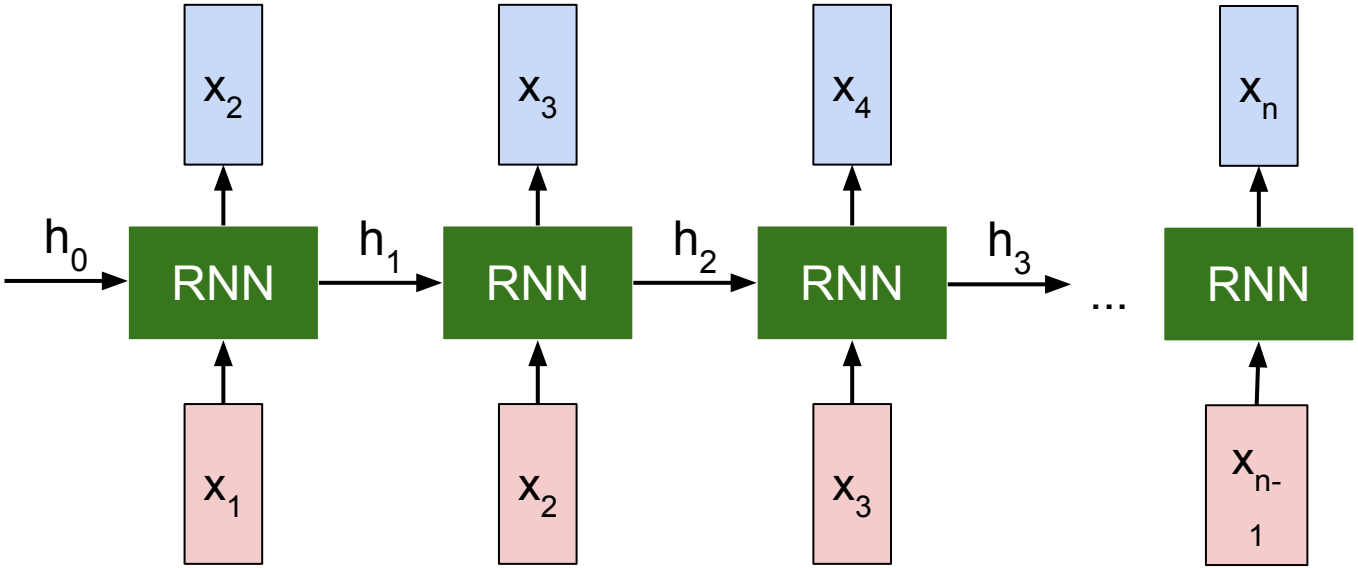


Then maximize likelihood of training data

Complex distribution over pixel values => Express using a neural network!

Recurrent Neural Network

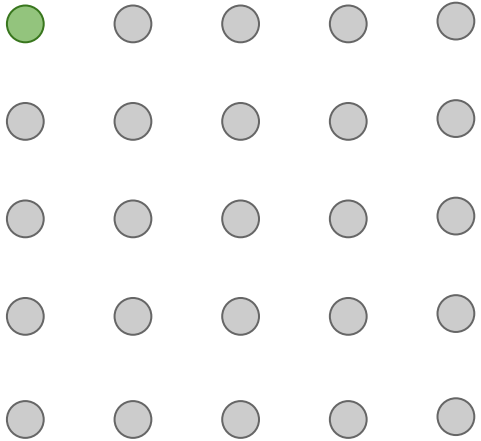


$$p(x_i|x_1, ..., x_{i-1})$$

PixelRNN *[van der Oord et al. 2016]*

Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)



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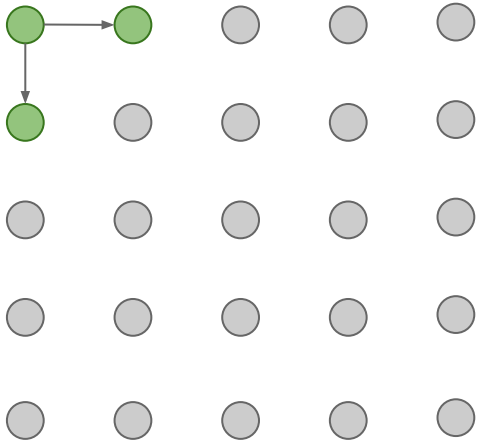

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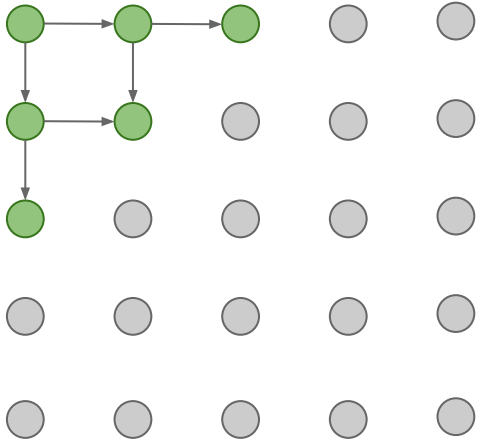

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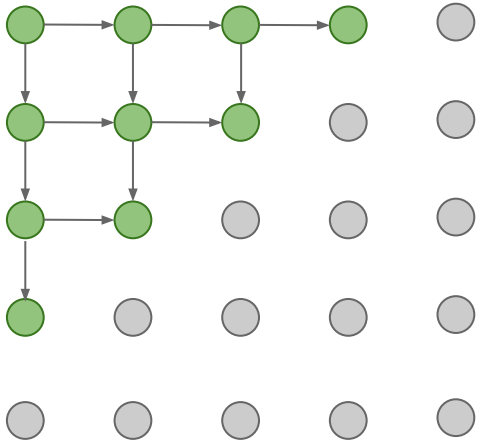
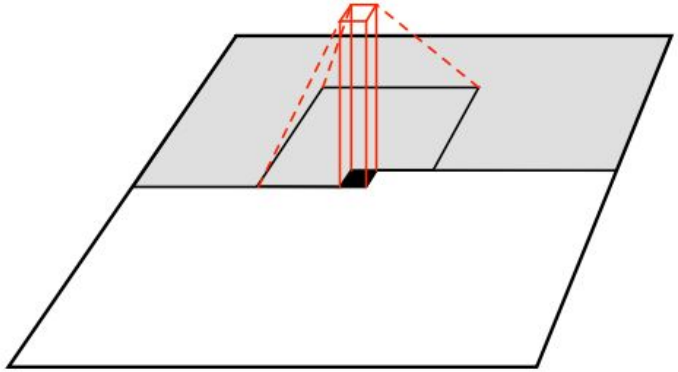


Drawback: sequential generation is slow in both training and inference!

PixelCNN *[van der Oord et al. 2016]*

Still generate image pixels starting from corner

Dependency on previous pixels now modeled using a CNN over context region (**masked convolution**)



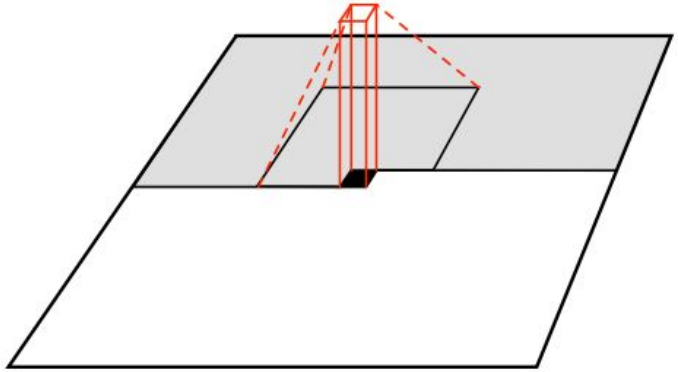
PixelCNN *[van der Oord et al. 2016]*

Still generate image pixels starting from corner

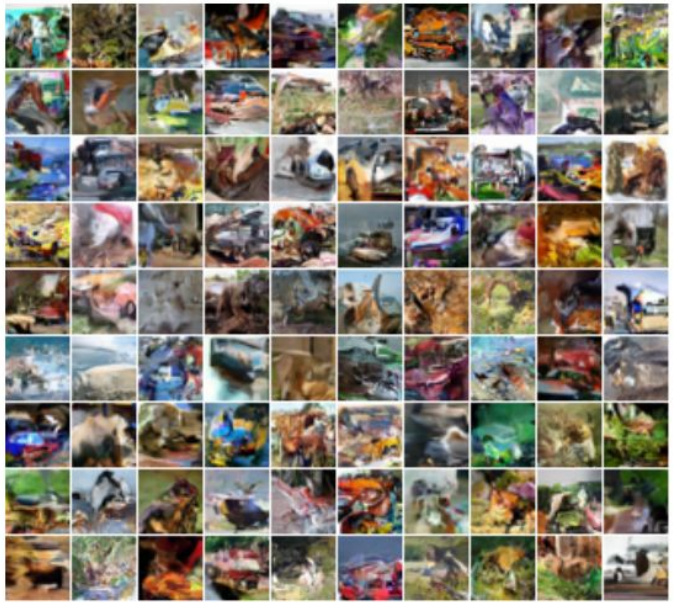
Dependency on previous pixels now modeled using a CNN over context region (masked convolution)

Training is faster than PixelRNN
(can parallelize convolutions since context region values known from training images)

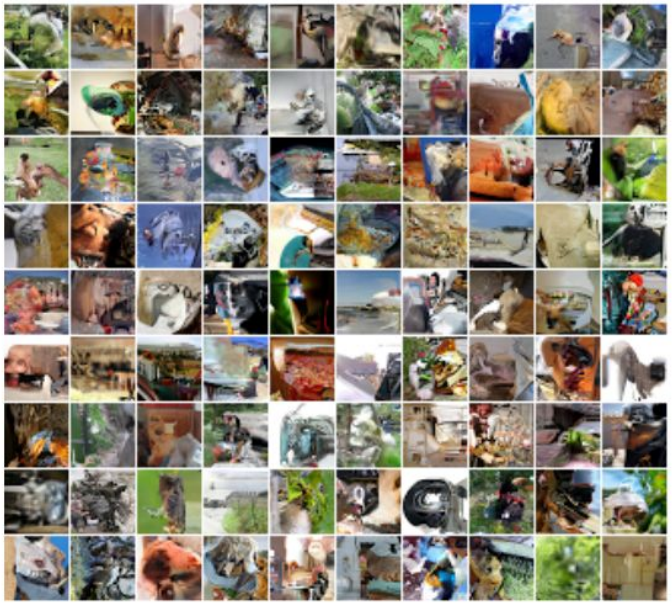
Generation is still slow:
For a 32x32 image, we need to do forward passes of the network 1024 times for a single image



Generation Samples



32x32 CIFAR-10



32x32 ImageNet

PixelRNN and PixelCNN

Pros:

- Can explicitly compute likelihood p(x)
- Easy to optimize
- Good samples

Con:

- Sequential generation => slow

Improving PixelCNN performance

- Gated convolutional layers
- Short-cut connections
- Discretized logistic loss
- Multi-scale
- Training tricks
- Etc…

See

- Van der Oord et al. NIPS 2016
- Salimans et al. 2017 (PixelCNN++)

Generative Adversarial Networks (GANs)

Generative Adversarial Networks

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Problem: Want to sample from complex, high-dimensional training distribution. No direct way to do this!

Solution: Sample from a simple distribution we can easily sample from, e.g. random noise. Learn transformation to training distribution.

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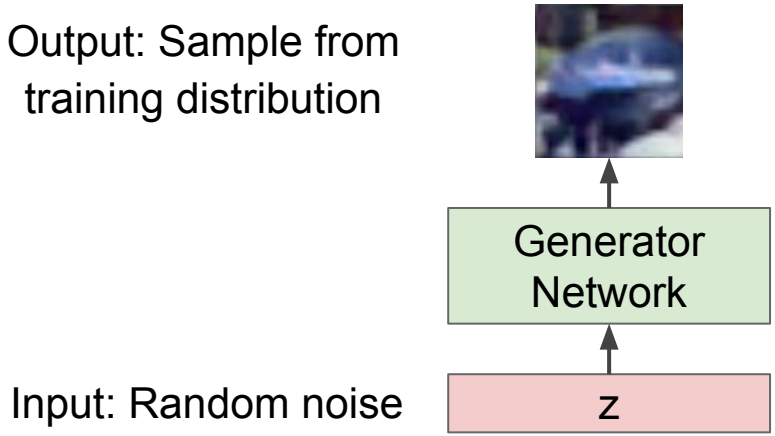

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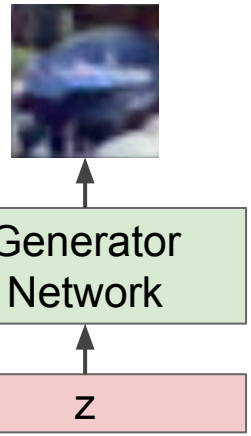
But we don’t know which sample z maps to which training image -> can’t learn by reconstructing training images

Output: Sample from training distribution



Input: Random noise

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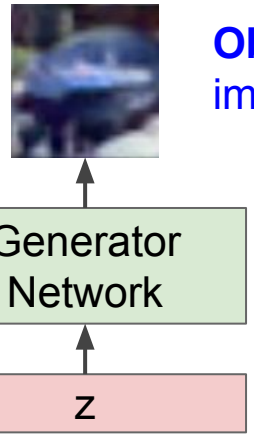

Input: Random noise

Objective: generated images should look “real”

Generative Adversarial Networks

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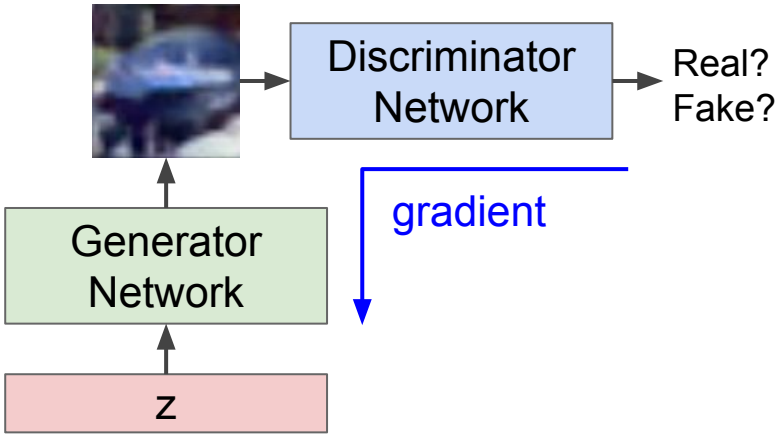
Solution: Sample from a simple distribution we can easily sample from, e.g. random noise. Learn transformation to training distribution.

But we don't know which sample z maps to which training image -> can't learn by reconstructing training images

Solution: Use a discriminator network to tell whether the generate image is within data distribution ("real") or not

Output: Sample from training distribution



Input: Random noise

Training GANs: Two-player game

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Discriminator network: try to distinguish between real and fake images
Generator network: try to fool the discriminator by generating real-looking images

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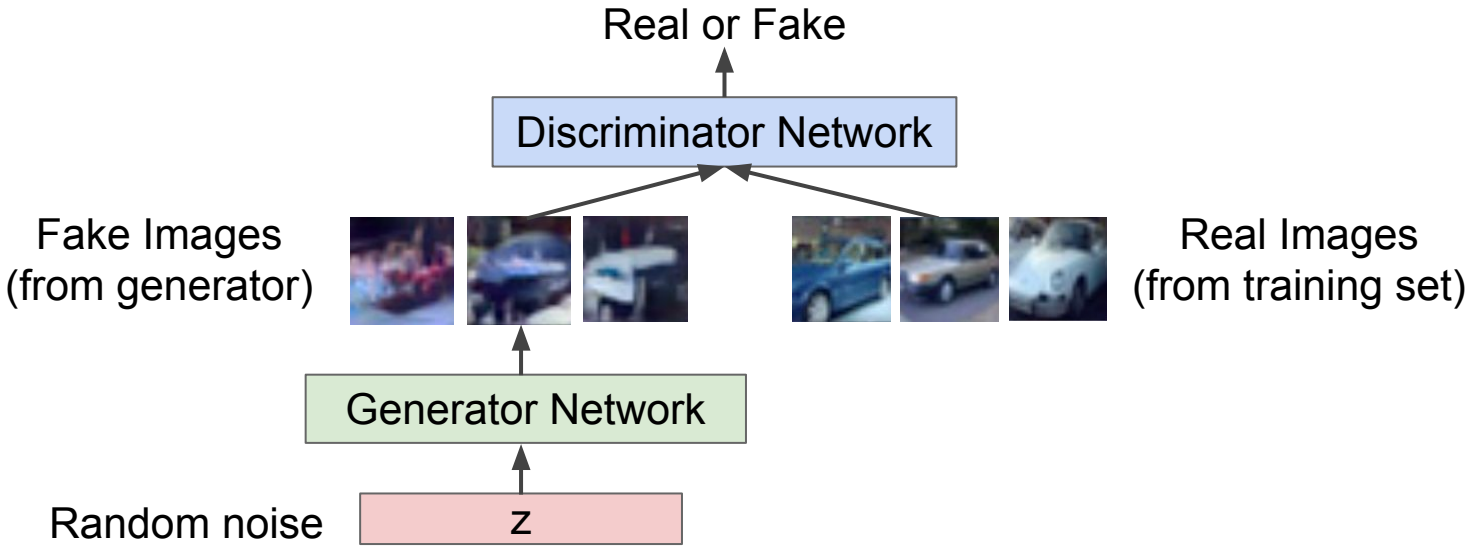

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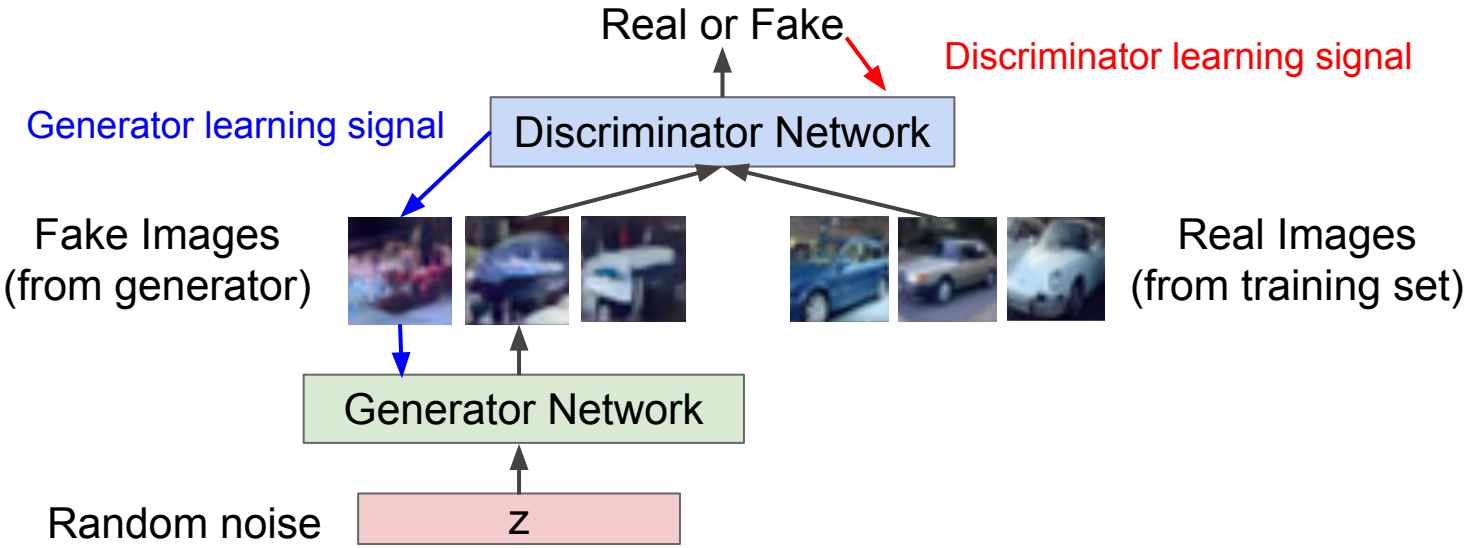

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Train jointly in **minimax game**

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Generator objective

Discriminator objective

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Discriminator output for real data x

Discriminator output for generated fake data G(z)

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Discriminator output for real data x

Discriminator output for generated fake data G(z)

- Discriminator (θ_d) wants to **maximize objective** such that D(x) is close to 1 (real) and D(G(z)) is close to 0 (fake)
- Generator (θ_g) wants to **minimize objective** such that D(G(z)) is close to 1 (discriminator is fooled into thinking generated G(z) is real)

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Alternate between:

1. **Gradient ascent** on discriminator

$$\max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

2. **Gradient descent** on generator

$$\min_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z)))$$

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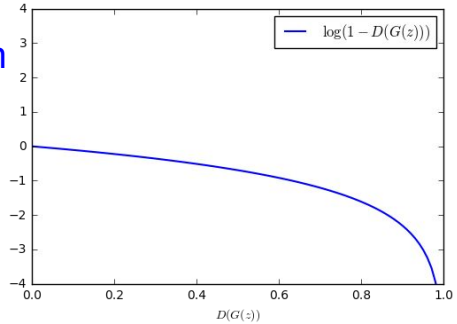
$$\min_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z)))$$

In practice, optimizing this generator objective does not work well!

When sample is likely fake, want to learn from it to improve generator (move to the right on X axis).



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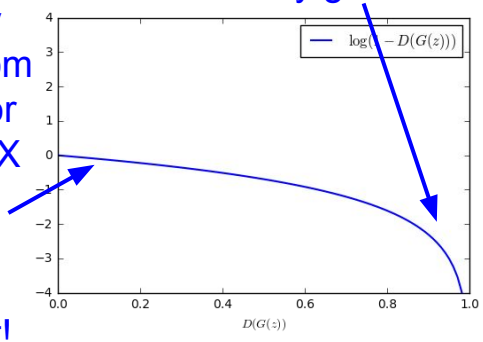
In practice, optimizing this generator objective does not work well!

When sample is likely fake, want to learn from it to improve generator (move to the right on X axis).

But gradient in this region is relatively flat!

Gradient signal dominated by region where sample is already good



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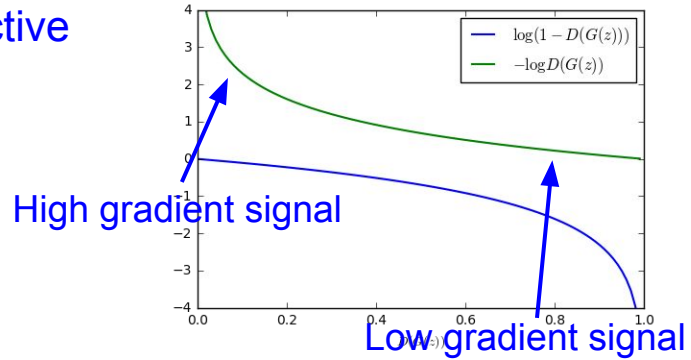
2. **Instead: Gradient ascent** on generator, different objective

$$\max_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(D_{\theta_d}(G_{\theta_g}(z)))$$

Instead of minimizing likelihood of discriminator being correct, now maximize likelihood of discriminator being wrong.
Same objective of fooling discriminator, but now higher gradient signal for bad samples => works much better! Standard in practice.



Training GANs: Two-player game

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Putting it together: GAN training algorithm

for number of training iterations **do**

for k steps **do**

- Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
- Sample minibatch of m examples $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ from data generating distribution $p_{\text{data}}(\boldsymbol{x})$.
- Update the discriminator by ascending its stochastic gradient:

$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[\log D_{\theta_d}(x^{(i)}) + \log(1 - D_{\theta_d}(G_{\theta_g}(z^{(i)}))) \right]$$

end for

- Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
- Update the generator by ascending its stochastic gradient (improved objective):

$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log(D_{\theta_d}(G_{\theta_g}(z^{(i)})))$$

end for

Training GANs: Two-player game

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Putting it together: GAN training algorithm

Some find k=1 more stable, others use k > 1, no best rule.

Followup work (e.g. Wasserstein GAN, BEGAN) alleviates this problem, better stability!

for number of training iterations **do**

  for k steps **do**

- Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
- Sample minibatch of m examples $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ from data generating distribution $p_{\text{data}}(\boldsymbol{x})$.
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- Update the generator by ascending its stochastic gradient (improved objective):

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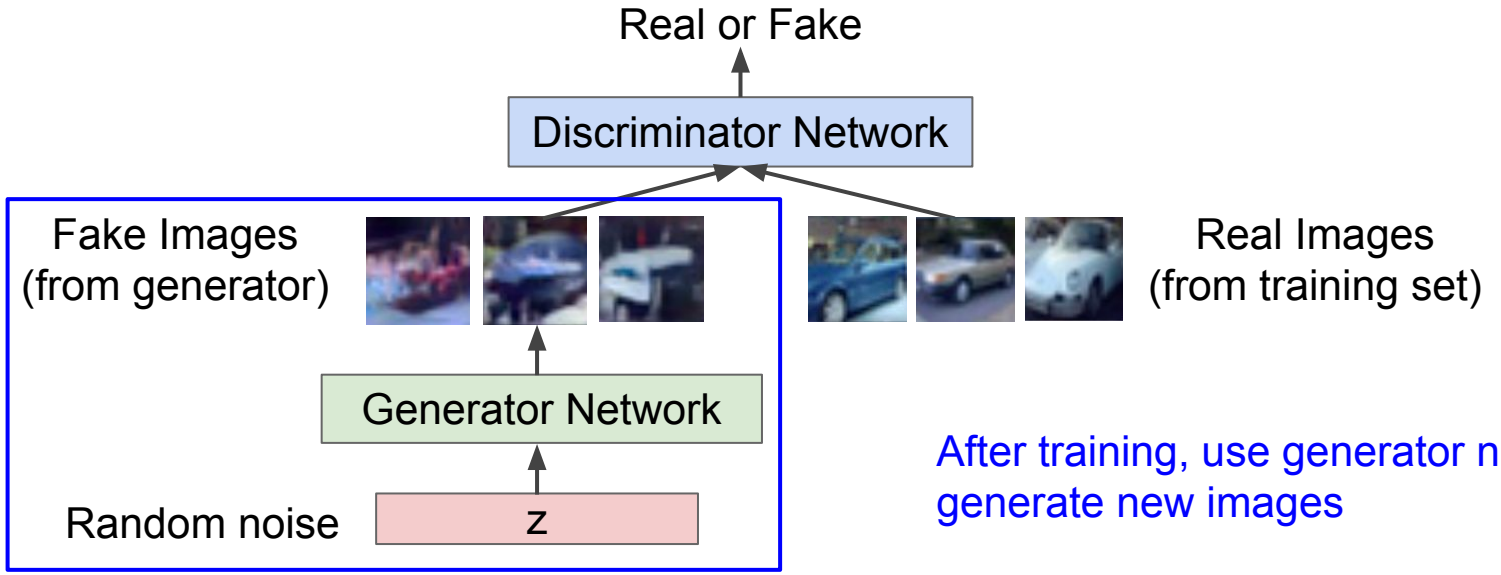
end for

Arjovsky et al. "Wasserstein gan." arXiv preprint arXiv:1701.07875 (2017)
Berthelot, et al. "Began: Boundary equilibrium generative adversarial networks." arXiv preprint arXiv:1703.10717 (2017)

Training GANs: Two-player game

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Generator network: try to fool the discriminator by generating real-looking images
Discriminator network: try to distinguish between real and fake images



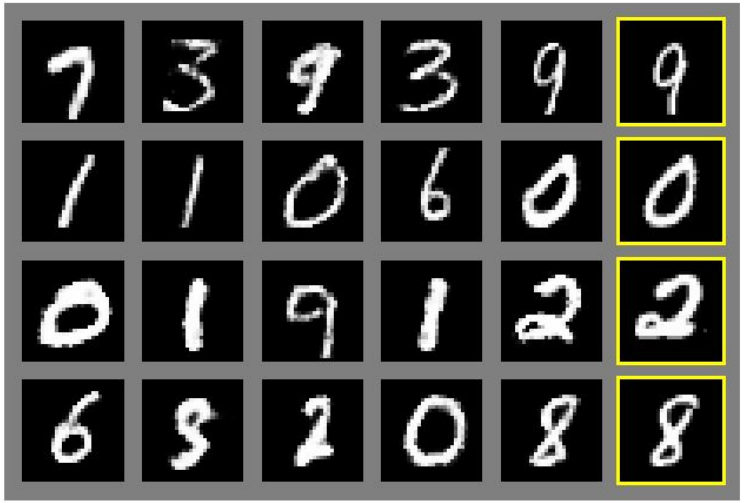
After training, use generator network to generate new images

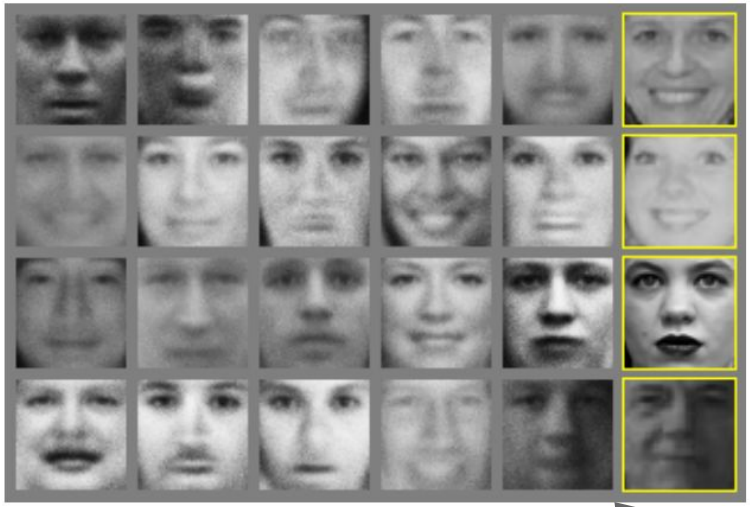
Fake and real images copyright Emily Denton et al. 2015. Reproduced with permission.

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Generative Adversarial Nets

Generated samples



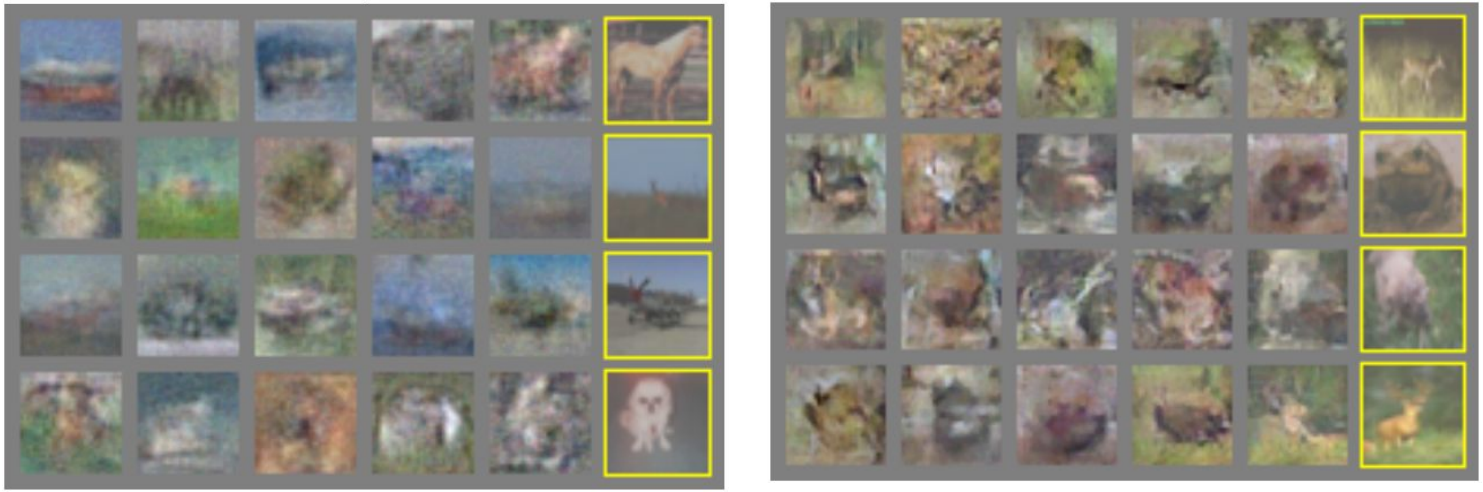


Nearest neighbor from training set

Generative Adversarial Nets

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Generated samples (CIFAR-10)



Nearest neighbor from training set

Generative Adversarial Nets: Convolutional Architectures

Samples from the model look much better!

Radford et al, ICLR 2016

Generative Adversarial Nets: Convolutional Architectures

Interpolating between random points in laten space

Radford et al, ICLR 2016

Generative Adversarial Nets: Interpretable Vector Math

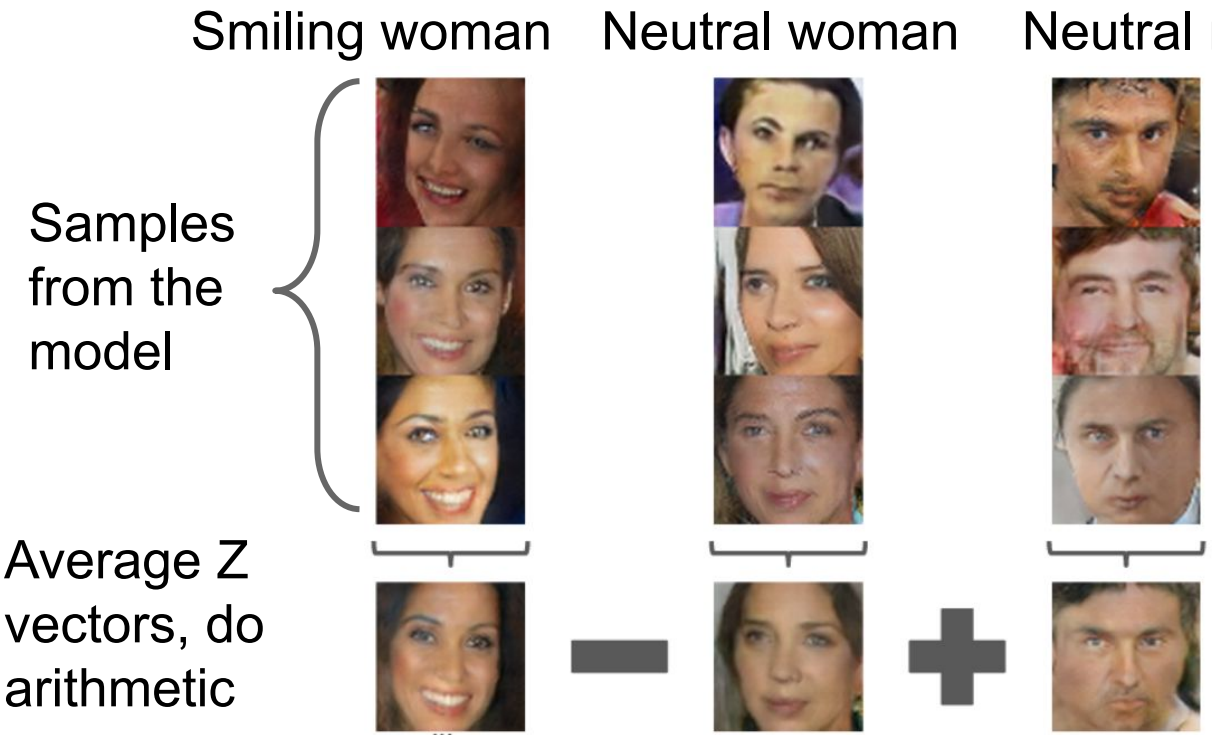
Radford et al, ICLR 2016

Smiling woman | Neutral woman | Neutral man

Samples from the model

Generative Adversarial Nets: Interpretable Vector Math

Radford et al, ICLR 2016



Generative Adversarial Nets: Interpretable Vector Math

Radford et al, ICLR 2016

Smiling woman | Neutral woman | Neutral man

Samples from the model

Average Z vectors, do arithmetic

Smiling Man

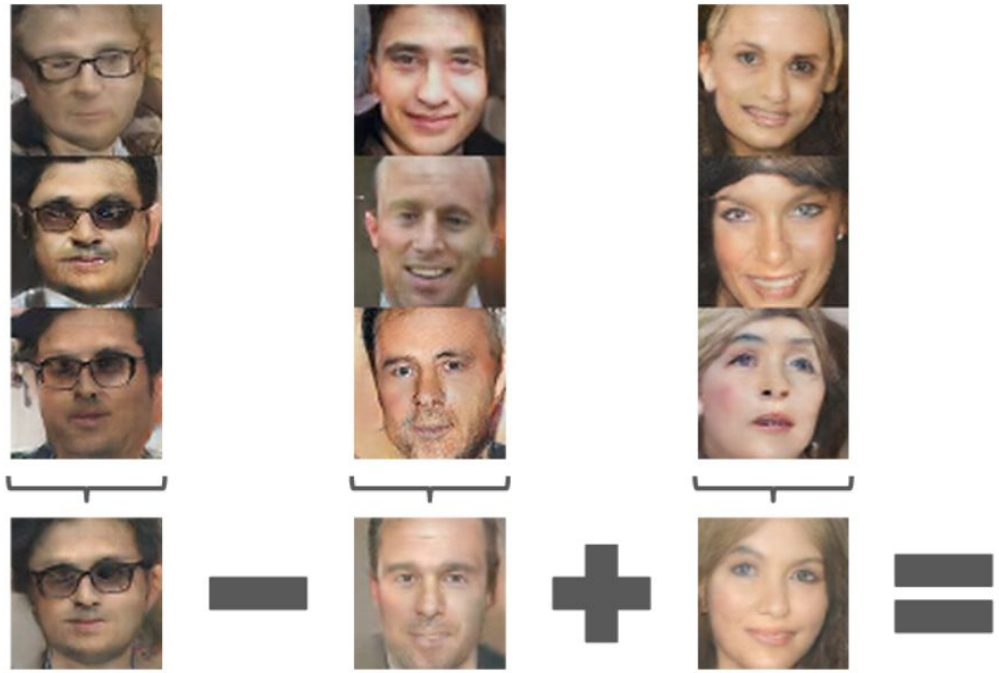
Generative Adversarial Nets: Interpretable Vector Math

Glasses man

No glasses man

No glasses woman

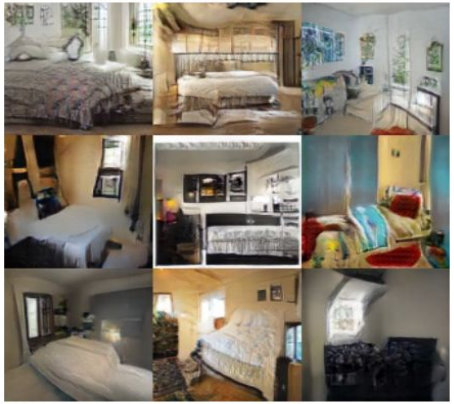
Radford et al, ICLR 2016



Woman with glasses

2017: Explosion of GANs

Better training and generation



LSGAN, Zhu 2017.

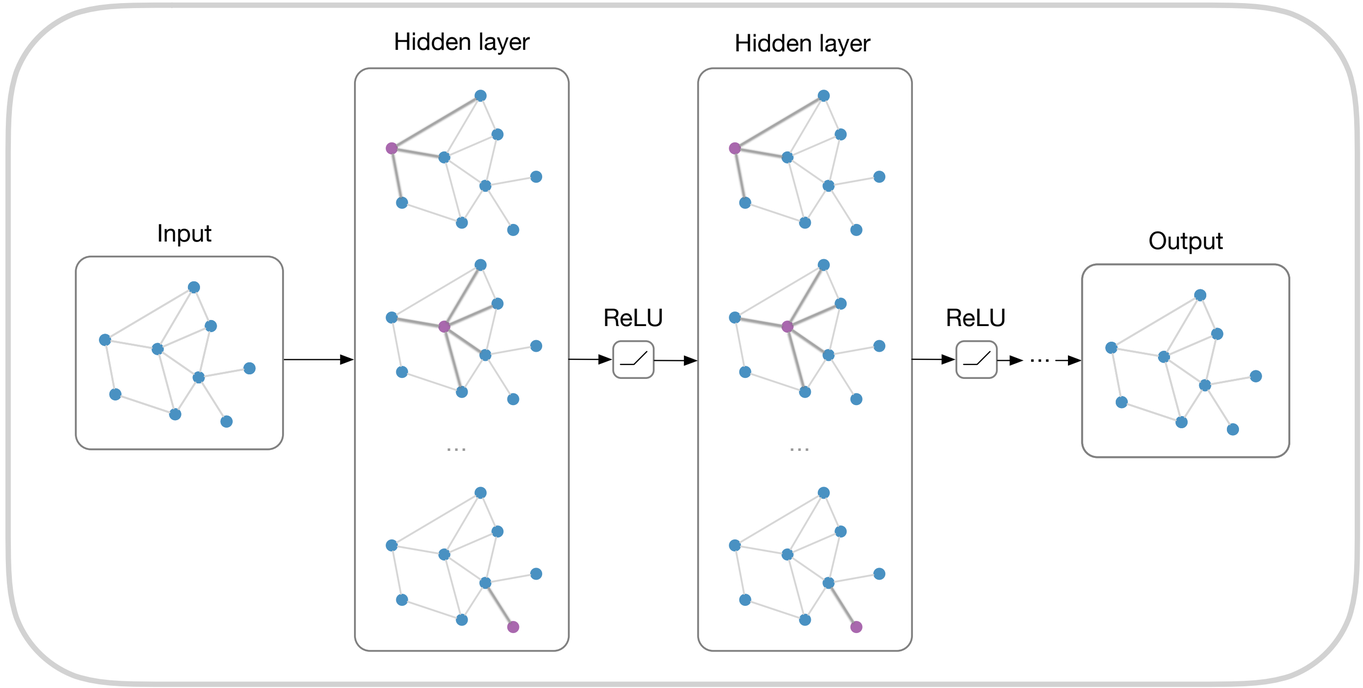
Wasserstein GAN, Arjovsky 2017. Improved Wasserstein GAN, Gulrajani 2017.

Progressive GAN, Karras 2018.

2019: BigGAN

Brock et al., 2019

Structured deep models:
Deep learning on graphs and beyond



Thomas Kipf, 25 May 2018

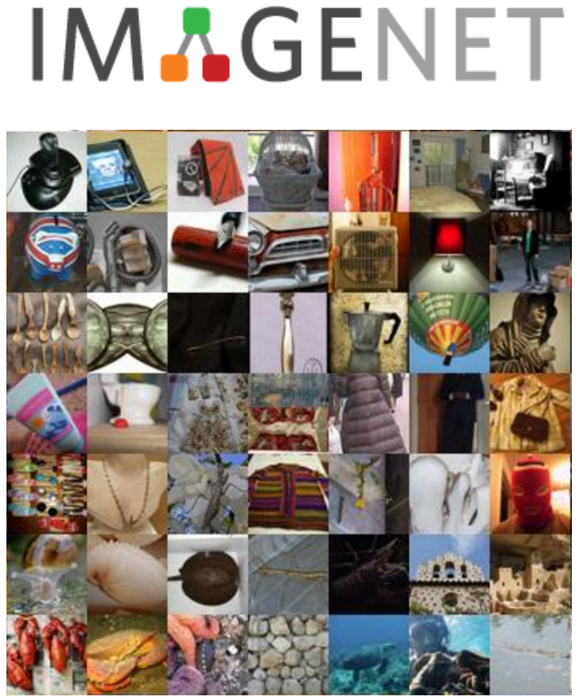
CompBio Seminar, University of Cambridge

In collaboration with Ethan Fetaya, Rianne van den Berg, Michael Schlichtkrull, Petar Veličković, Ivan Titov, Max Welling, Richard Zemel and others

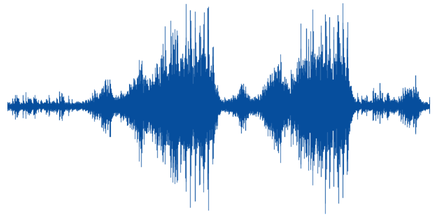
UNIVERSITEIT VAN AMSTERDAM

AMLAB Amsterdam Machine Learning Lab

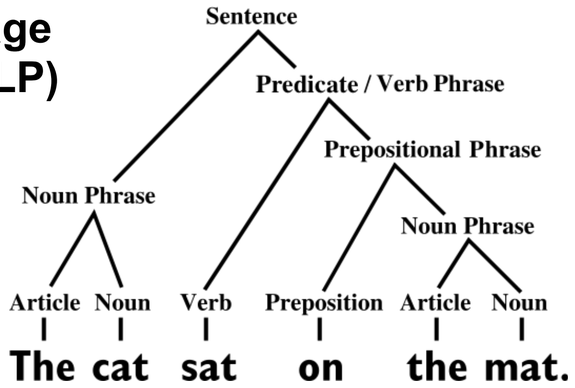
The Deep Learning slide



Speech data



Natural language processing (NLP)



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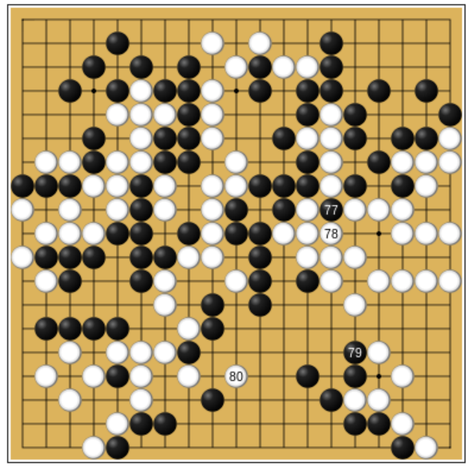
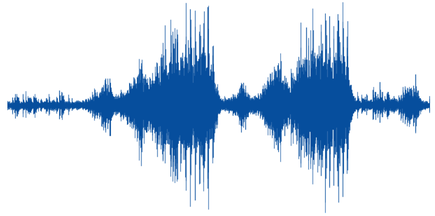
Grid games



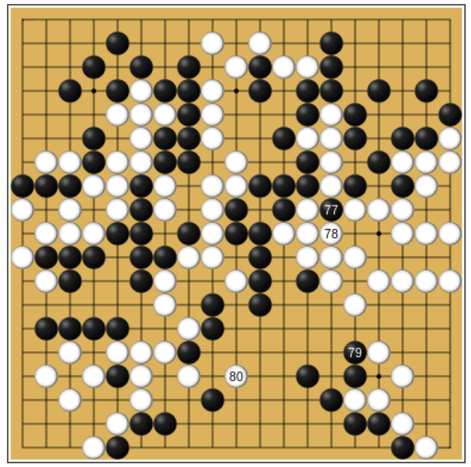
The Deep Learning slide

IMAGENET

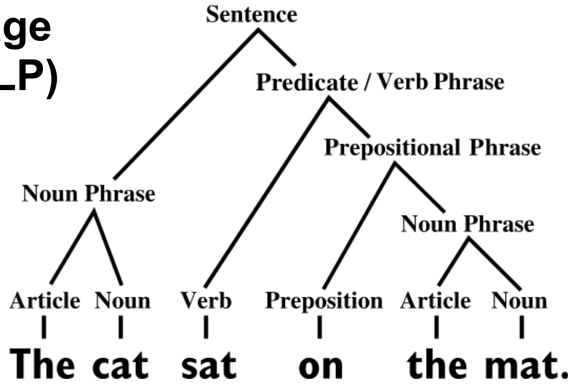
Speech data



Grid games



Natural language processing (NLP)



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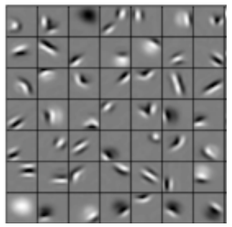
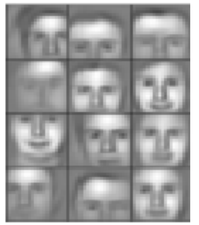
Deep neural nets that exploit:

- translation equivariance (weight sharing)
- hierarchical compositionality





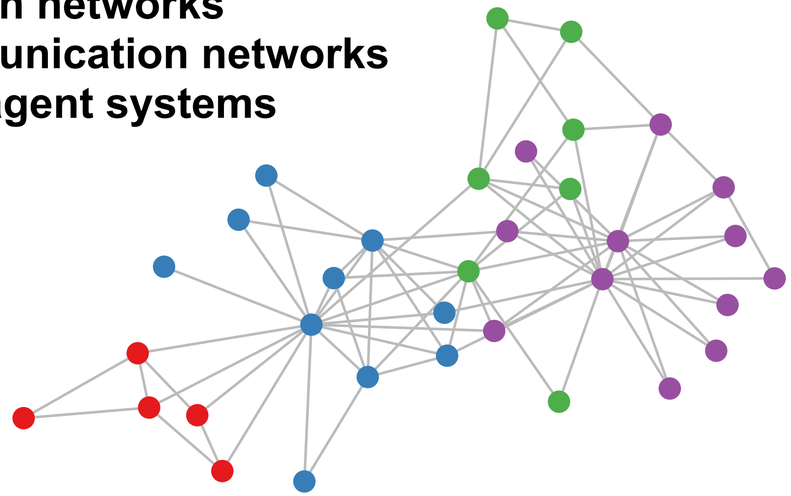
Graph-structured data

A lot of real-world data does not “live” on grids

Graph-structured data

A lot of real-world data does not “live” on grids

Social networks
Citation networks
Communication networks
Multi-agent systems



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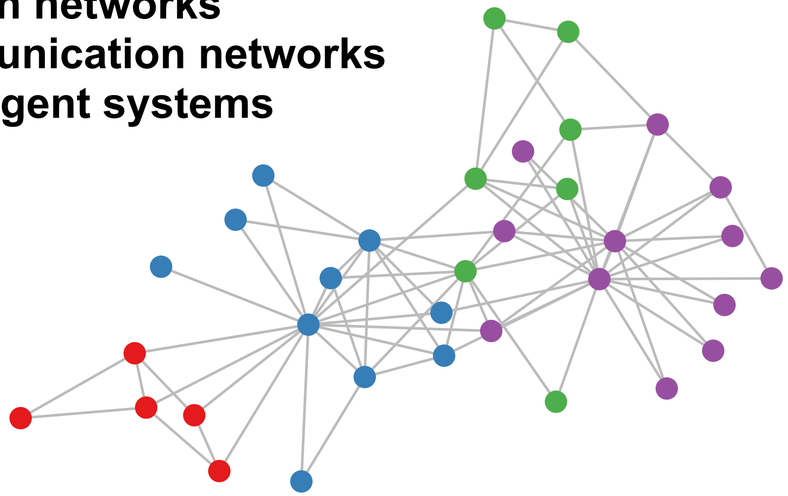

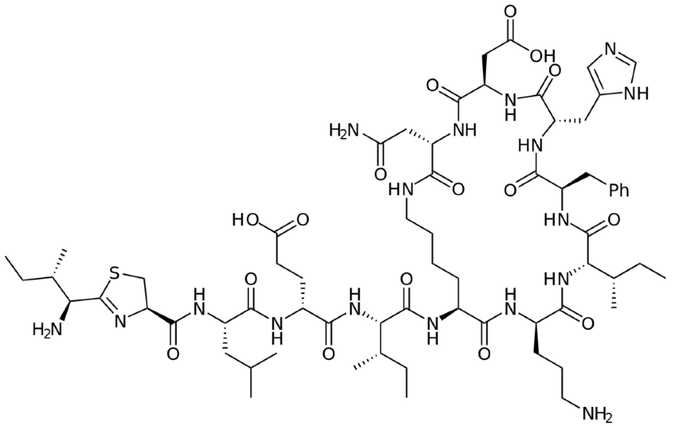

Molecules

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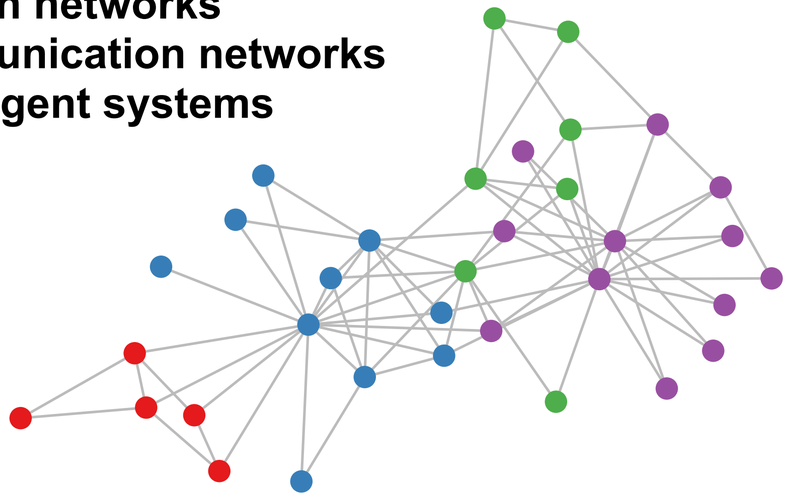
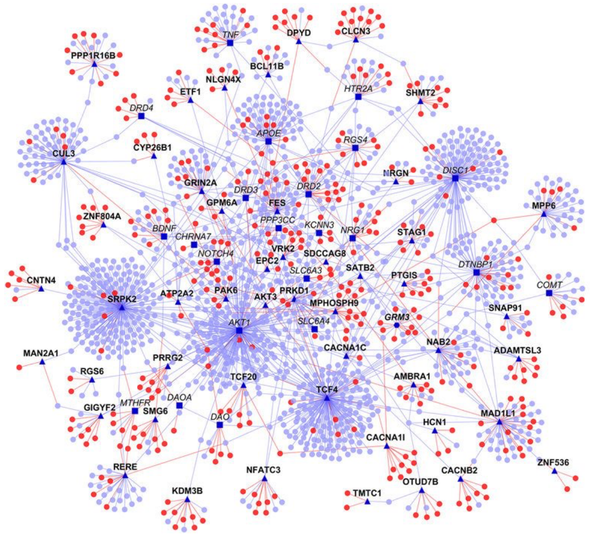
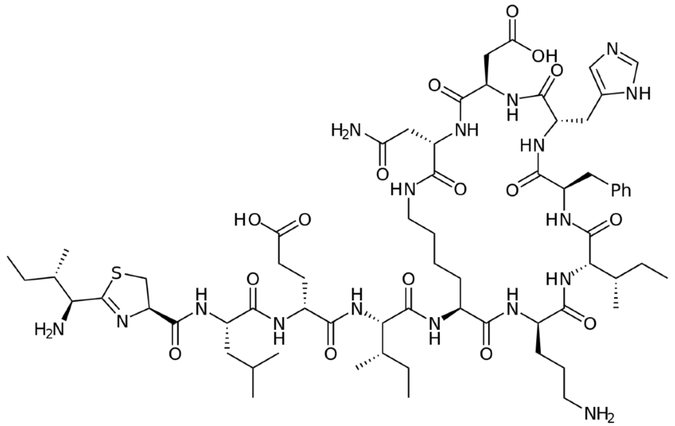




Protein interaction networks



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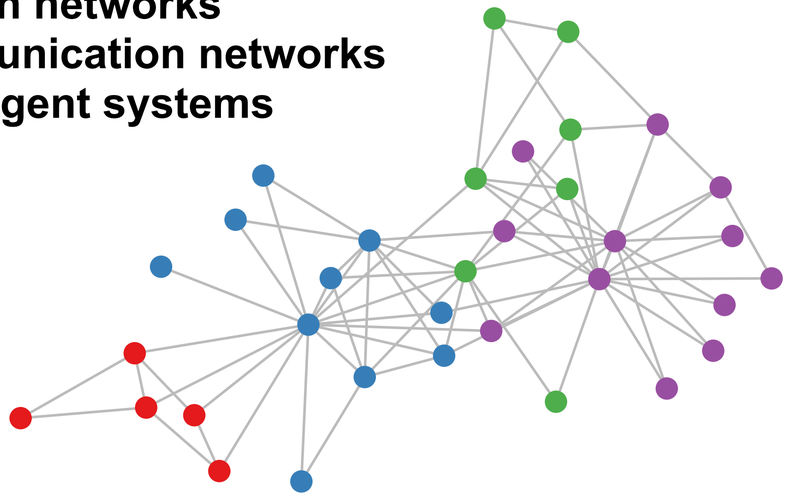
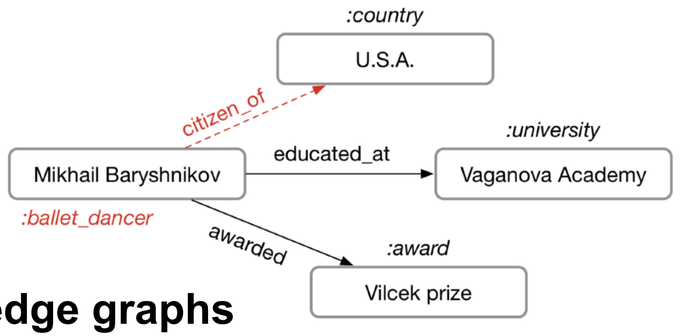
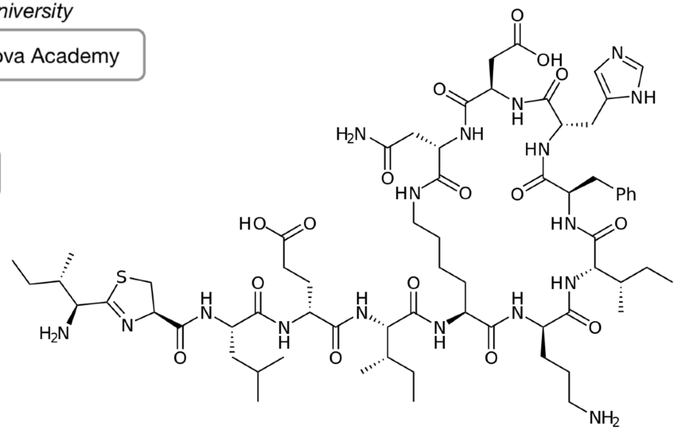
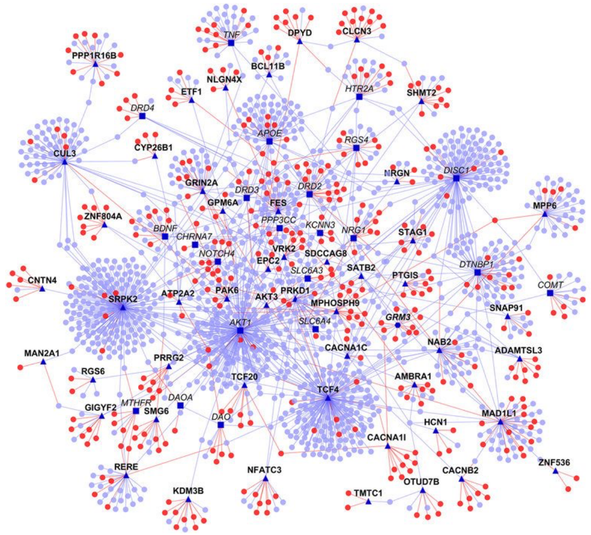




Knowledge graphs



Molecules



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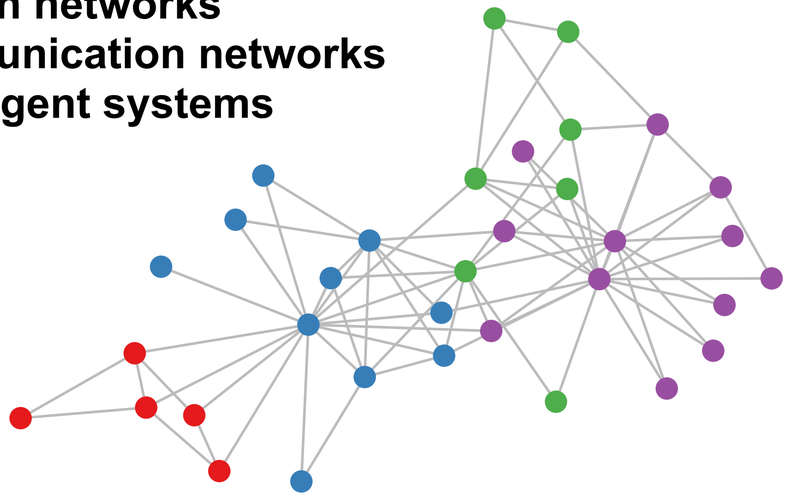

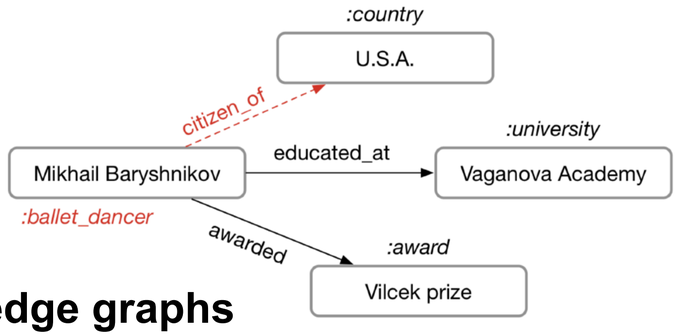

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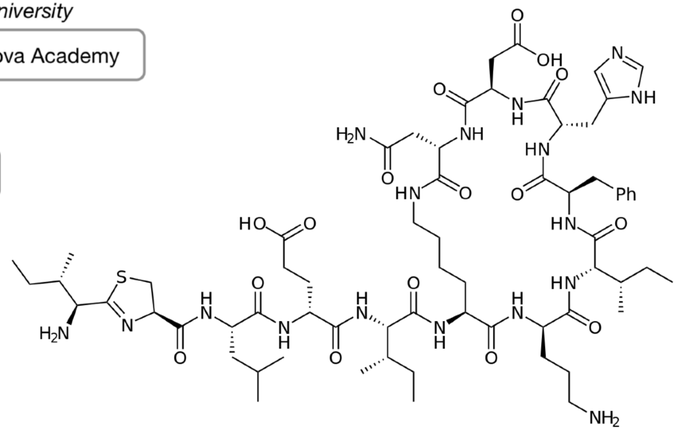
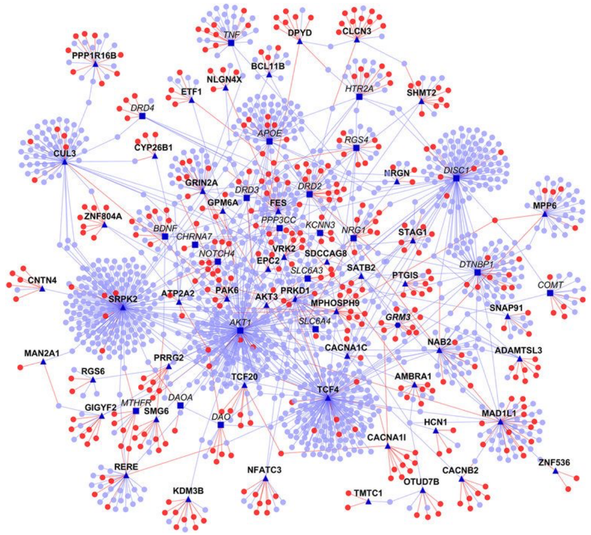
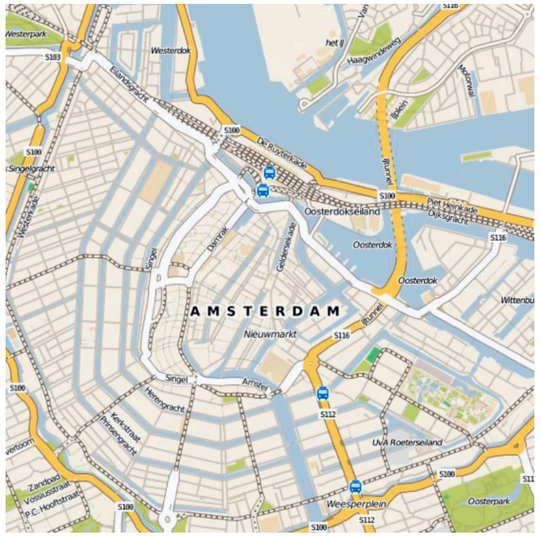


Molecules



Protein interaction networks



Road maps

Graph-structured data

A lot of real-world data does not “live” on grids

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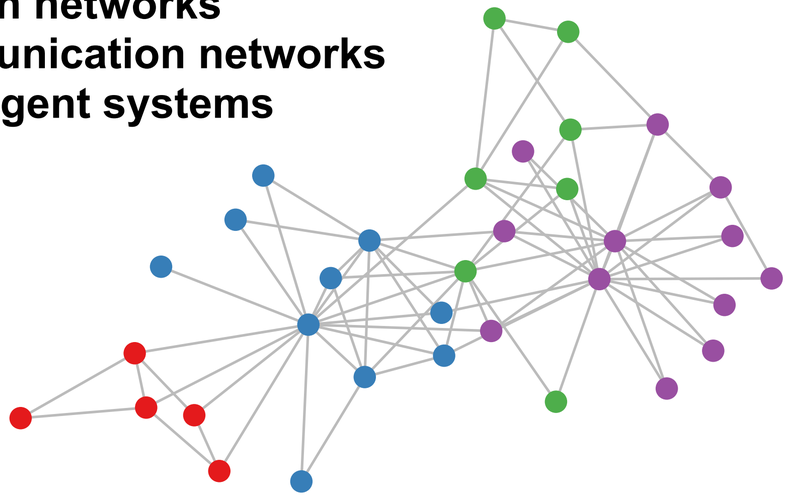
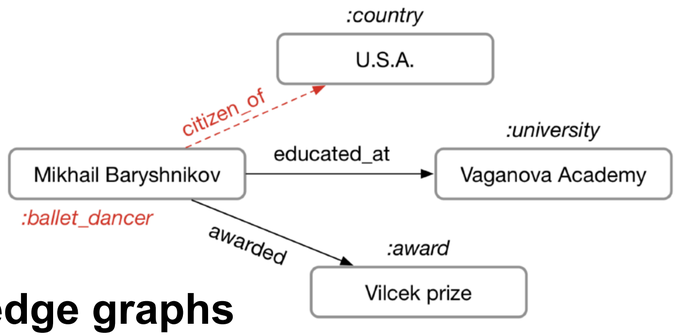
Citation networks
Communication networks
Multi-agent systems





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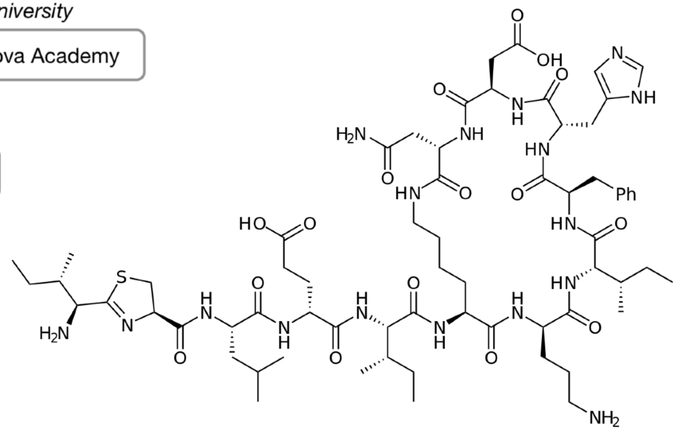
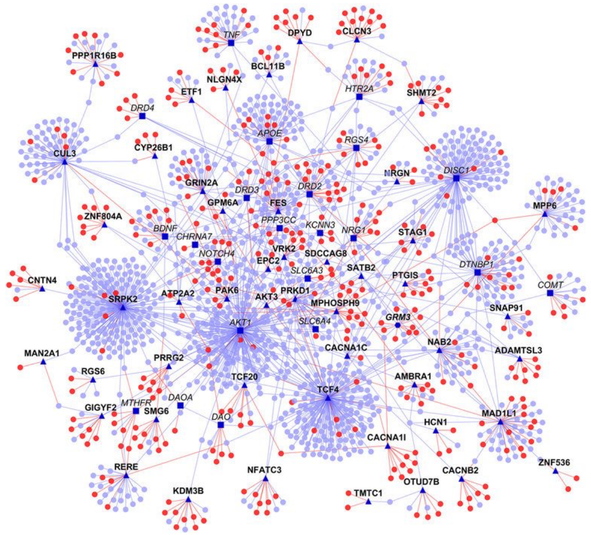
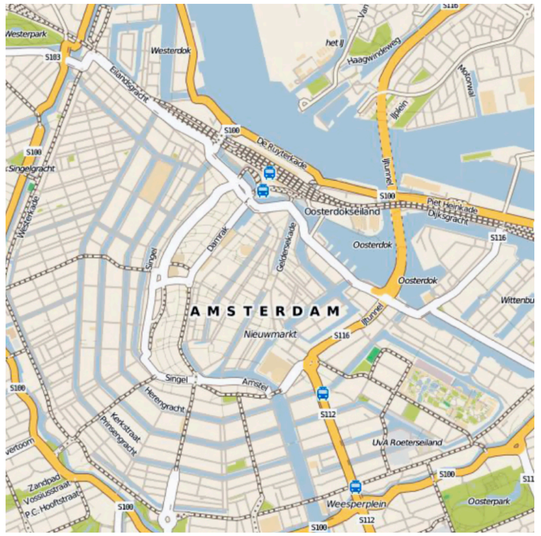


Molecules



Protein interaction networks



Road maps

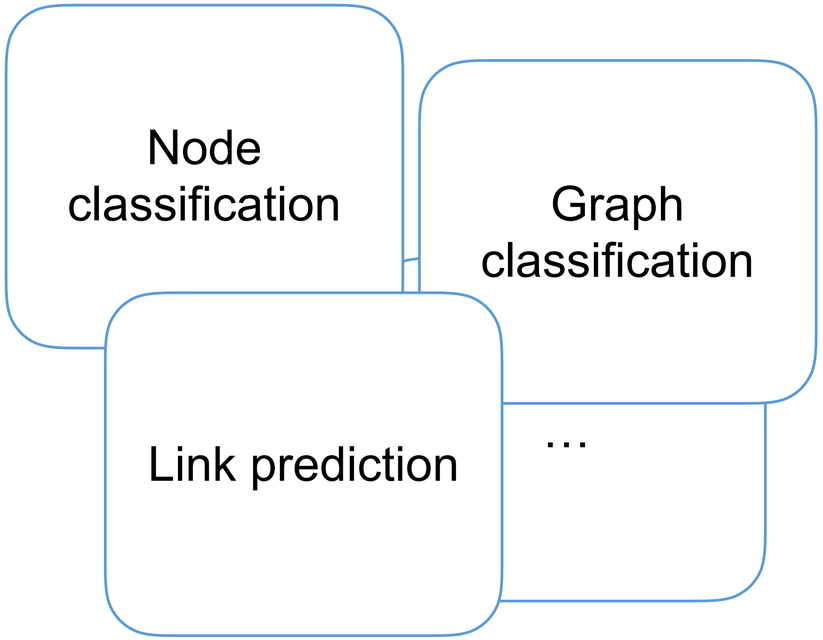
Standard deep learning architectures like CNNs and RNNs don’t work here!

Talk overview

1) Graph neural nets (GNNs):

Introduction & some history

2) GNNs for "classical" network problems



Talk overview

1) Graph neural nets (GNNs):
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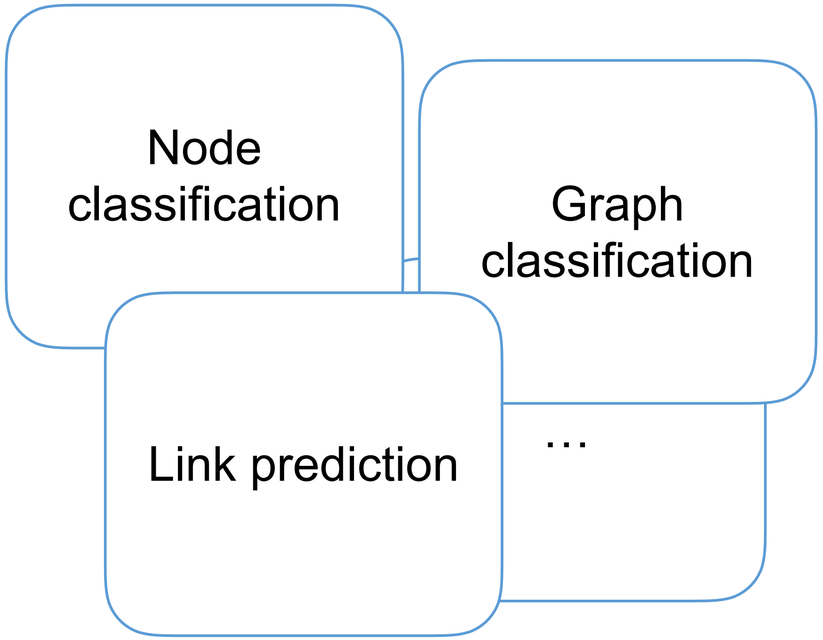
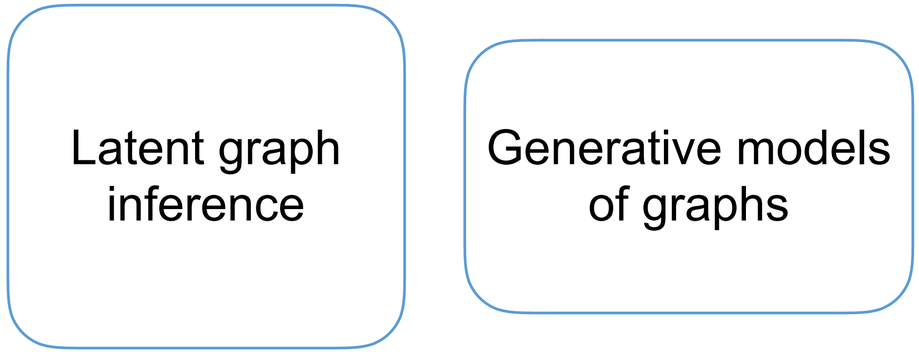


3) Emerging research directions

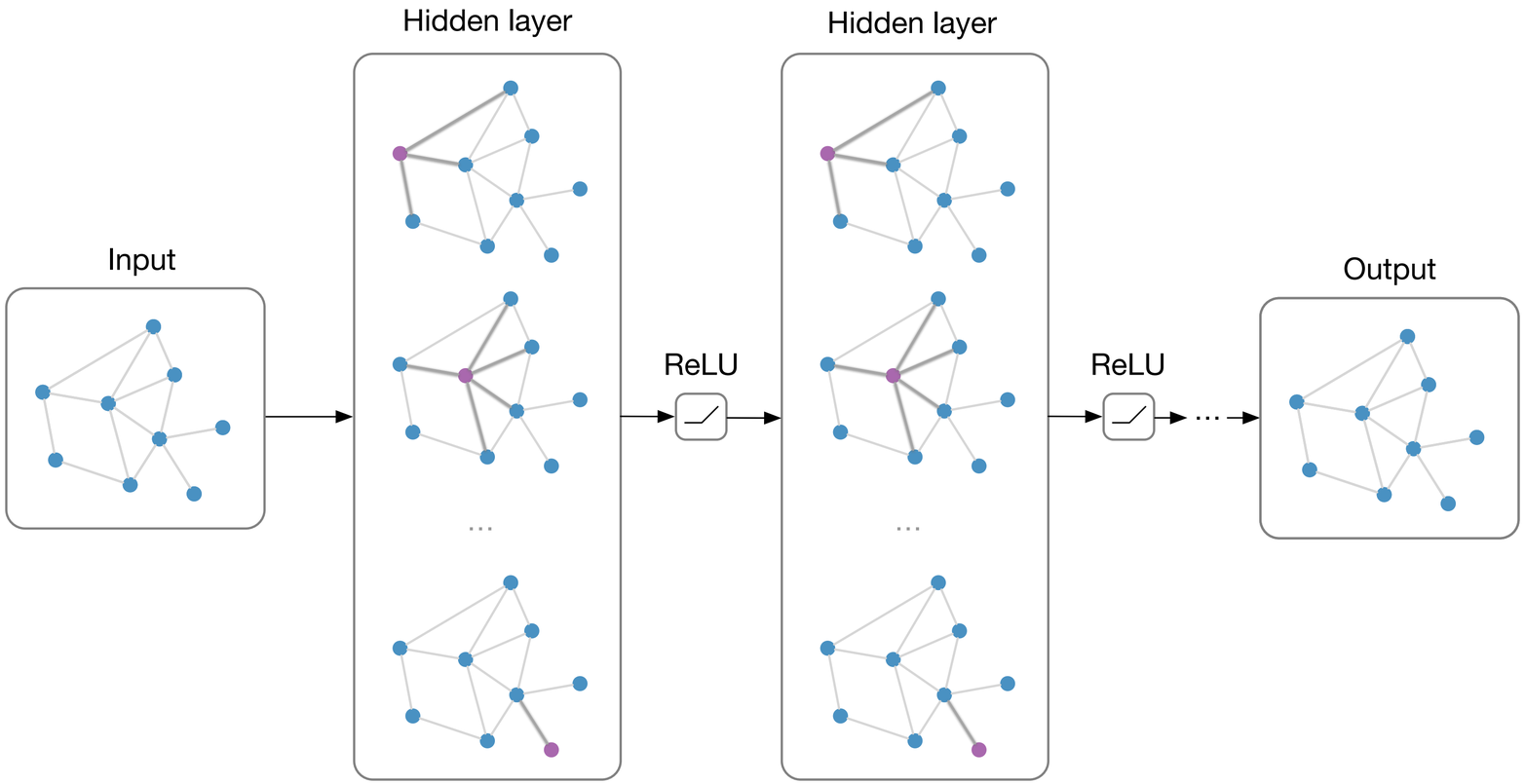


(Potential) applications:

- Interacting systems (physics/multi-agent),
- Causal inference
- Program induction,
- Chemical synthesis,

Graph Neural Networks (GNNs)

The bigger picture:



Main idea: Pass messages between pairs of nodes & agglomerate

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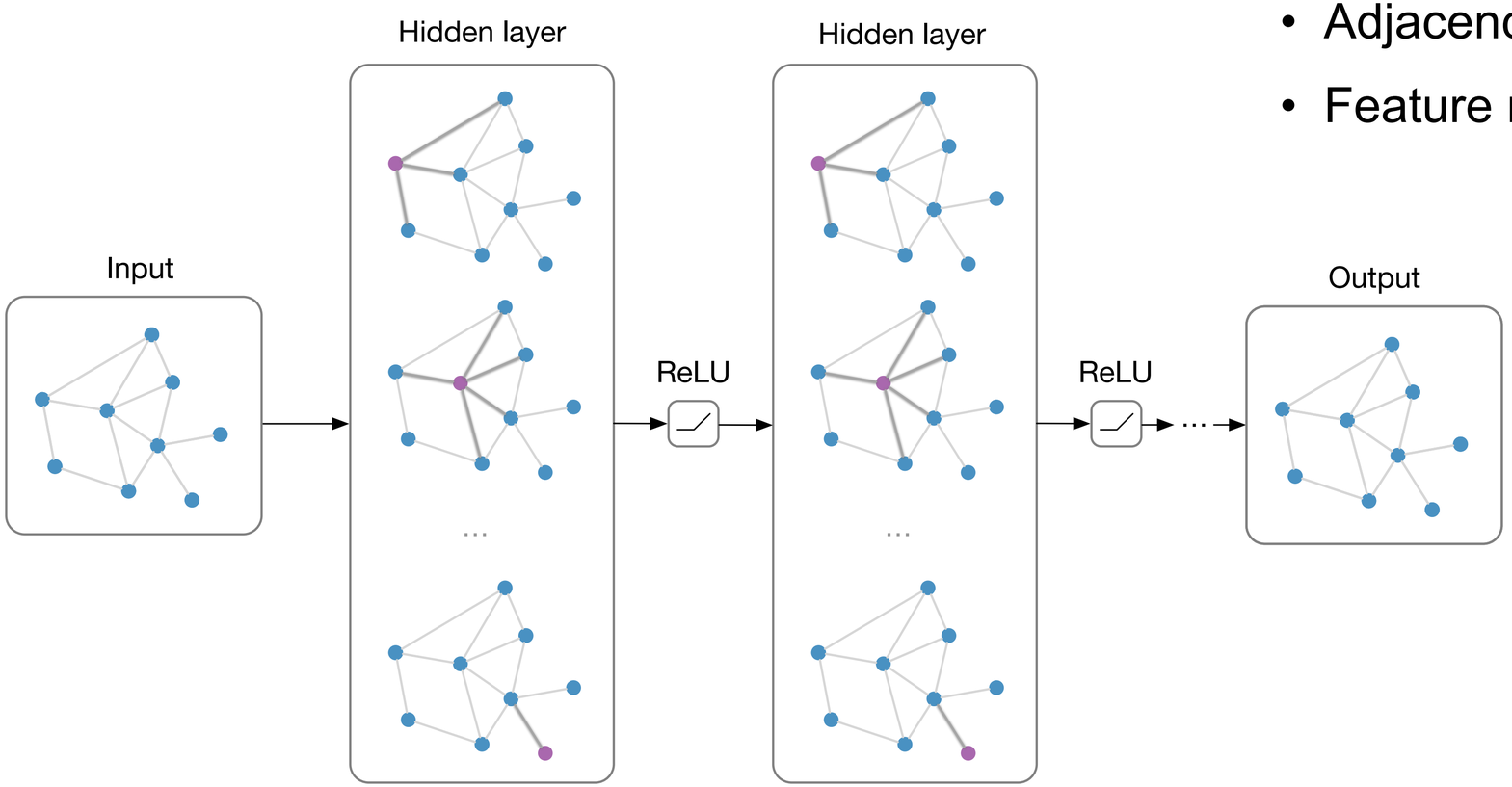


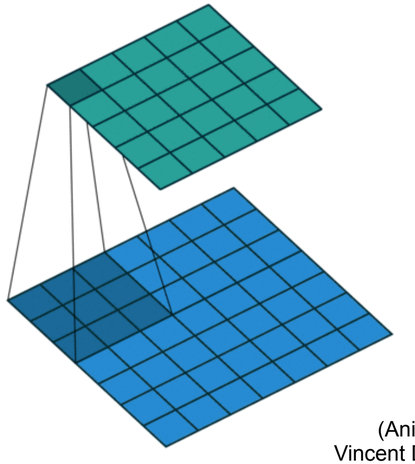
Notation: $\mathcal{G} = (\mathbf{A}, \mathbf{X})$

- Adjacency matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$
- Feature matrix $\mathbf{X} \in \mathbb{R}^{N \times F}$

Main idea: Pass messages between pairs of nodes & agglomerate

Recap: Convolutional neural networks (on grids)

Single CNN layer with 3x3 filter:



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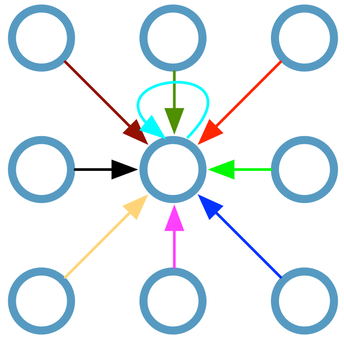

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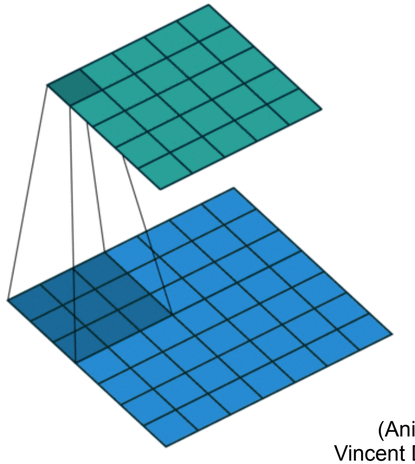

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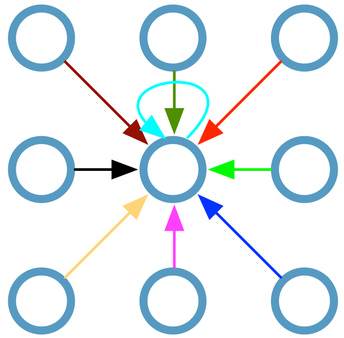

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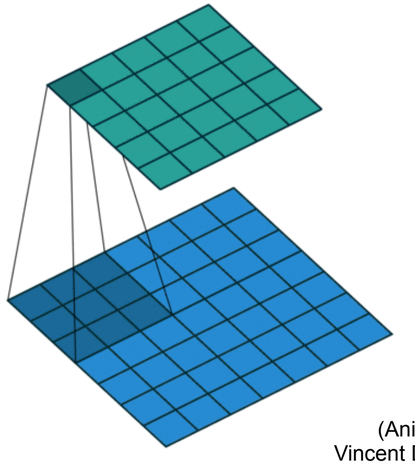

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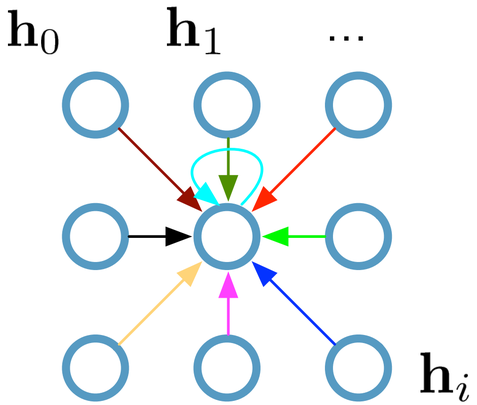

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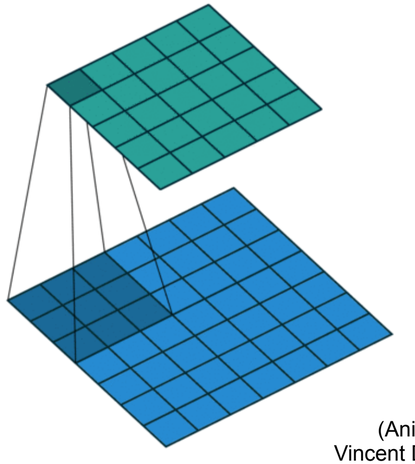

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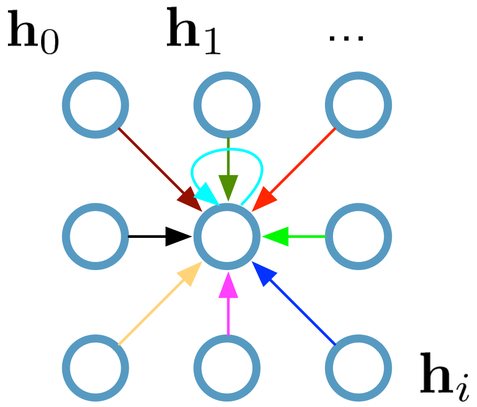

$\mathbf{h}_i \in \mathbb{R}^F$ are (hidden layer) activations of a pixel/node

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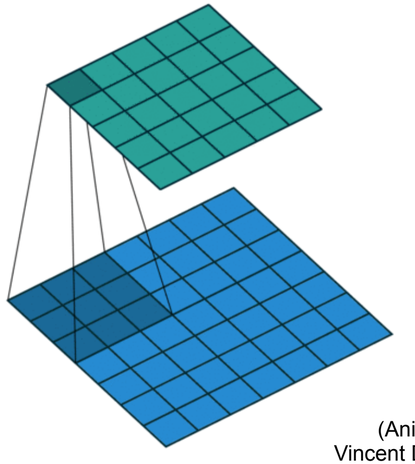

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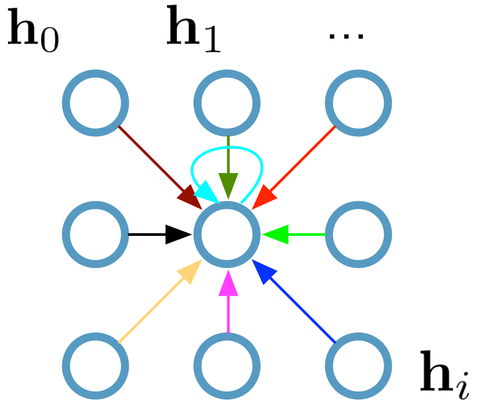

Update for a single pixel:

- Transform messages individually $\mathbf{W}_i\mathbf{h}_i$
- Add everything up $\sum_i \mathbf{W}_i\mathbf{h}_i$

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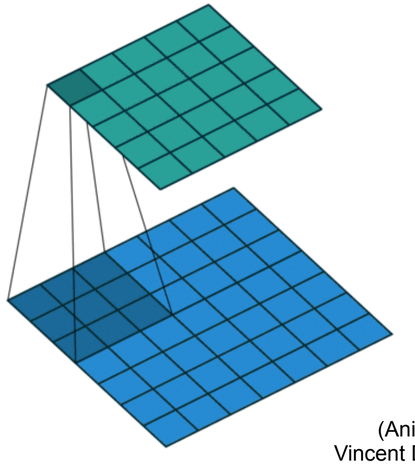

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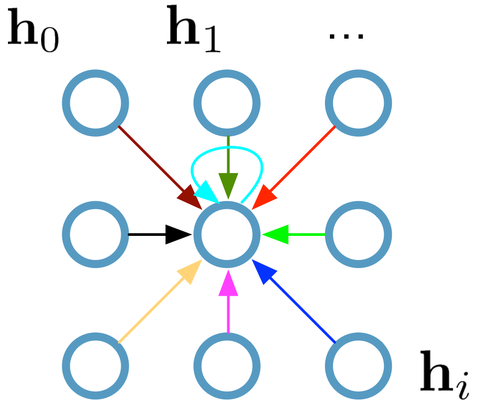

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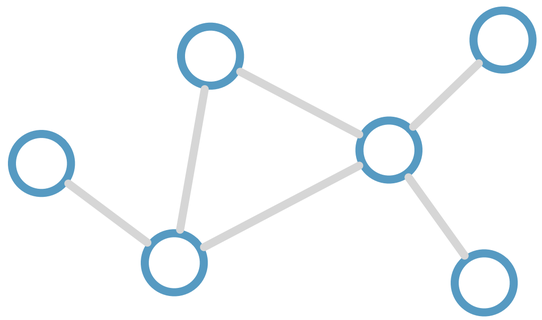
Full update:

$$\mathbf{h}_4^{(l+1)} = \sigma\left(\mathbf{W}_0^{(l)}\mathbf{h}_0^{(l)} + \mathbf{W}_1^{(l)}\mathbf{h}_1^{(l)} + \cdots + \mathbf{W}_8^{(l)}\mathbf{h}_8^{(l)}\right)$$

Graph convolutional networks (GCNs)

Kipf & Welling (ICLR 2017), related previous works by Duvenaud et al. (NIPS 2015) and Li et al. (ICLR 2016)

Consider this undirected graph:



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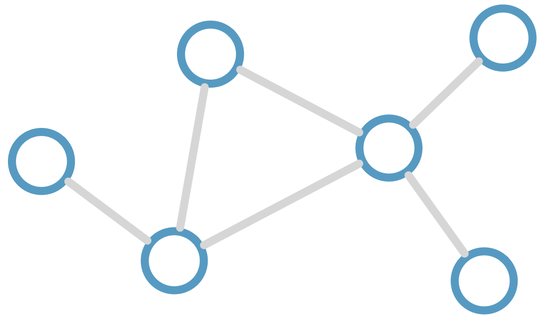
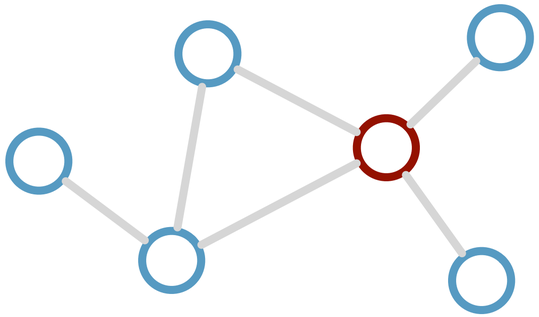


Calculate update for node in red:



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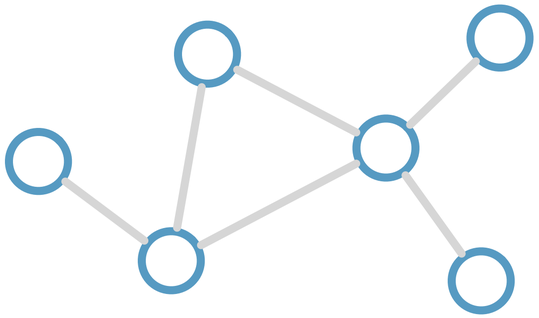

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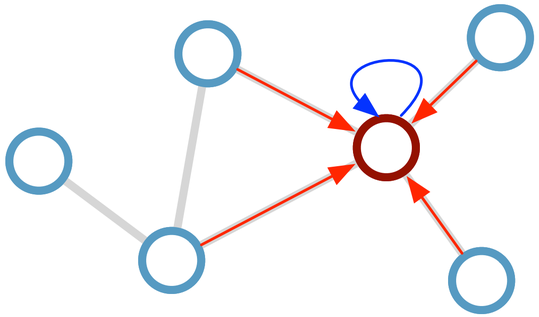

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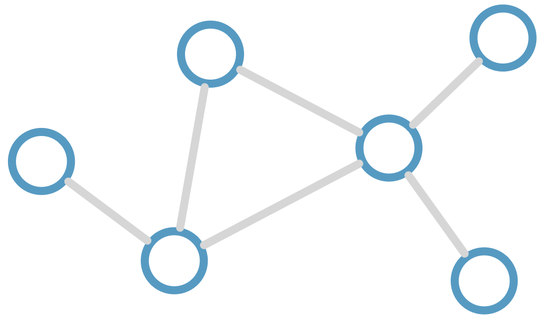

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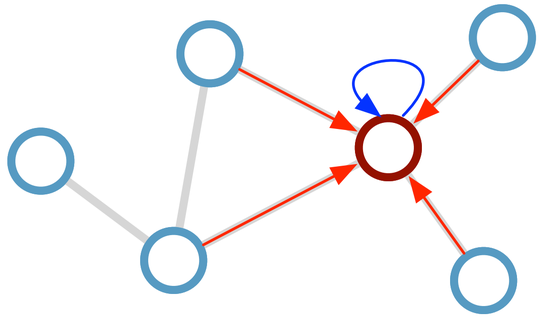

Update rule:

$$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \sum_{j\in\mathcal{N}_i}\frac{1}{c_{ij}}\mathbf{h}_j^{(l)}\mathbf{W}_1^{(l)}\right)$$

$\mathcal{N}_i$: neighbor indices

c_{ij} : norm. constant (fixed/trainable)

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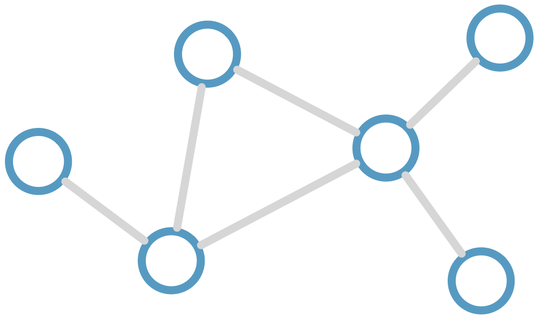

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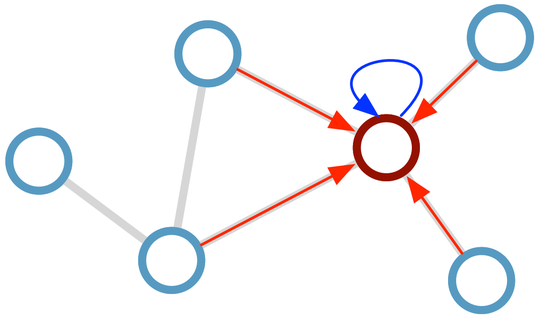

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Scalability: subsample messages [Hamilton et al., NIPS 2017]

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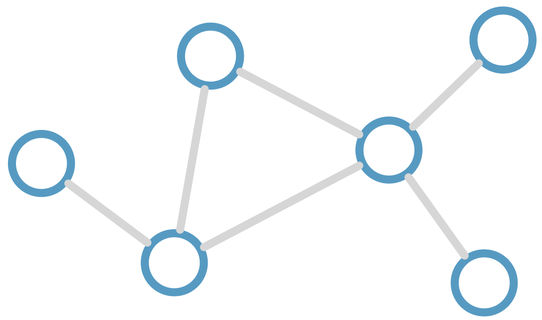

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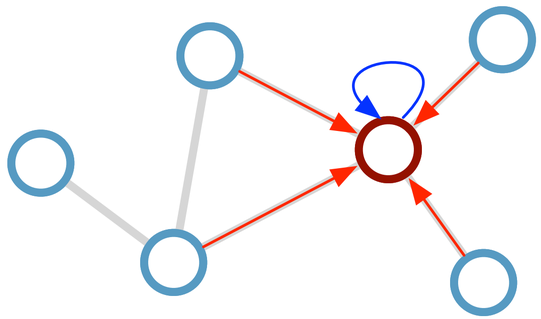

Desirable properties:

- Weight sharing over all locations
- Invariance to permutations
- Linear complexity O(E)
- Applicable both in transductive and inductive settings

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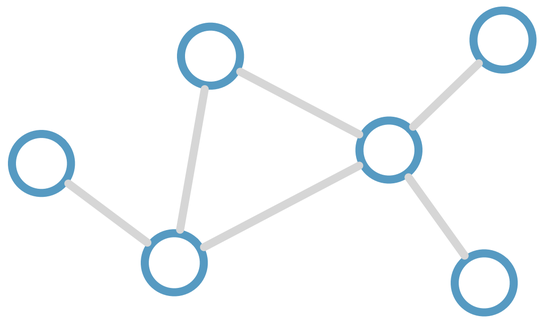

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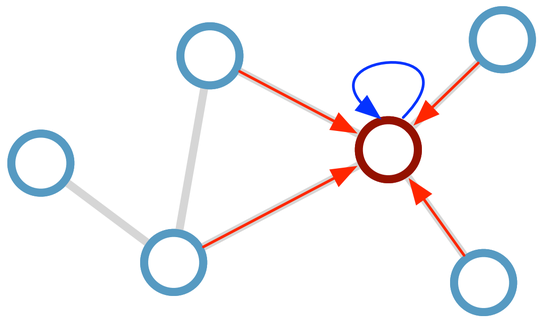

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Desirable properties:

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Limitations:

- Requires gating mechanism / residual connections for depth
- Only indirect support for edge features

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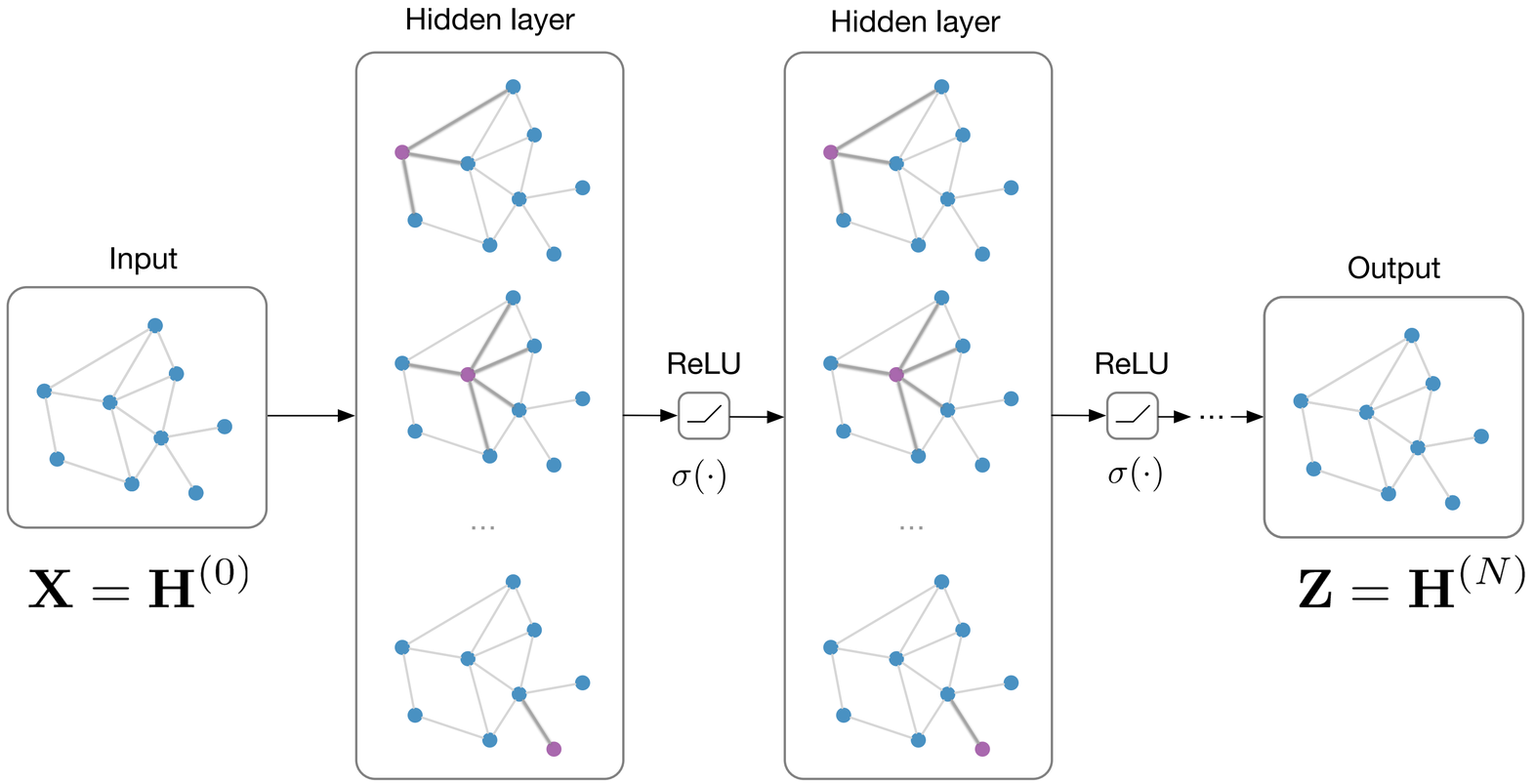
Part 2: Application to “classical” network problems

Node classification **Graph classification**

Link prediction

One fits all: Classification and link prediction with GNNs/GCNs

Input: Feature matrix $\mathbf{X} \in \mathbb{R}^{N \times E}$, preprocessed adjacency matrix $\hat{\mathbf{A}}$



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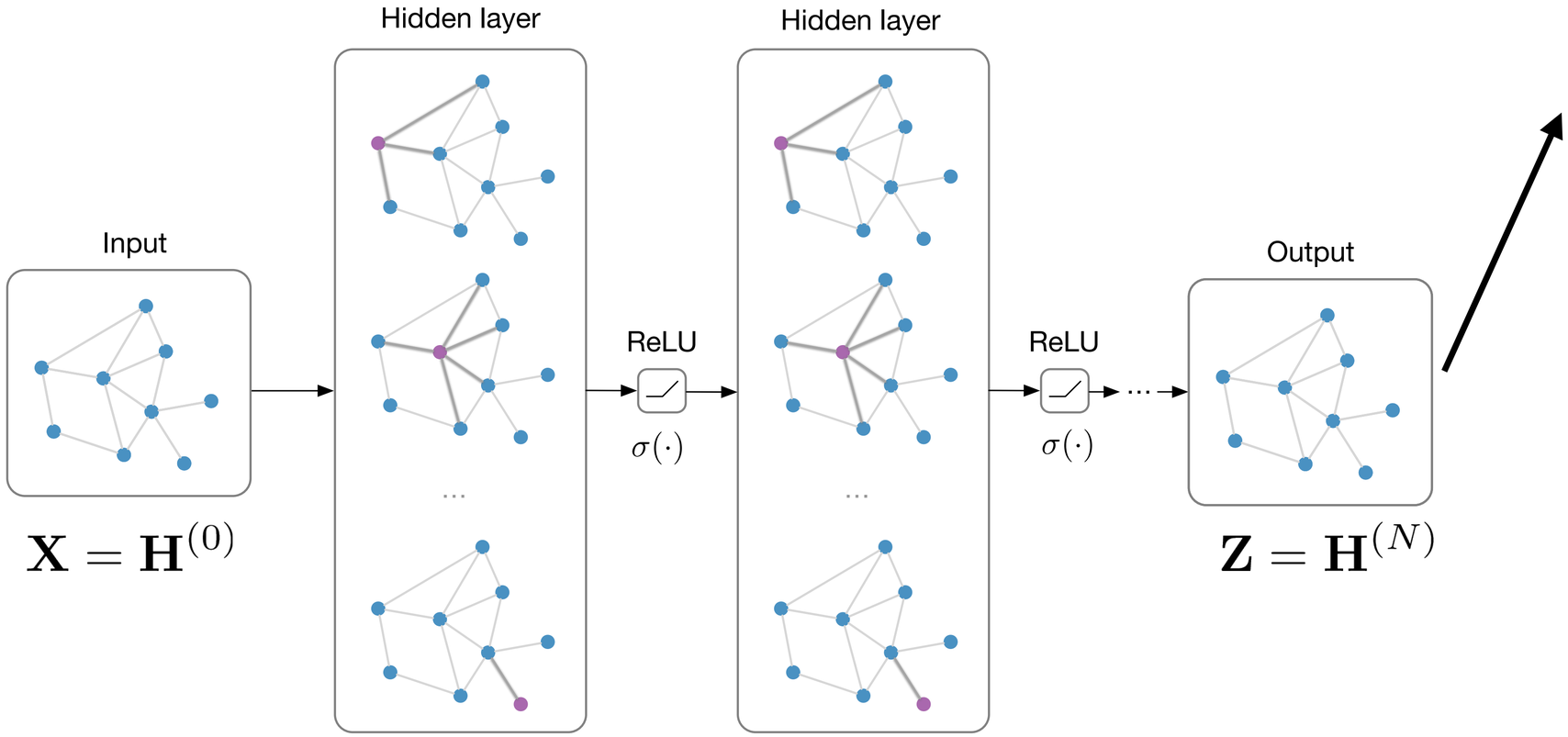

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Node classification:

$$\mathrm{softmax}(\mathbf{z_n})$$

e.g. Kipf & Welling (ICLR 2017)

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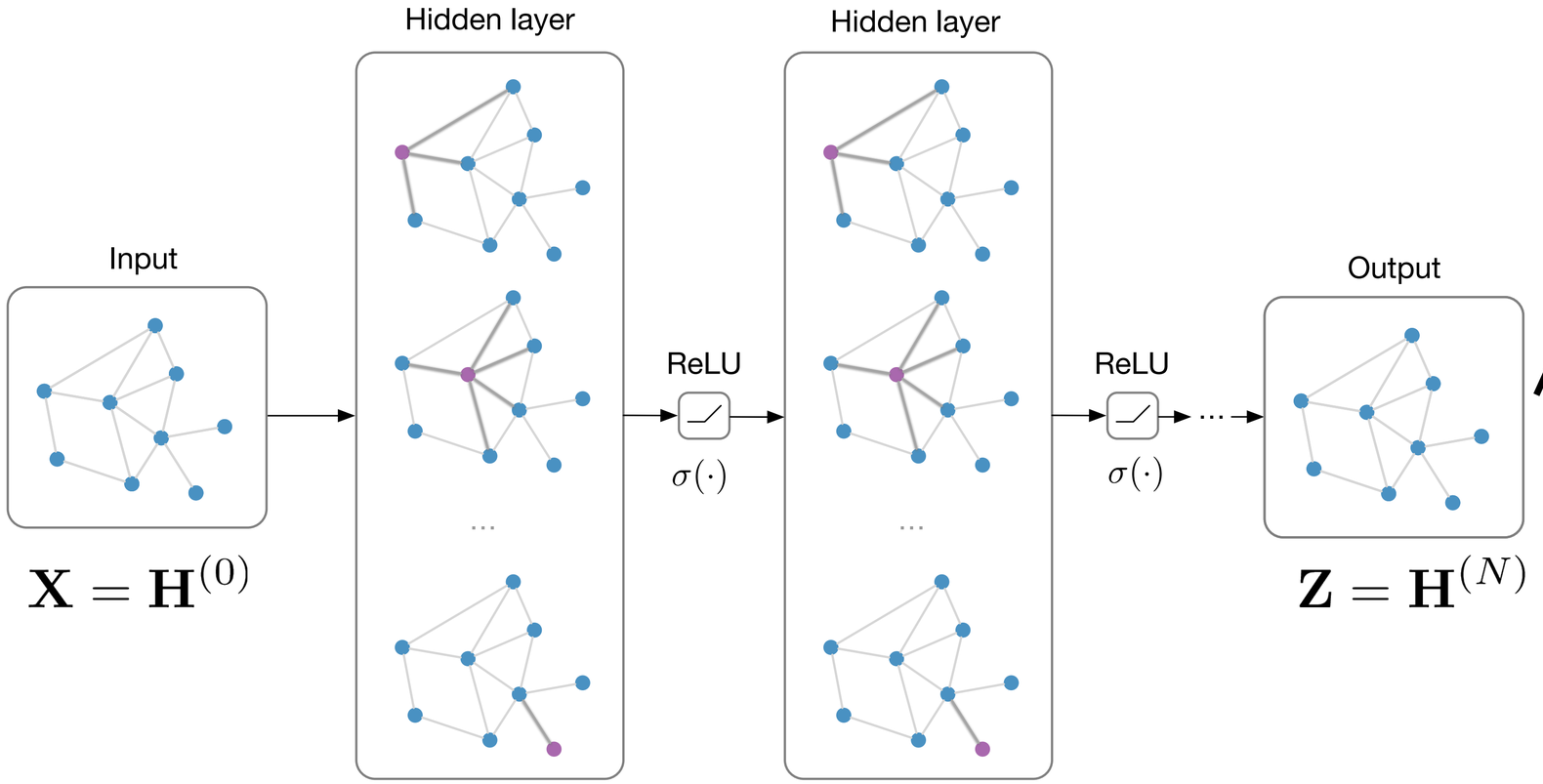

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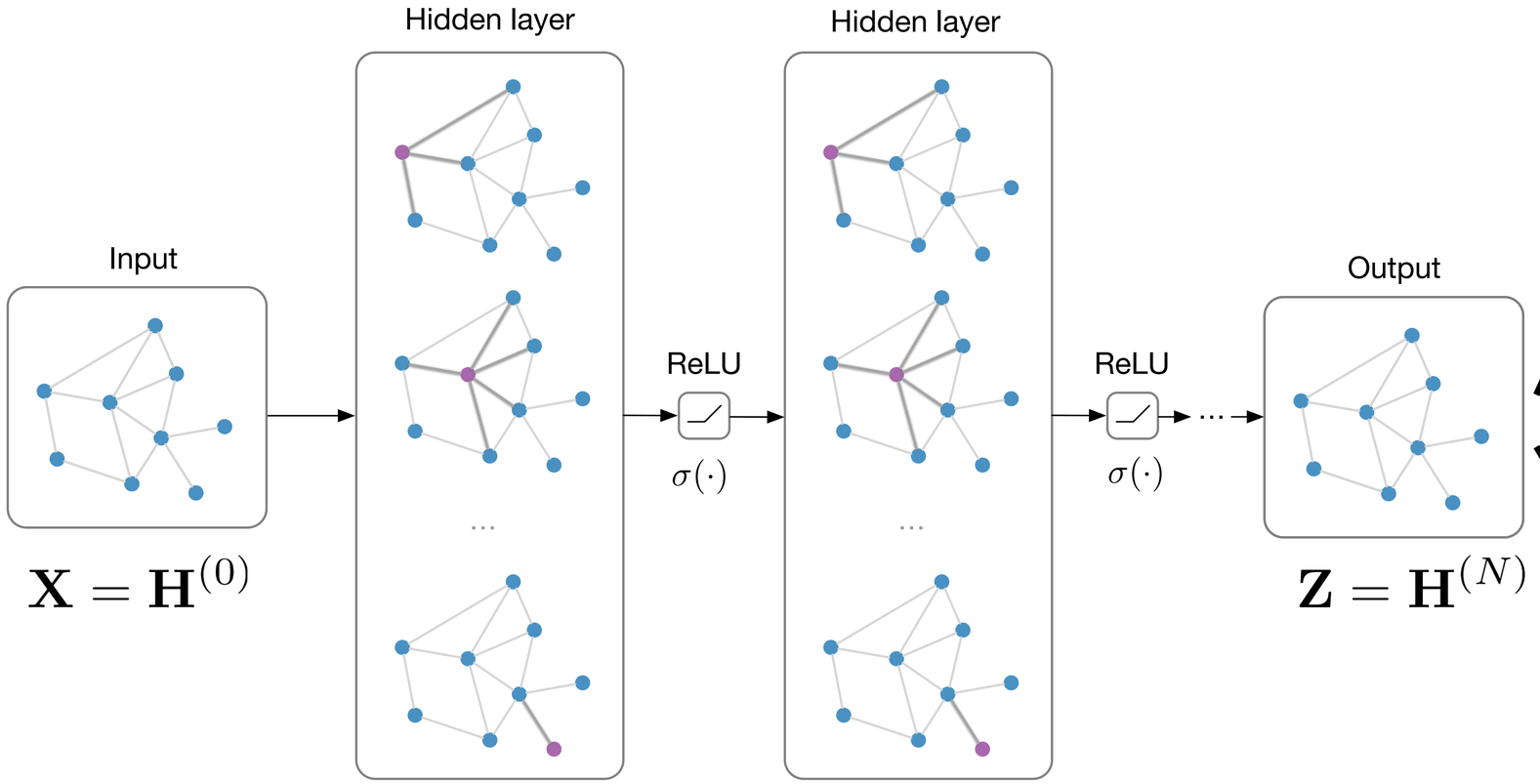

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Link prediction:

$p(A_{ij}) = \sigma(\mathbf{z_i^T z_j})$

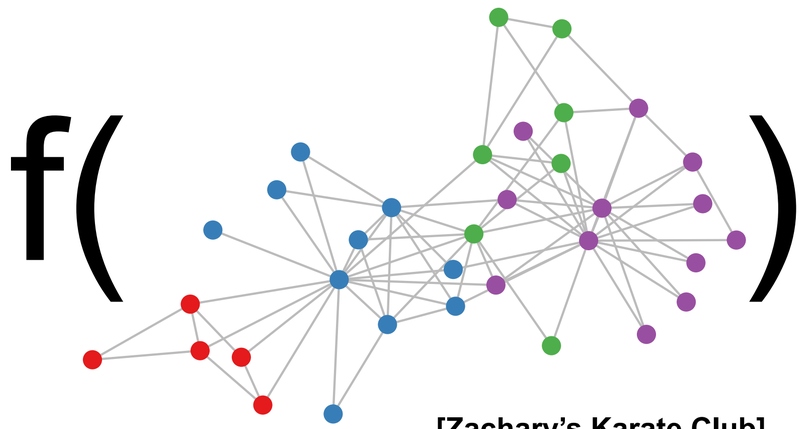
Kipf & Welling (NIPS BDL 2016)

"Graph Auto-Encoders"

What do learned representations look like?

Forward pass through **untrained** 3-layer GCN model

Parameters initialized randomly



[Zachary's Karate Club]

2-dim output per node