Interpretability in Deep Learning

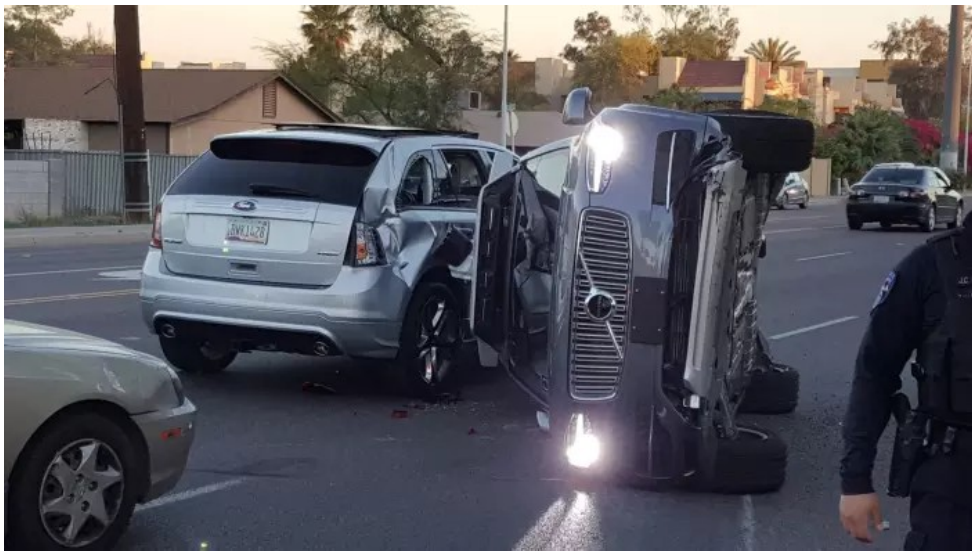
2023

Yandex
Research

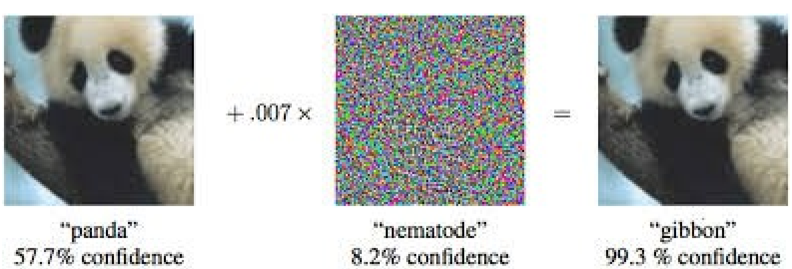
LAMBDA

British Hedgehog
Preservation Society

ML mistakes have a cost



Uber self-driving car crashes dur
US tests



3. Robot injured a child

A so-called "crime fighting robot," created by the platform
into a child in a Silicon Valley mall in July, injuring the 16-

Chinese billionaire's face identified as jaywalker

Traffic police in major Chinese cities are using AI to address jaywalking. They deploy smart cameras using facial recognition techniques at

The question of trust

How can I explain my model’s prediction?
Why did it make this decision/mistake?
What features does it rely on?

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Can I trust this data?
Is something missing?
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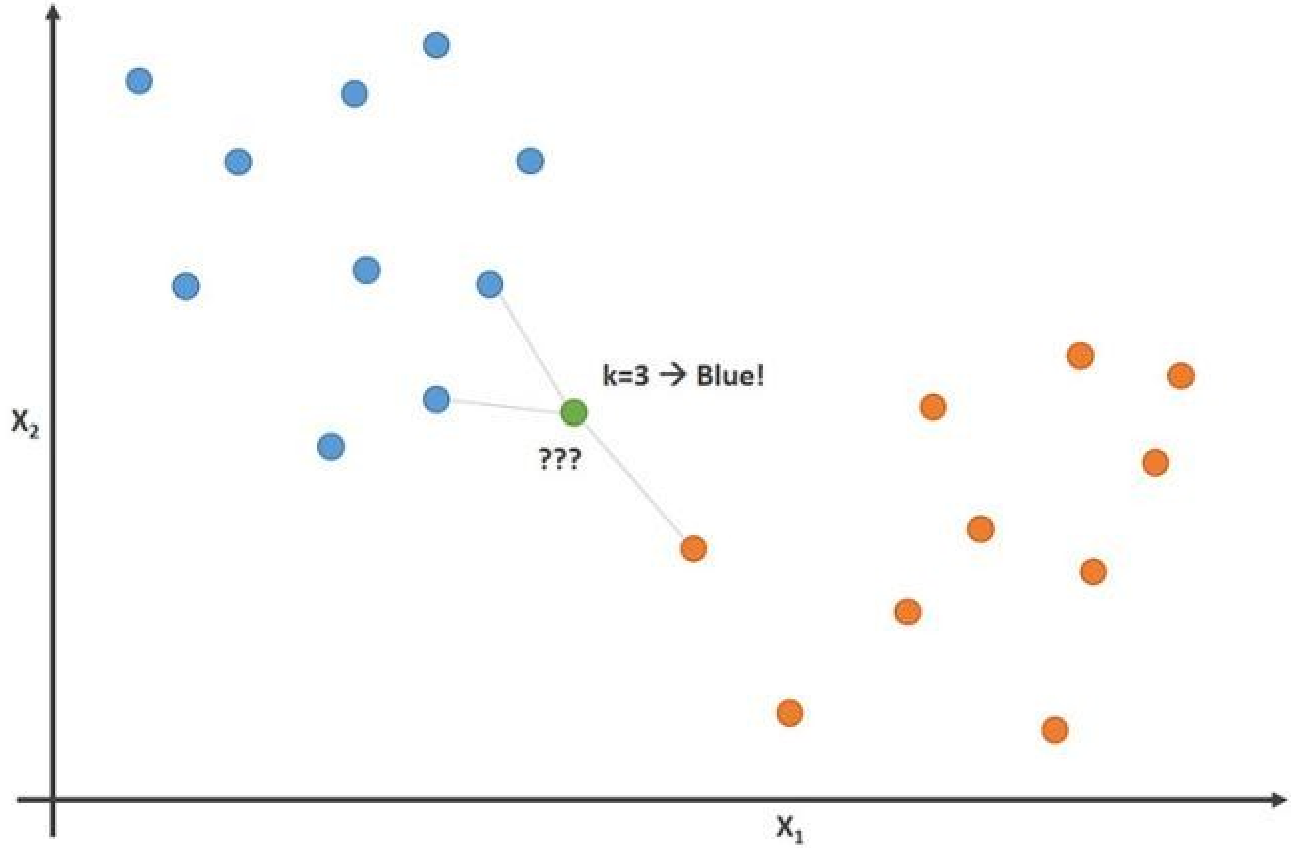
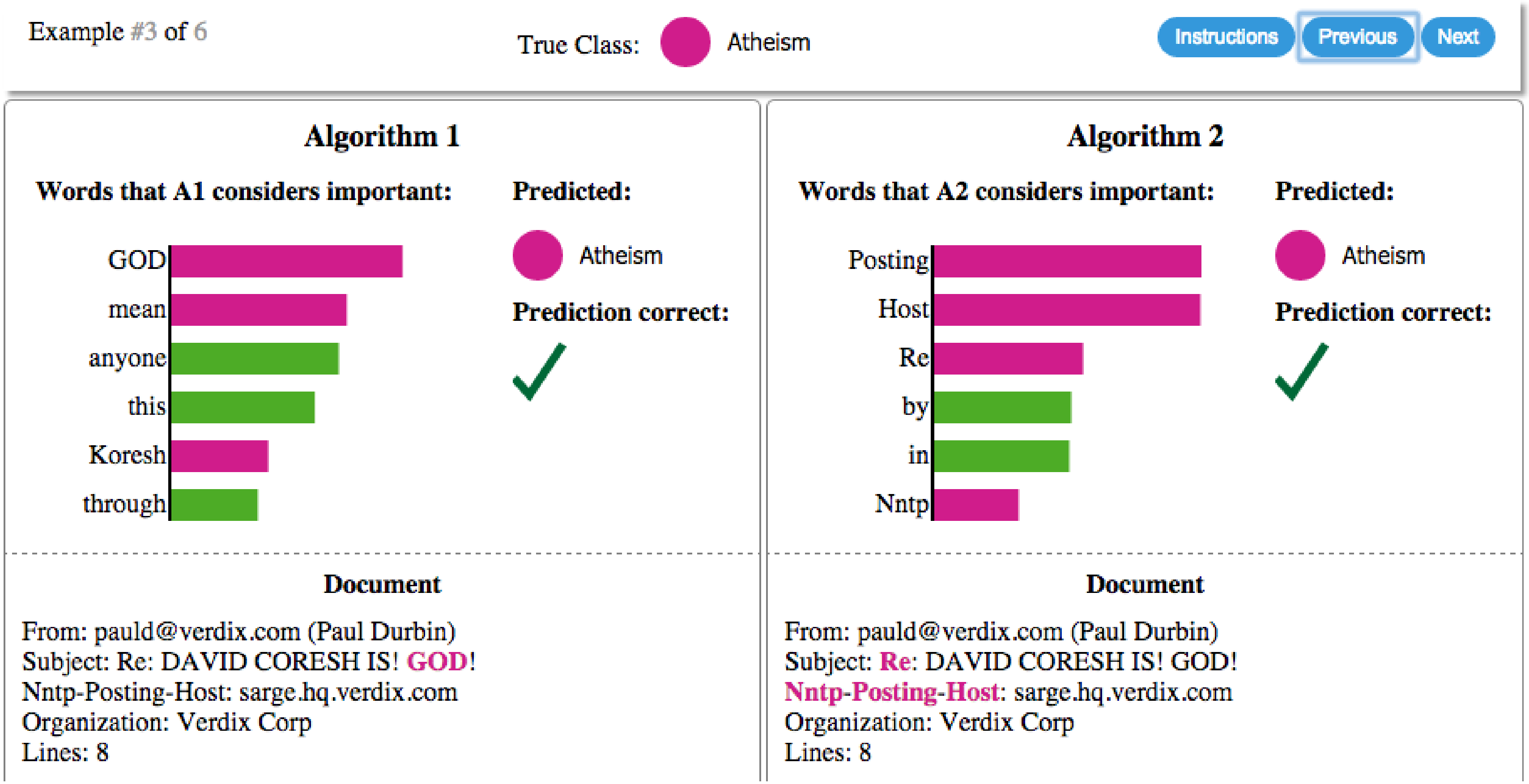
What is interpretable?

Simple stuff like **K Nearest Neighbors**



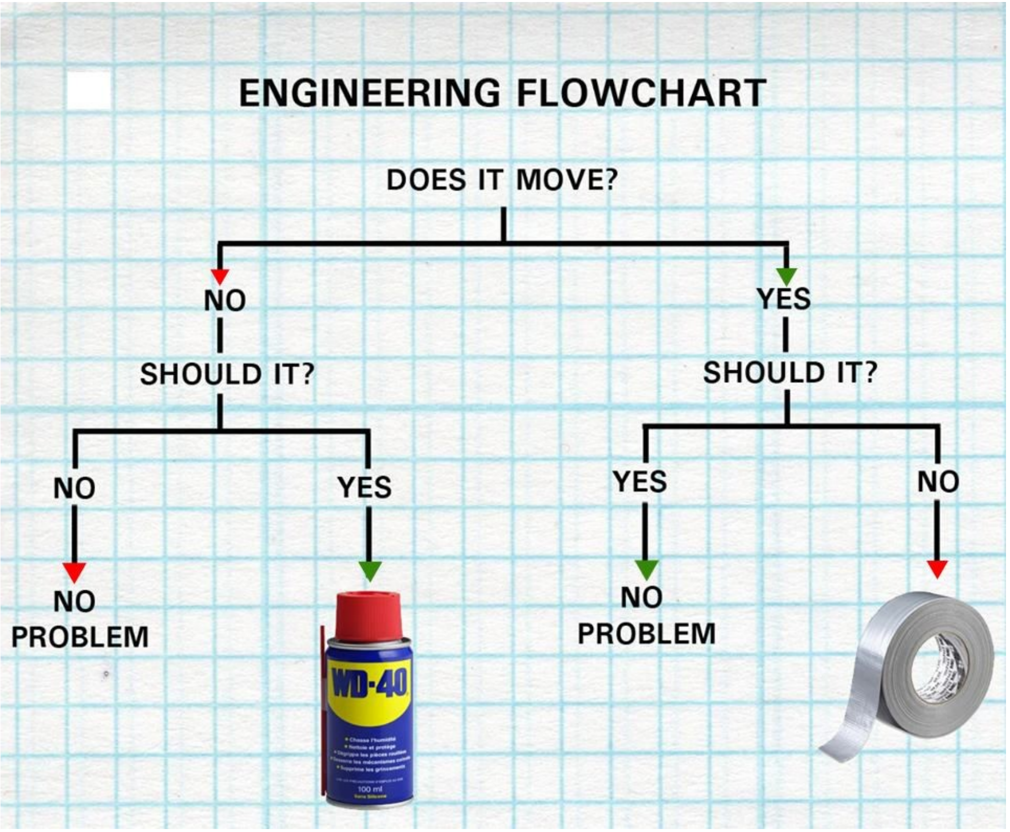
What is interpretable?

Simple stuff like **Linear models**

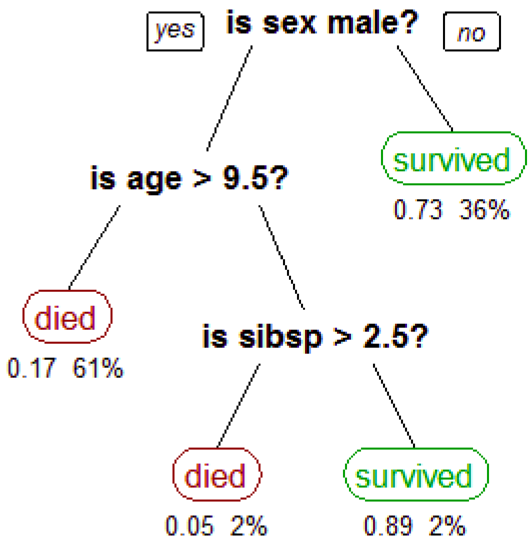


What is interpretable?

Simple stuff like **Decision Trees**



Survival on Titanic



What is interpretable?

Neural networks are **not** naturally interpretable

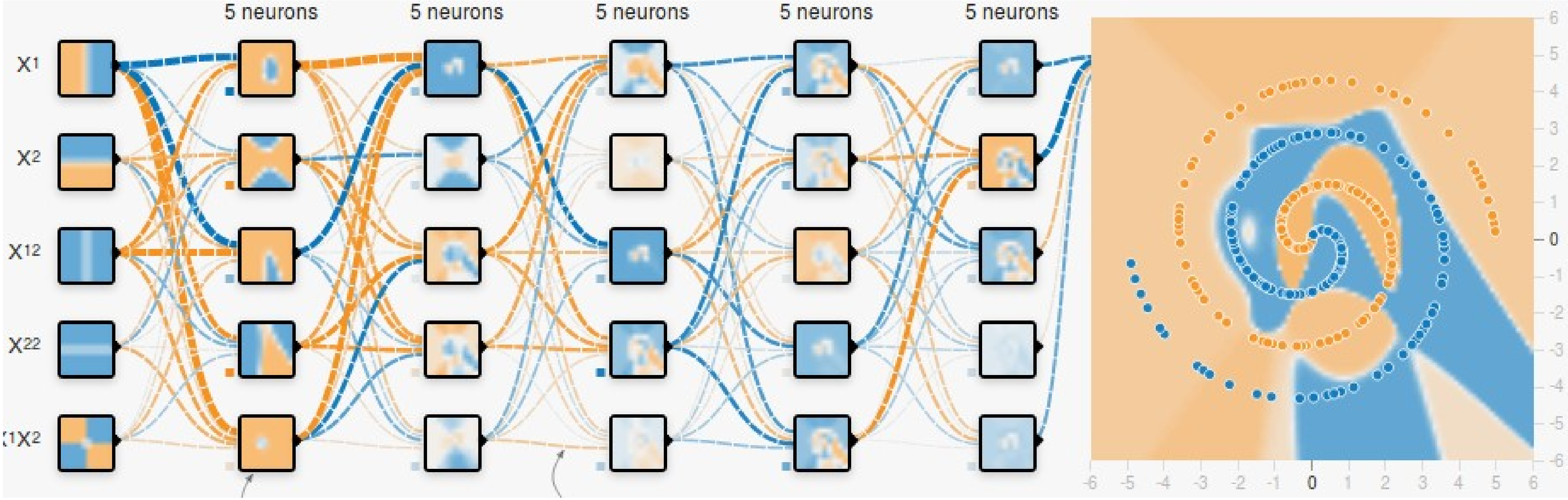
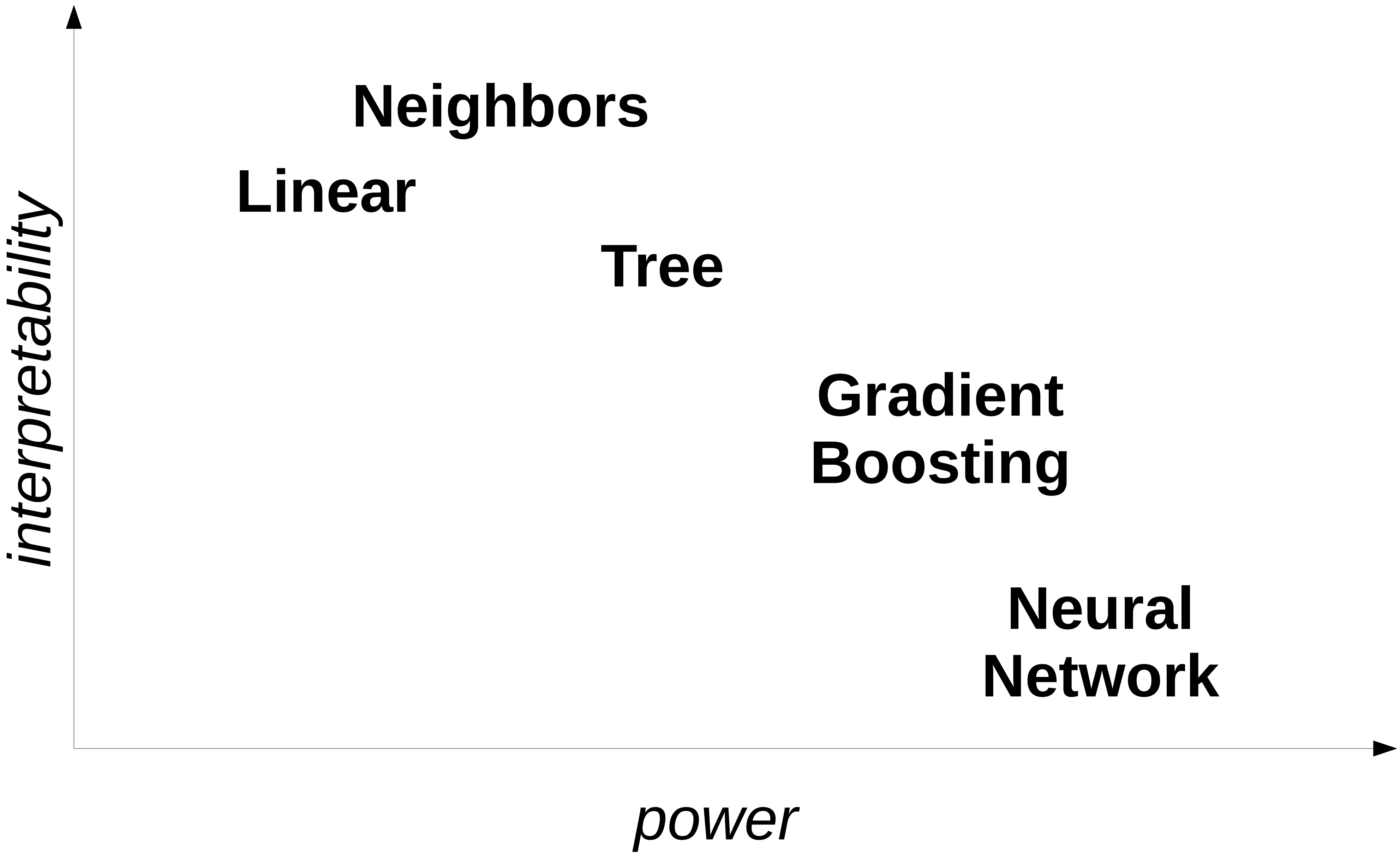
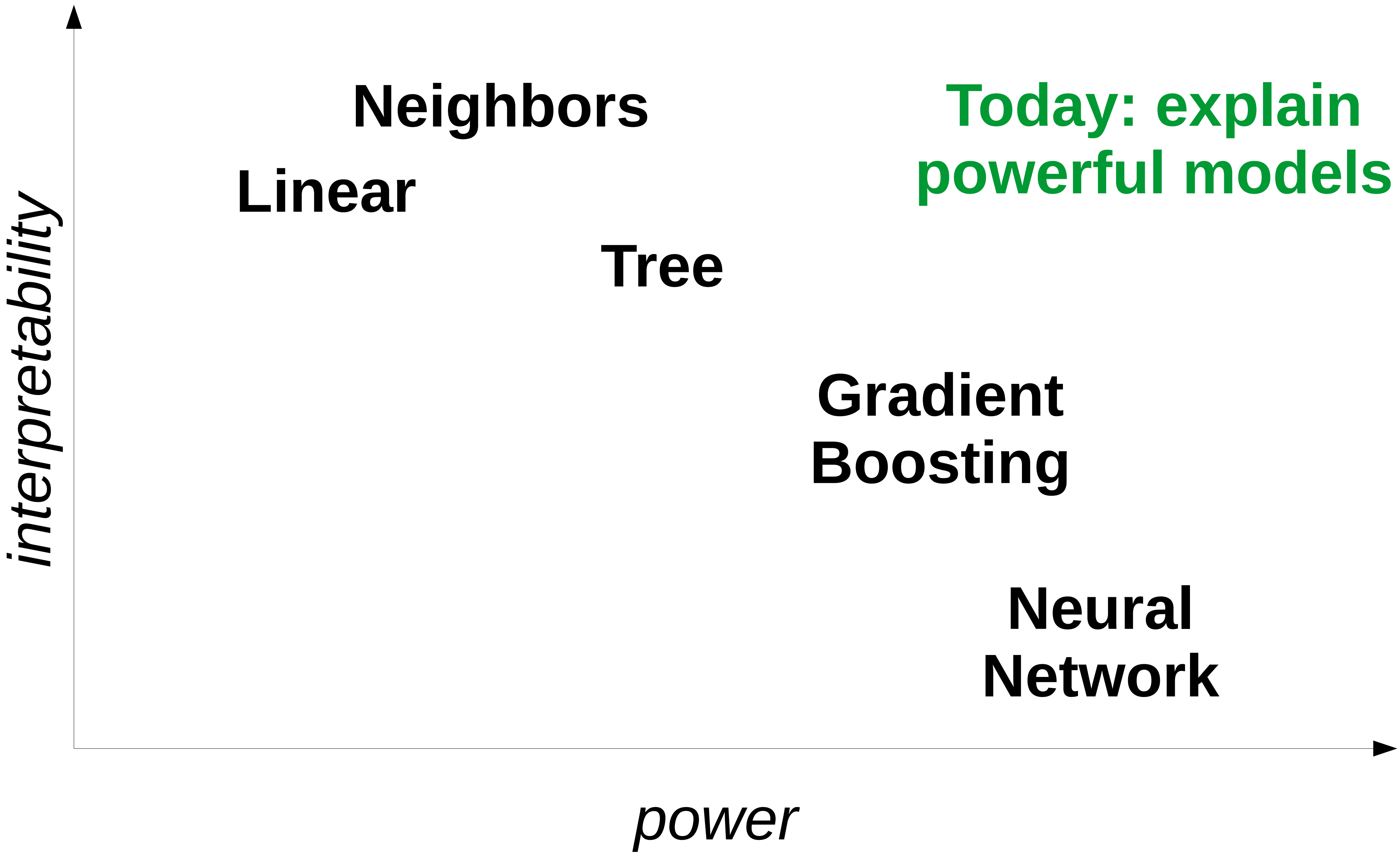


Image source: https://playground.tensorflow.org

Power vs interpretability



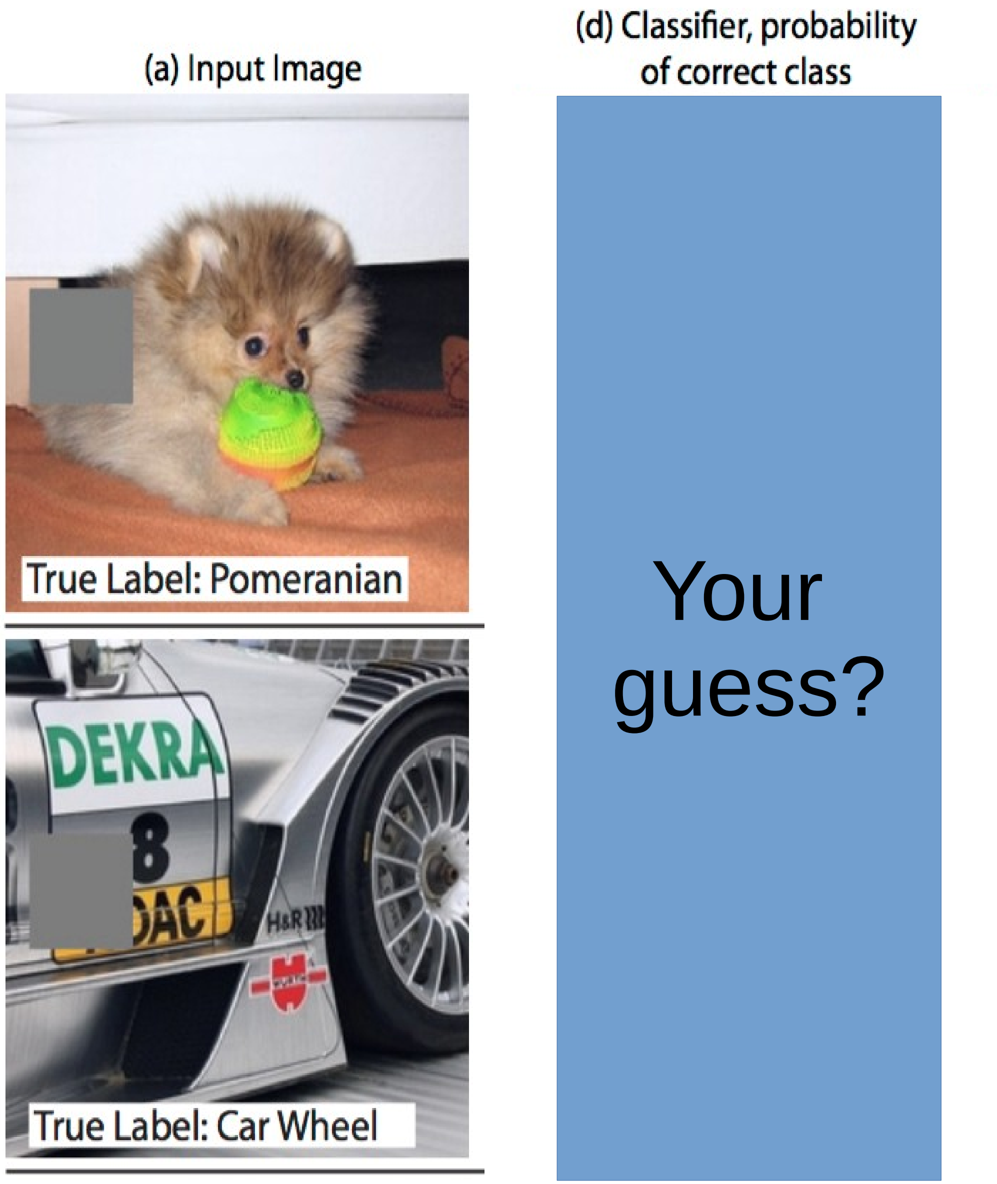
Power vs interpretability



Explanation by occlusion

Idea:

- Let’s add noise to inputs and see what happens!
- For images: slide a gray square over the image, measure how it affects predictions



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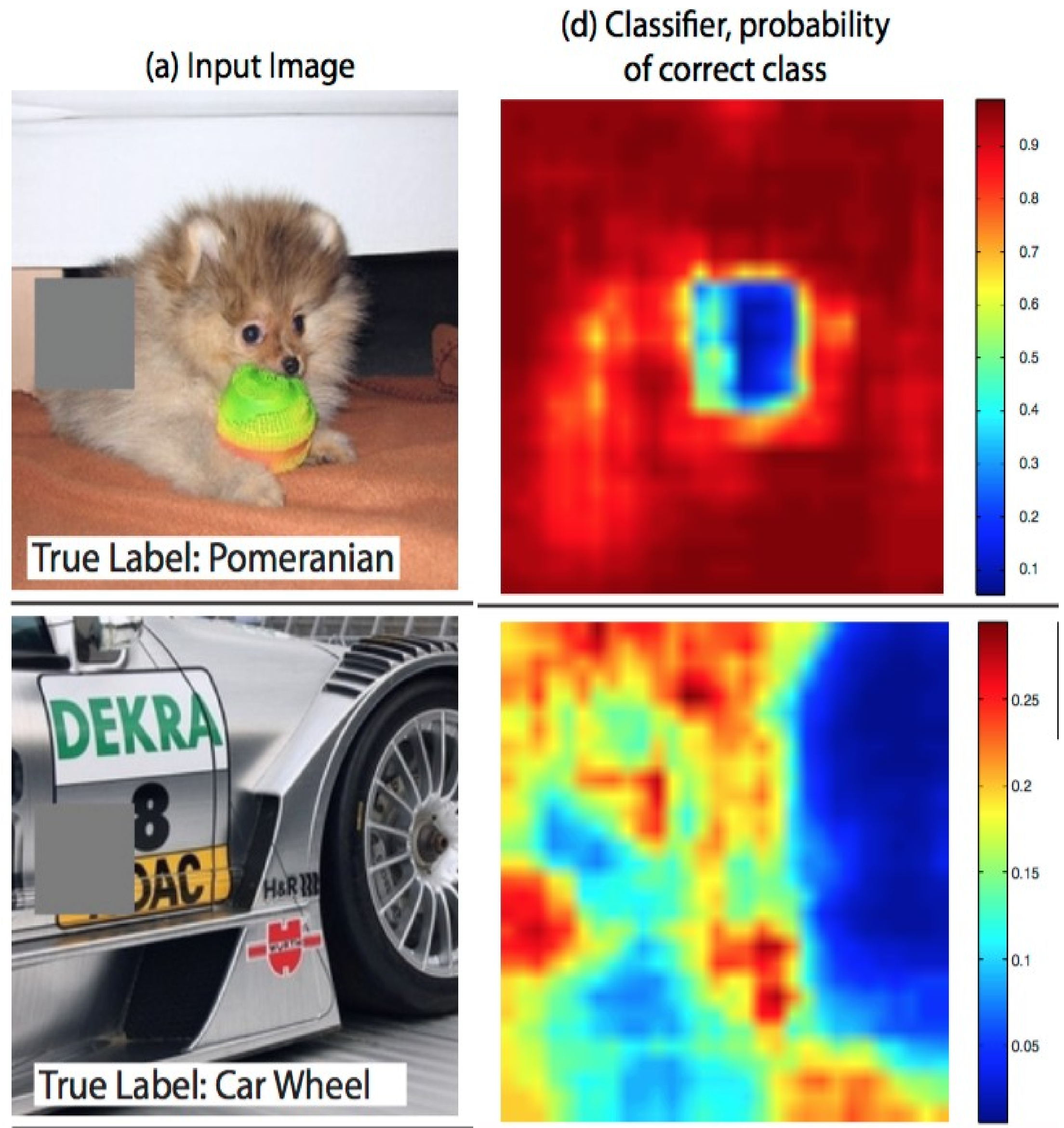


Explanation by occlusion

Idea:

- Let's add noise to inputs and see what happens!
- For texts: drop individual words and measure how it affects predictions

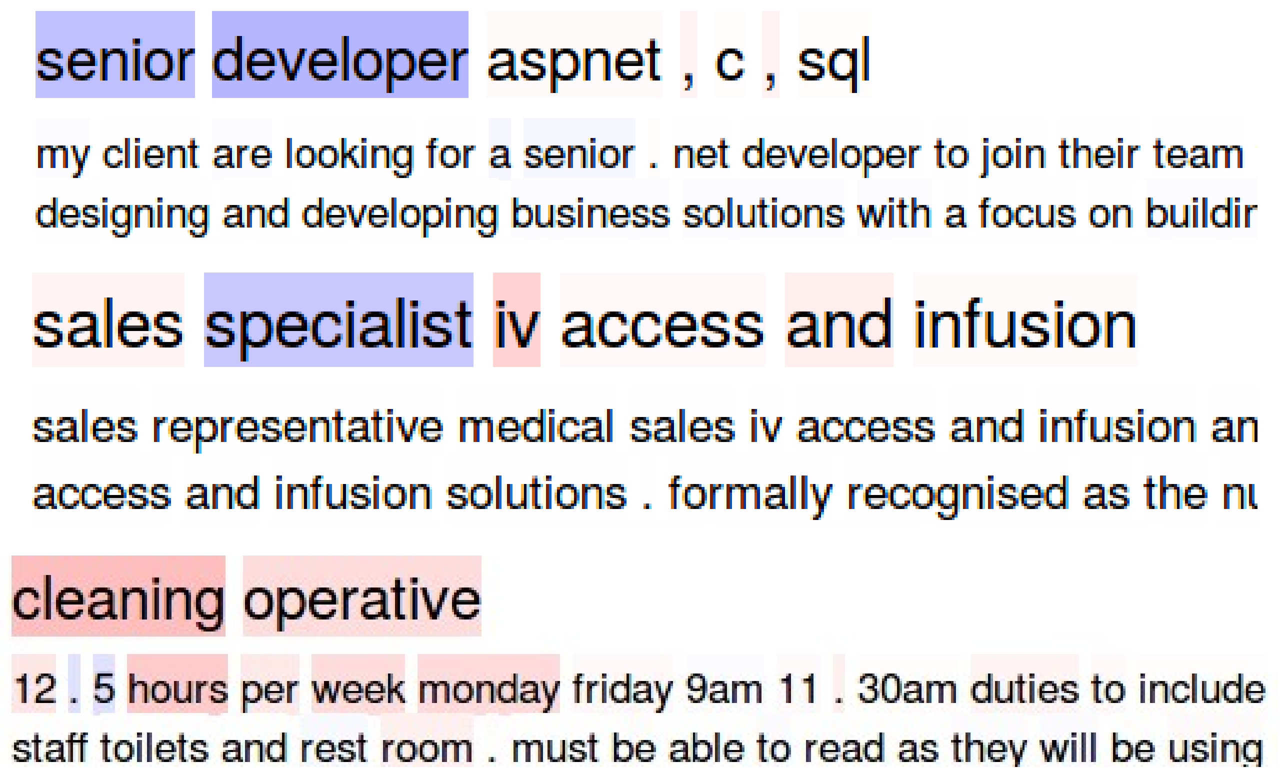
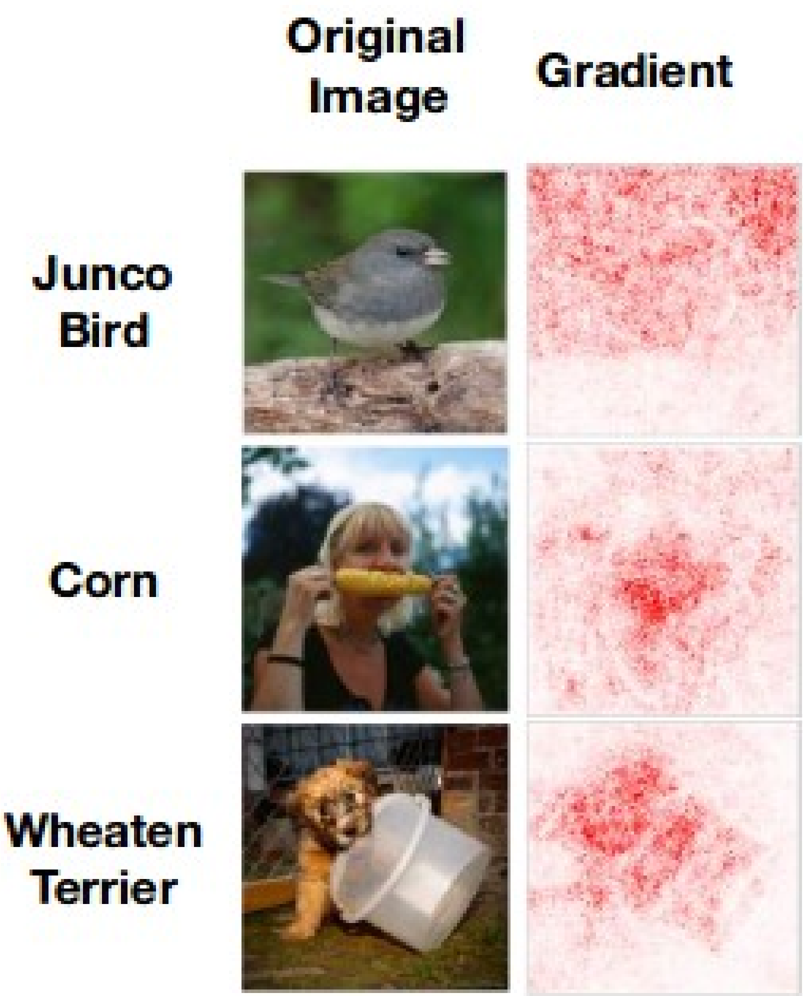


Image: salary prediction

Explanation by gradients

Idea: use gradients!

$$\nabla_{x_i} model(x) = \frac{\partial\, model(x)}{\partial x_i}$$



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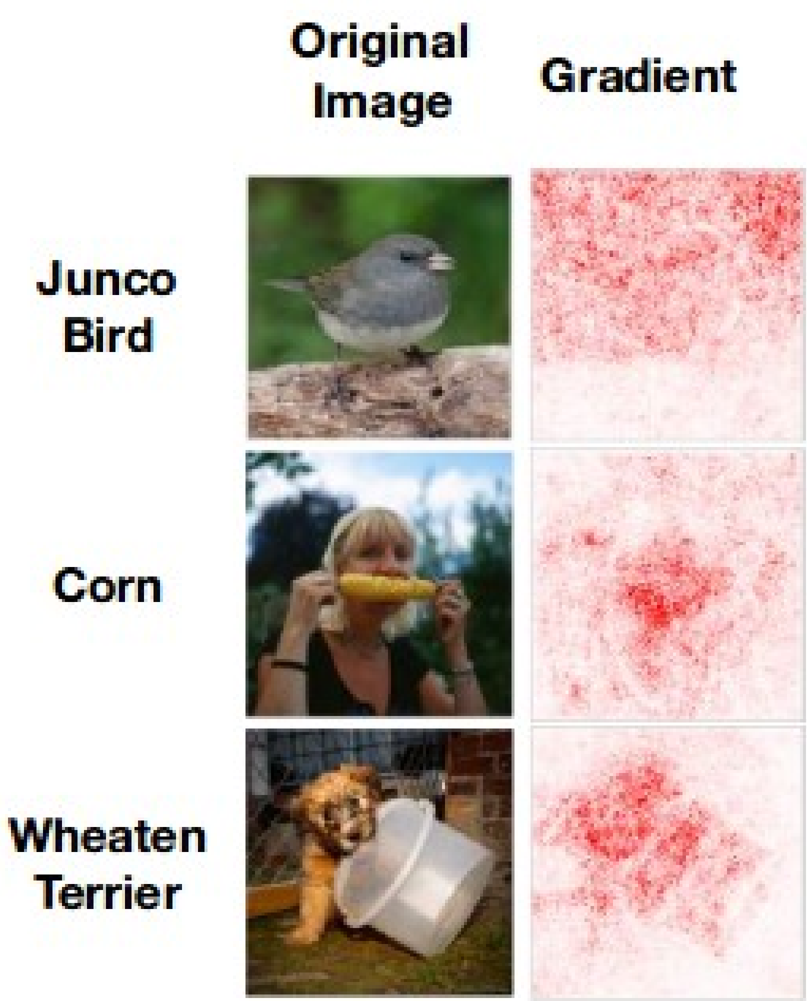

Gradients are too sensitive to small changes in **x**

Q: How would you fix that?

Explanation by gradients

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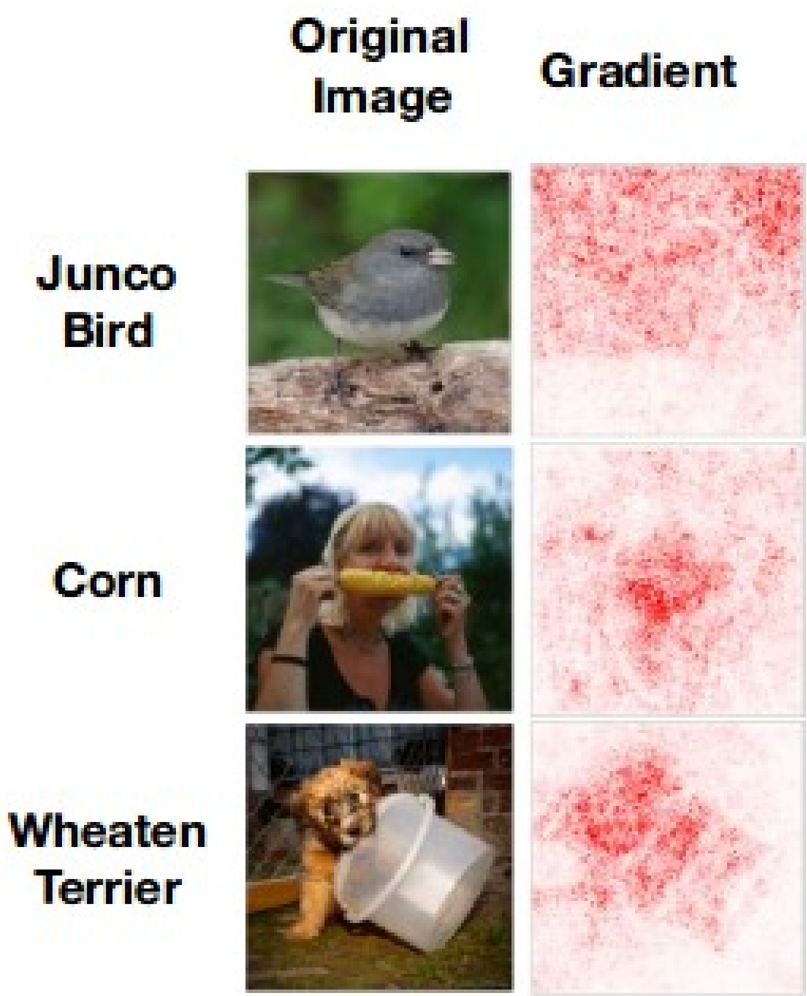

Gradients are too sensitive to small changes in **x**

Smoothgrad: average gradients over several **noisy** copies of **x**

(one of many heuristics)

Explanation by gradients

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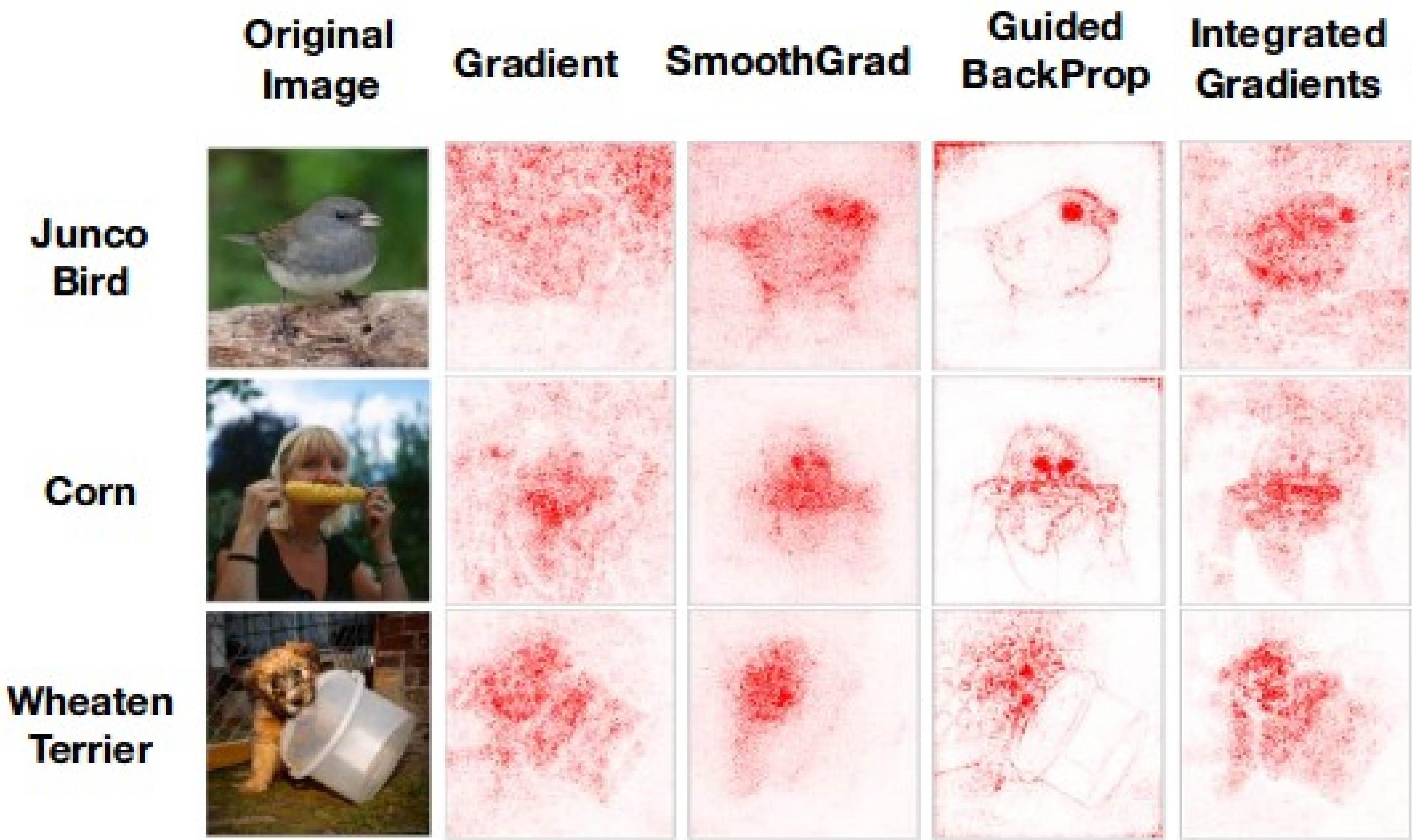
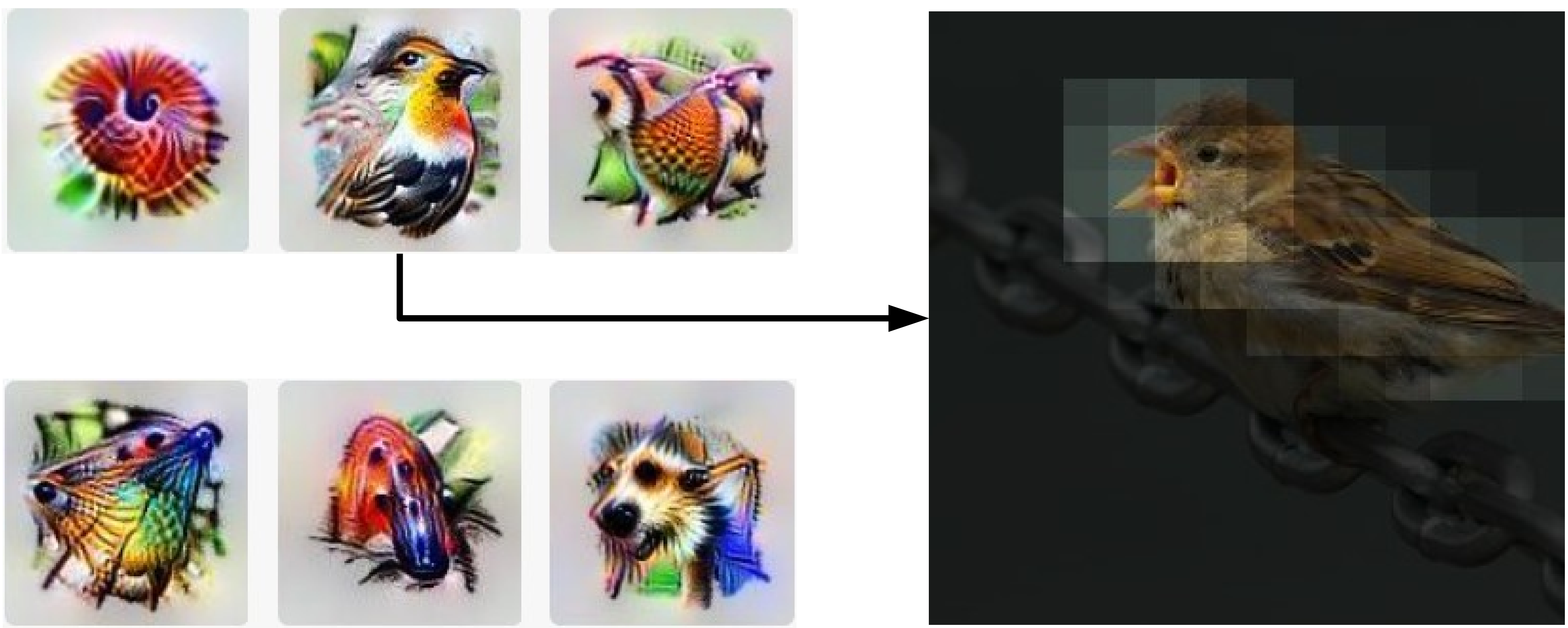


Explanation by optimization

Idea: build an image that maximizes the activation of a particular neuron
Must read: distill.pub/2018/building-blocks



Explanation by optimization

Idea: build an image that maximizes
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Must read: **distill.pub/2018/building-blocks**

More:

https://distill.pub

https://poloclub.github.io

https://karpathy.github.io

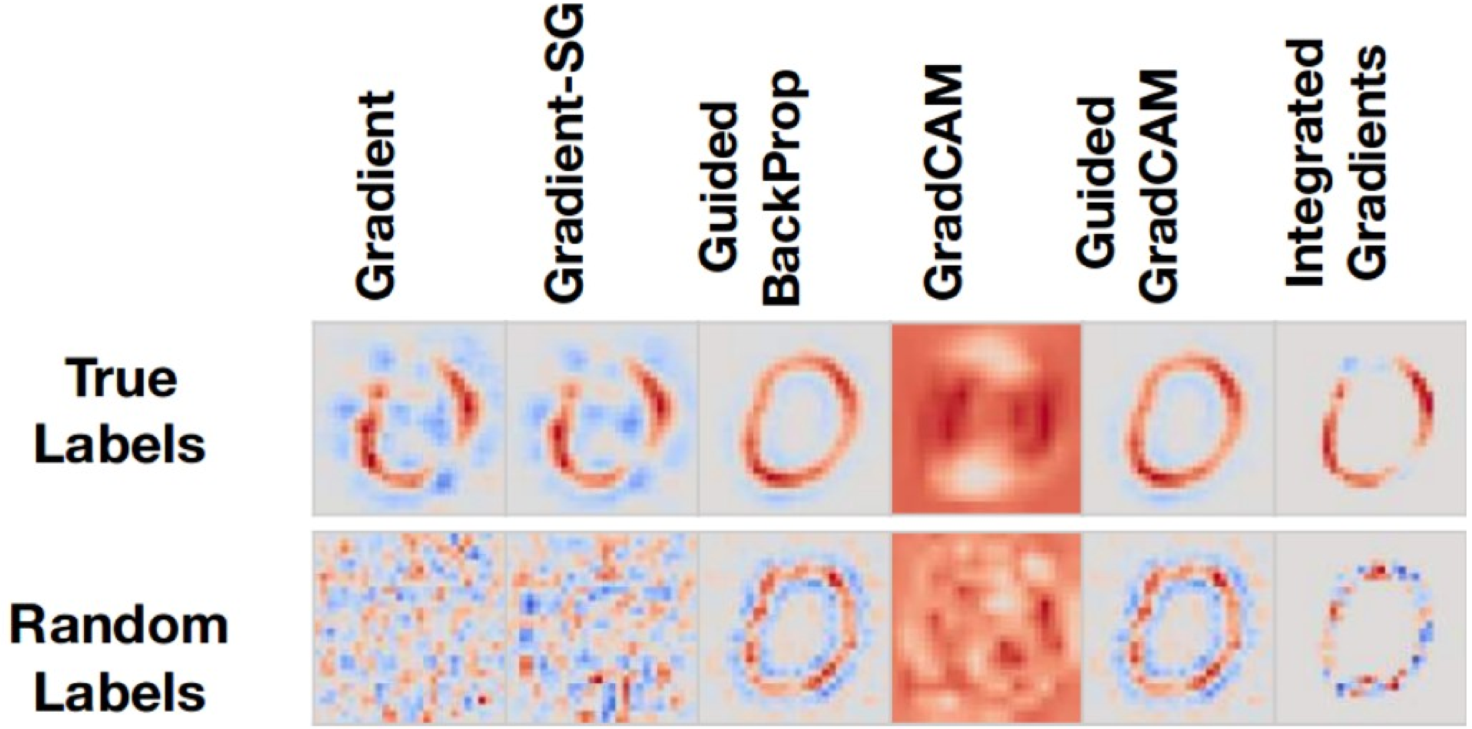
Don’t trust yourself!

The method outputs a noisy image
you see something reasonable
should you be satisfied?

How can you **verify** the explanation?

Don’t trust yourself!

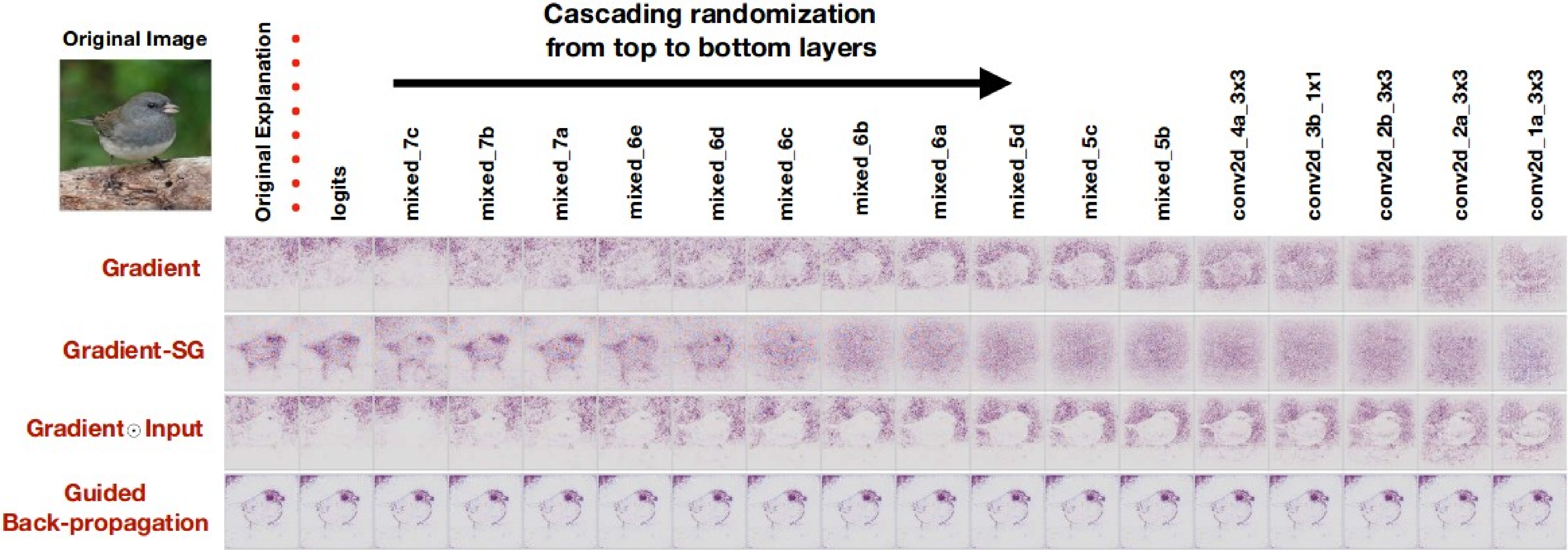
Idea: train a bogus model to see
if the method can “explain” the fake model



Source: Sanity Checks for Saliency Maps

Don’t trust yourself!

Idea: replace weights with random one layer at a time (top to bottom)



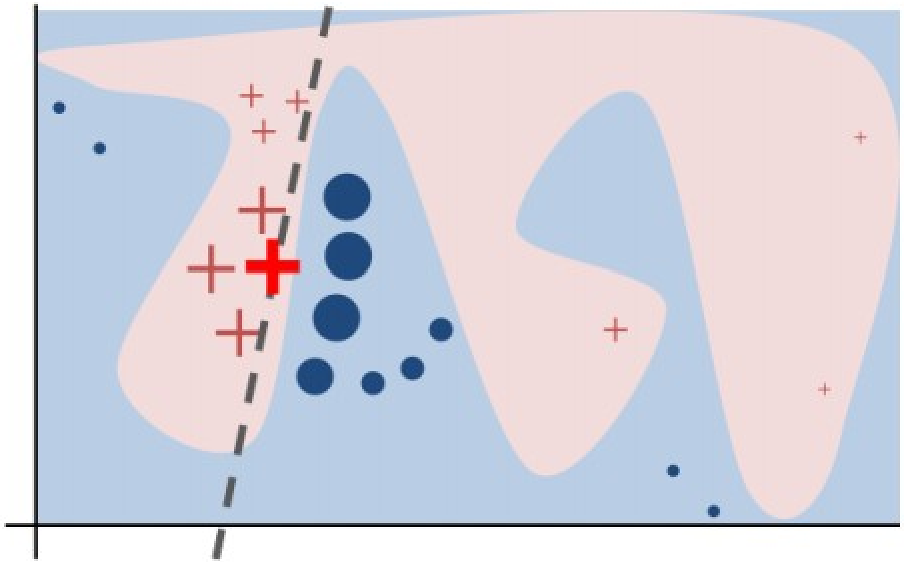
Source: *Sanity Checks for Saliency Maps*

Explanation by approximation

Idea:

- Approximate your model with something explainable
  e.g. linear model

- The approximation only needs to hold **locally**
  i.e. on similar inputs



Read more in the paper

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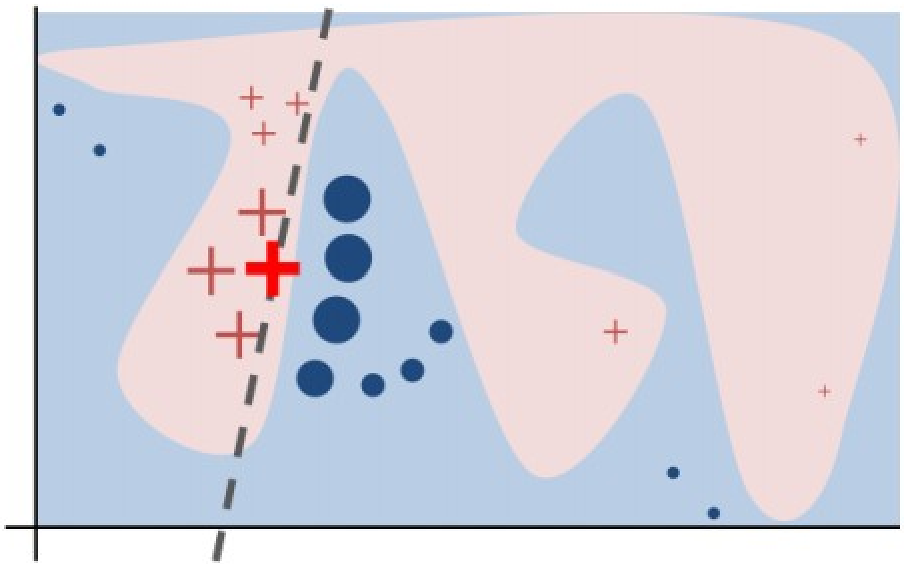

Read more in the paper

(a) Original Image (b) Explaining *Electric guitar* (c) Explaining *Acoustic guitar* (d) Explaining *Labrador*

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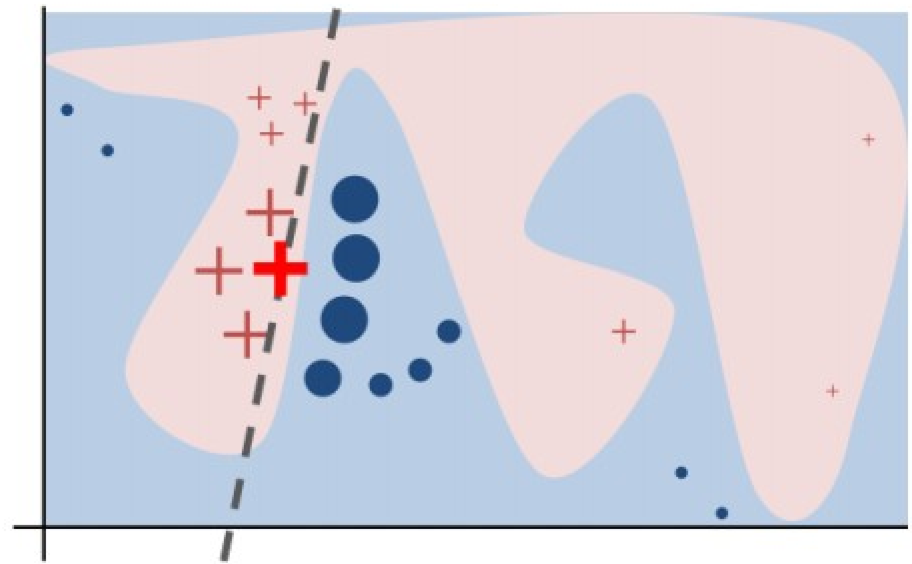

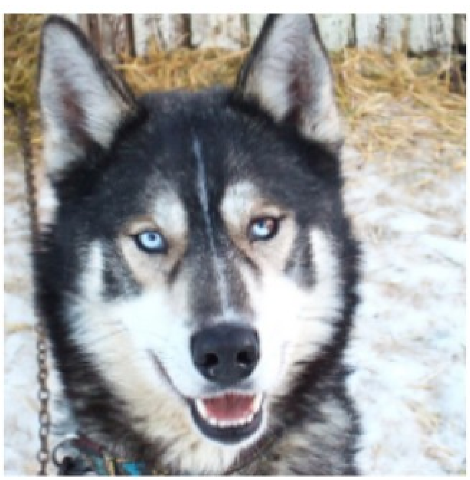

(a) Husky classified as wolf

(b) Explanation

Left image: model mislabeled a husky dog as a wolf; explanation: snow :)

Figures taken from the paper [Why Should I Trust You?]

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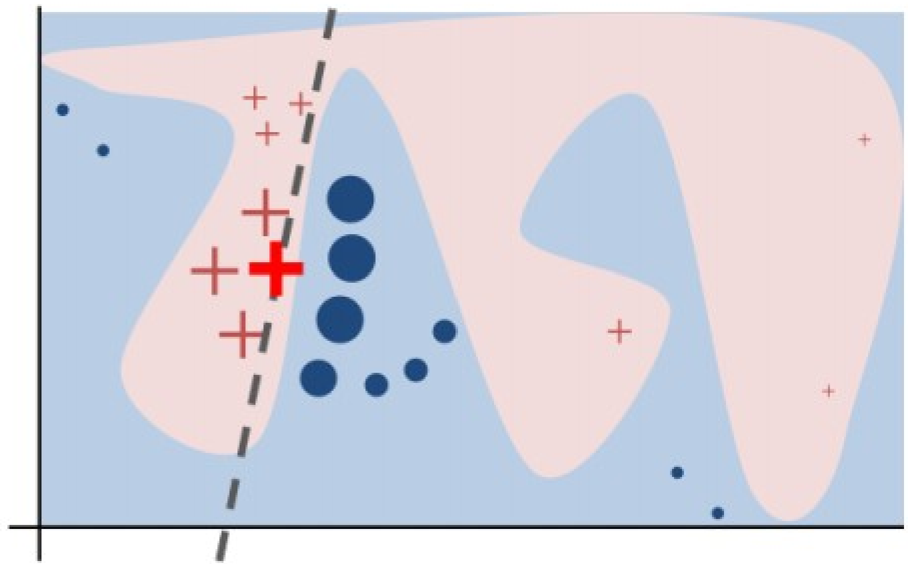

(a) Husky classified as wolf (b) Explanation

Read more:
arxiv.org/abs/1602.04938
arxiv.org/abs/1705.07874
arxiv.org/abs/1904.12991

Explanation by game theory

Idea: features are a “players” that play
a cooperative game of making a prediction

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Equivalent “game”:
Alice, **B**ob and **C**arol ordered a $1000 meal at a restaurant
Q: How should they split the bill?

Hint: here’s what it would cost for them individually & in pairs

Who goes	**A**lice	**B**ob	**C**arol	**A** & **B**	**A** & **C**	**B** & **C**	**A**, **B** & **C**
Total price	400	560	720	740	780	980	1000

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Game theorist's answer: Shapley values!

$$\phi_i(v) = \sum_{S \subseteq N \setminus \{i\}} \frac{|S|!(|N| - |S| - 1)!}{|N|!}(v(S \cup \{i\}) - v(S))$$

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Game the

$\phi_i(v) =$ … $v(S))$

WARNING
Do **NOT** take your game theorist friend
to a restaurant! You'll thank me later.

Shapley values explained

Same old table

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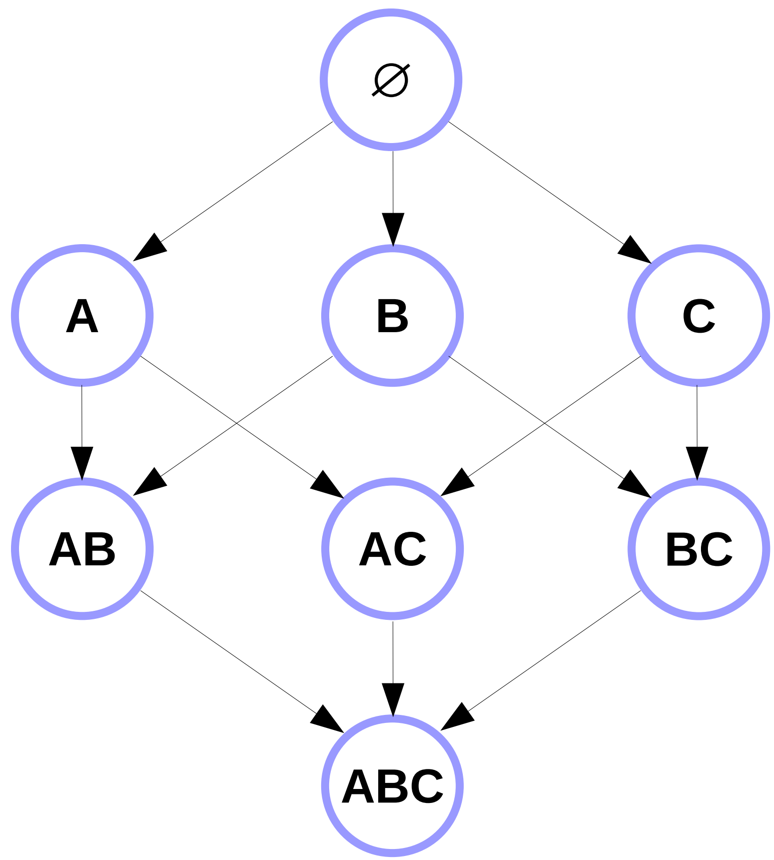
Shapley(X) = average increase in cost from adding X to a group

Note: average over all ***paths***.



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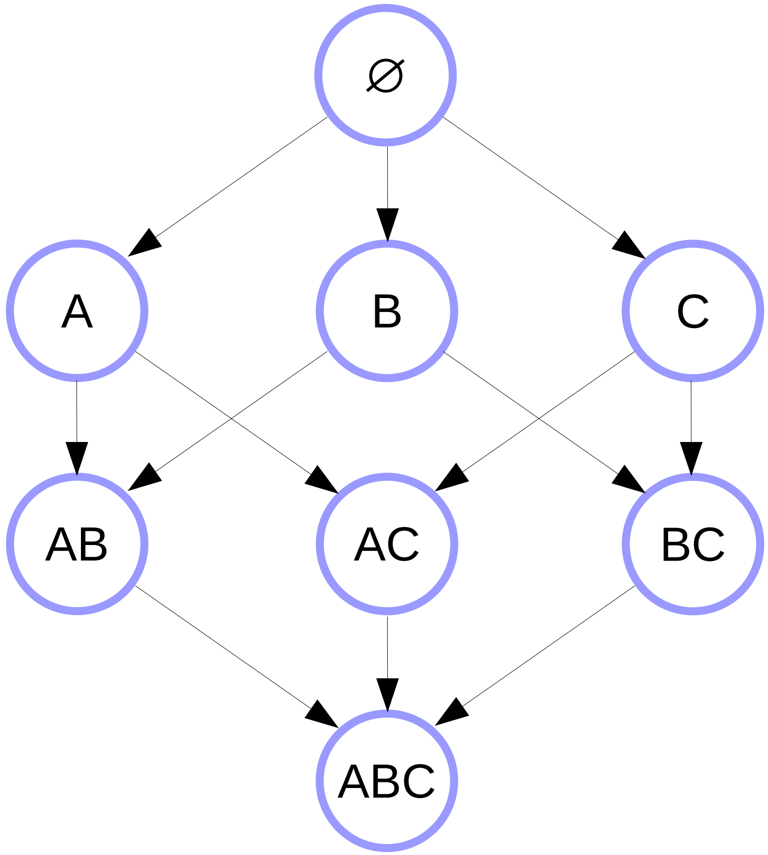
Shapley(A) = $\frac{2}{6} \cdot 400$ + …

Q: What else?



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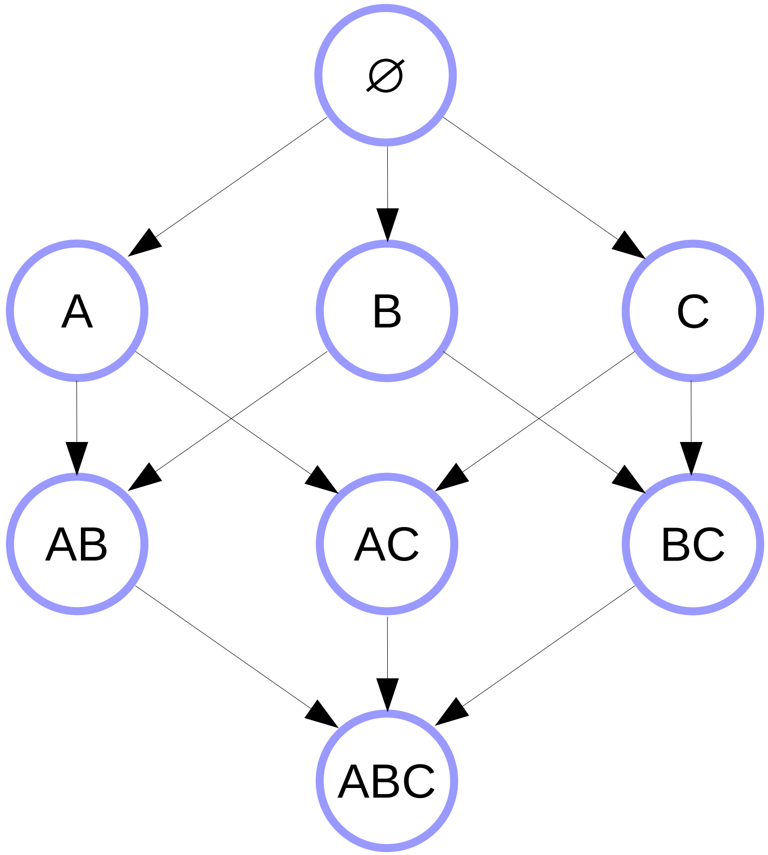
Note: average over all ***paths***.

$$\text{Shapley(A)} = \frac{2}{6}\cdot 400 + \ldots$$

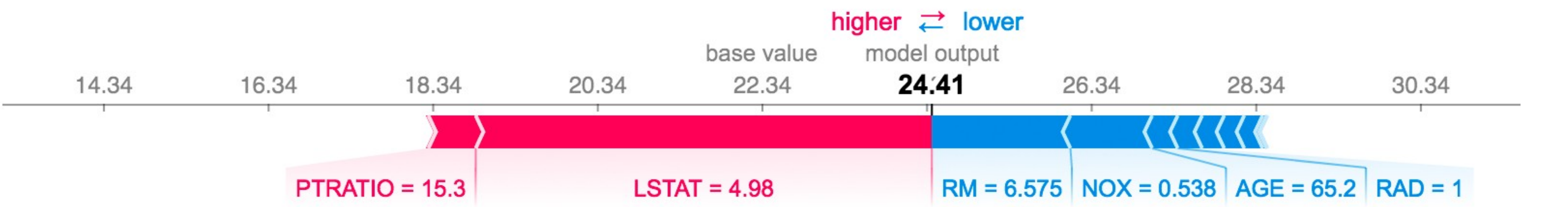
$$+ \frac{1}{6}\cdot\left(740-560\right) + \frac{1}{6}\cdot\left(780-720\right) +$$

$$+ \frac{2}{6}\cdot\left(1000-990\right) = 180$$



Explanation by game theory

SHAP *= Shapley values for features + clever approximation*
State of the art in after-the-fact model explanation

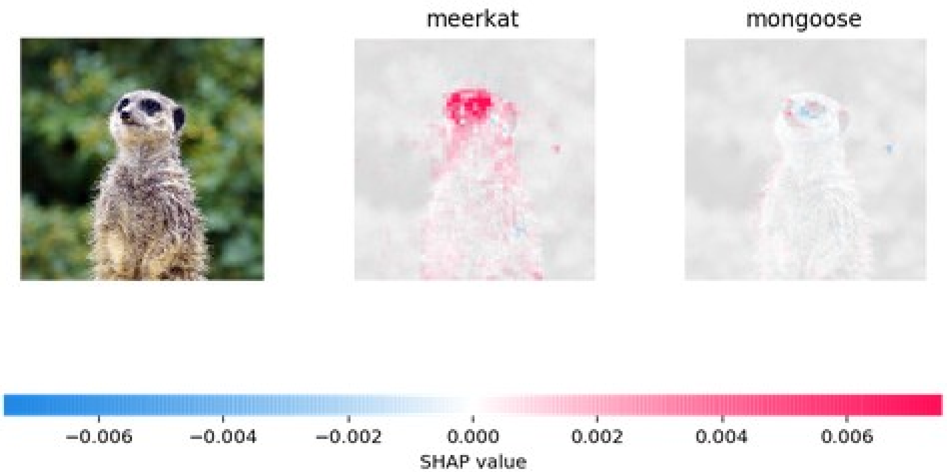


MOAR:

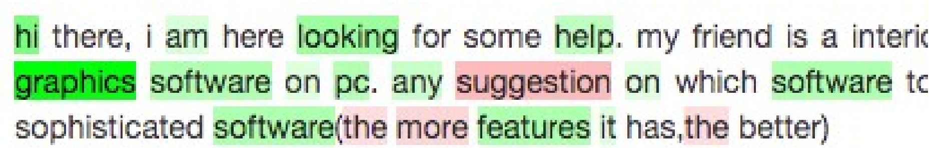
- SHAP original paper: tinyurl.com/shap-paper (NeurIPS'17)
- SHAP explained by paper author: youtu.be/ngOBhhINWb8
- Shapley values in game theory: youtu.be/w9O0fkfMkx0

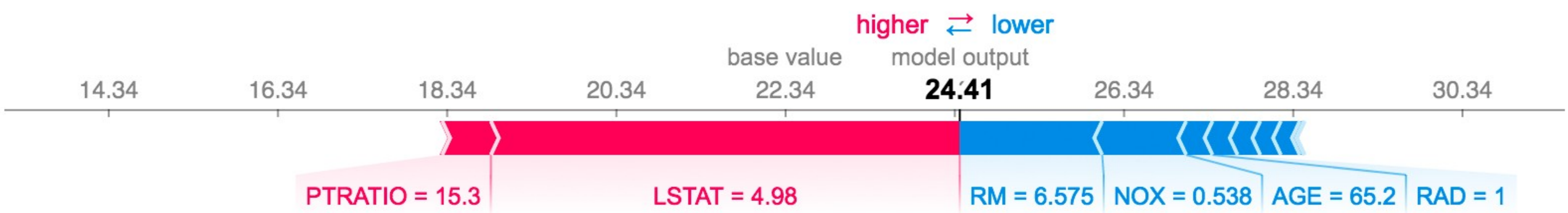
Frameworks

SHAP - https://github.com/slundberg/shap
(tensorflow, keras, pytorch, sklearn-like)
ELI5 - https://github.com/TeamHG-Memex/eli5
(popular explainers for keras/tf, sklearn-like)



Left, bottom – shap
Right - ELI5



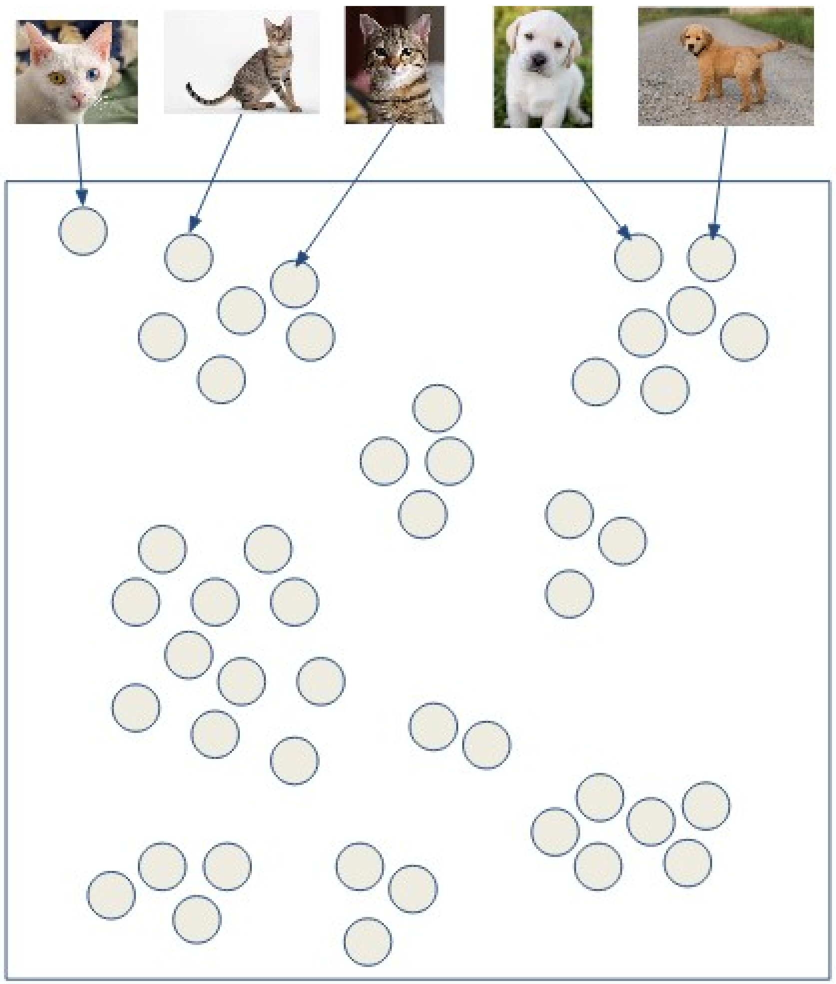


So far: explaining black-box models

Now: model-specific methods

Explanation by design

Idea: design architecture to be interpretable



hidden layer activations

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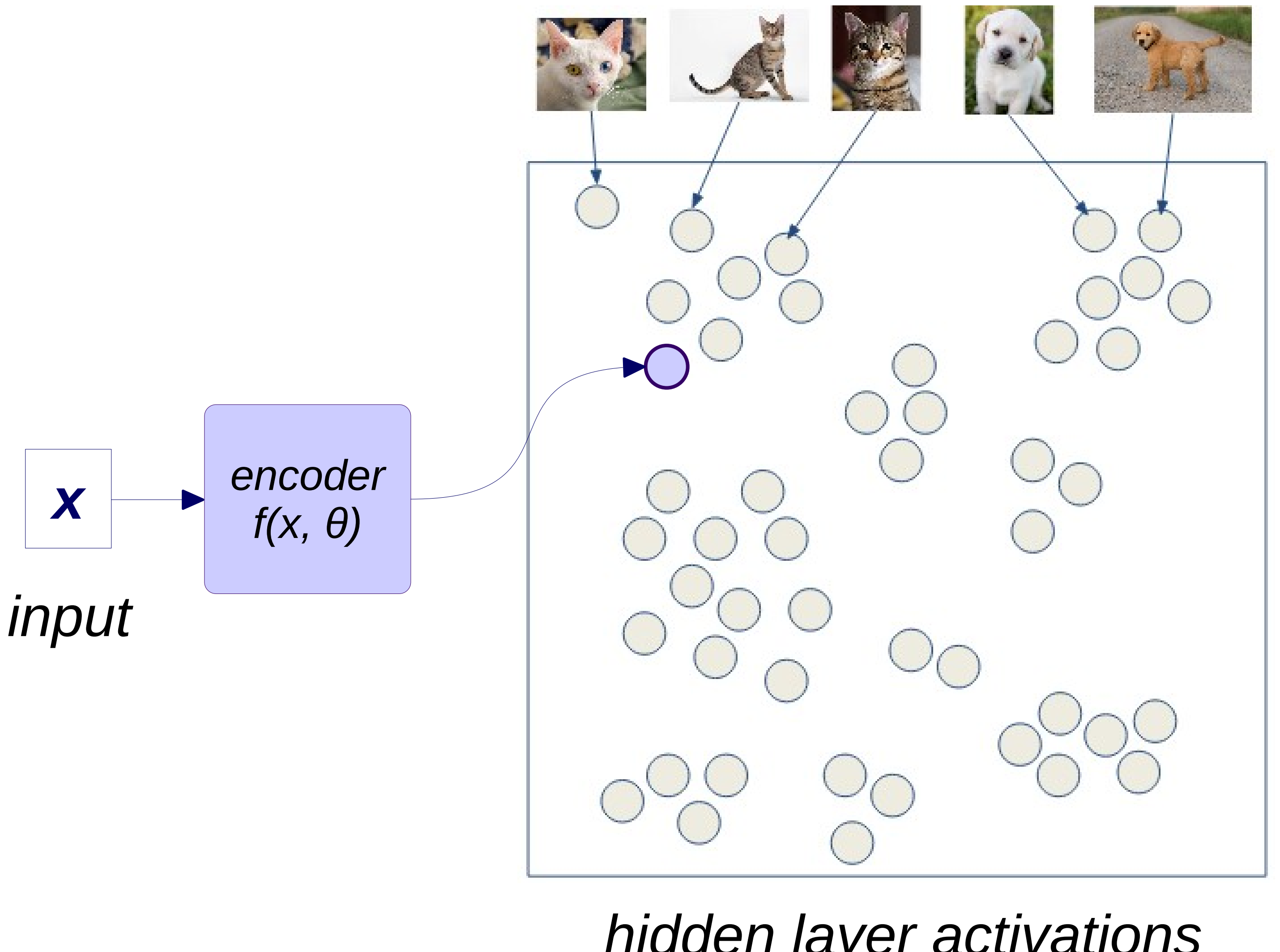

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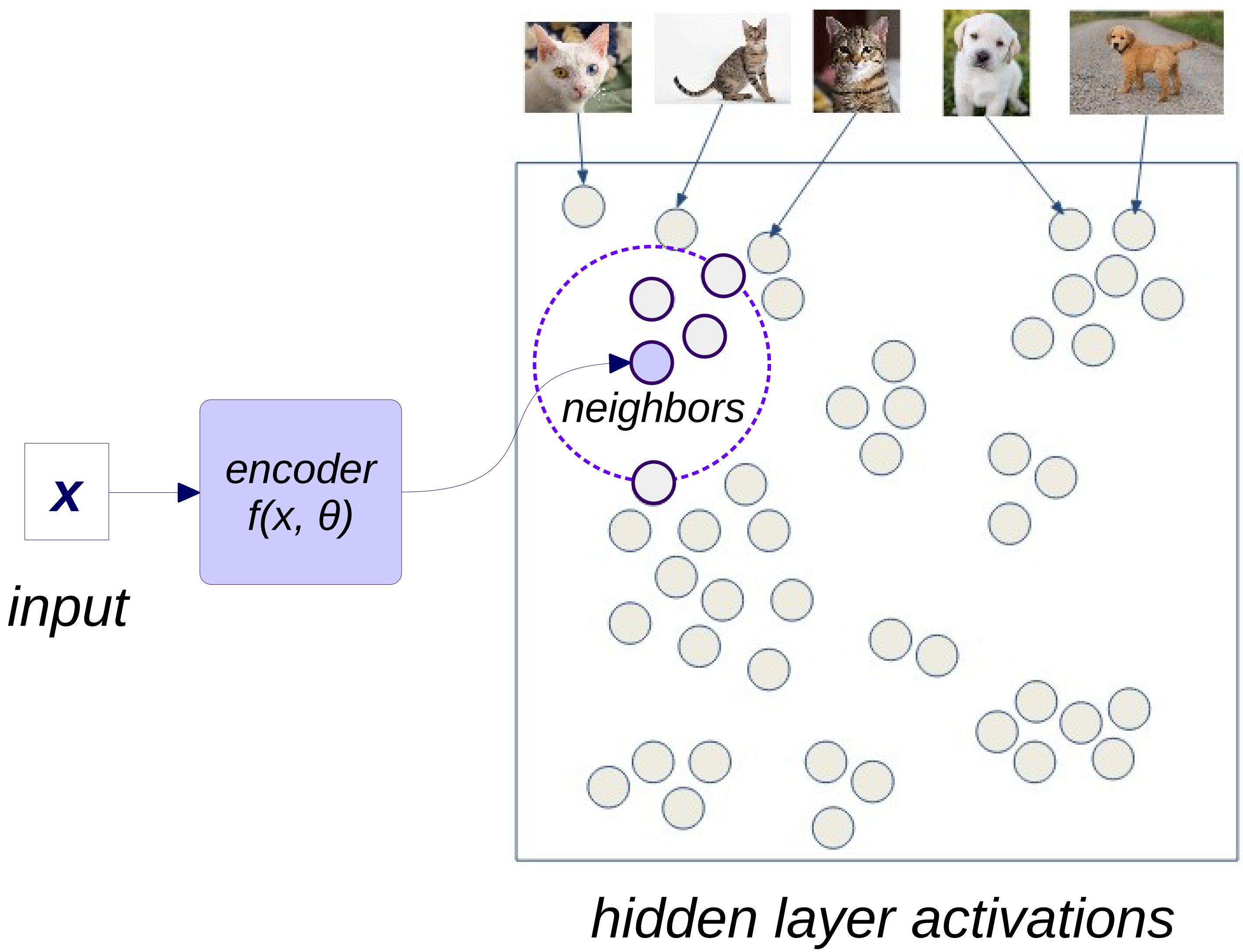

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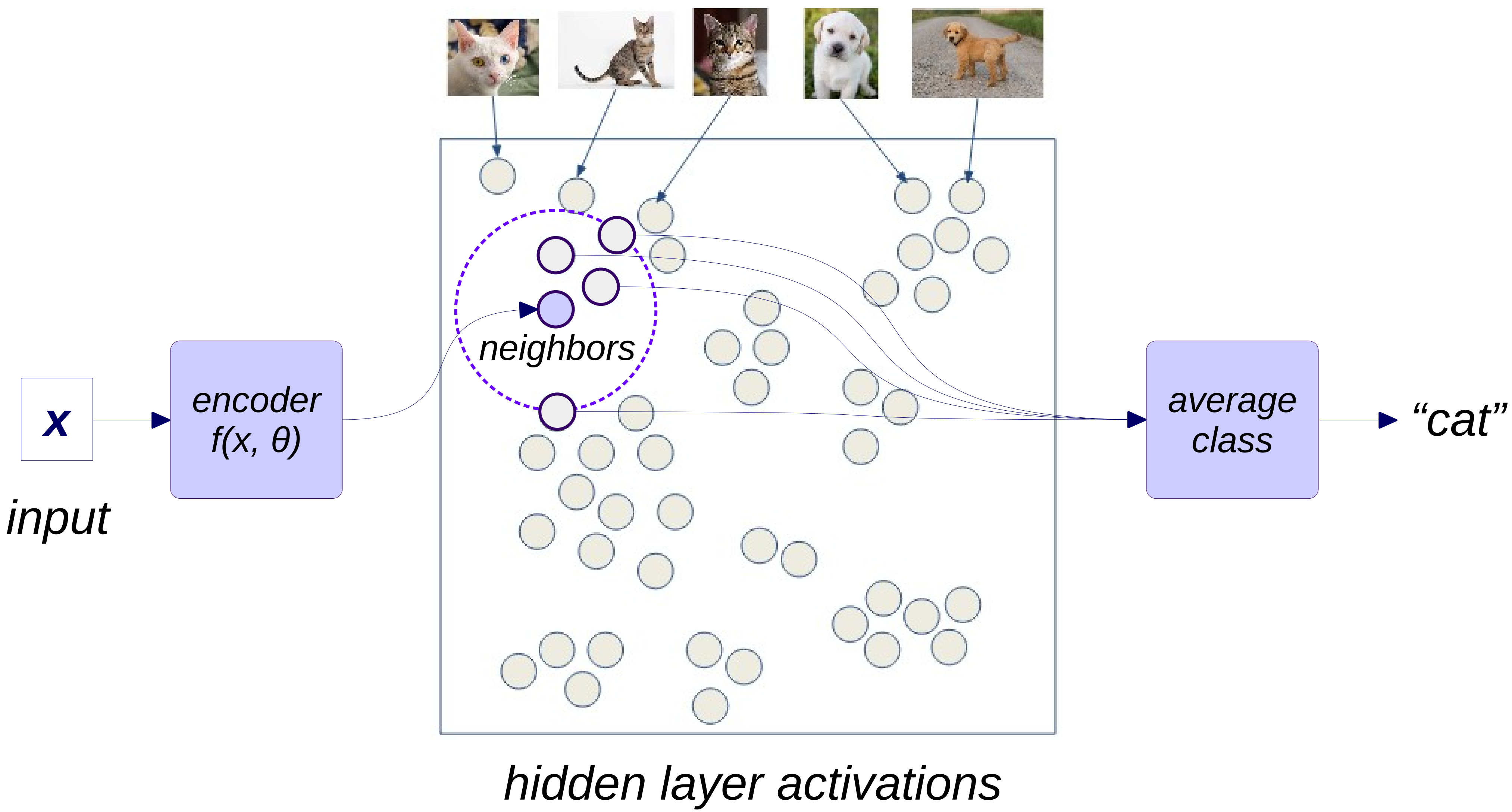

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Idea: design architecture to be interpretable

Prototype objects and answers: $(\hat{x}_{0,} \hat{y}_0), \ldots, (\hat{x}_N, \hat{y}_N)$

"Attention" weights: $a(x, \hat{x}_i) = \frac{e^{\langle f(x, theta), f(\hat{x}_i, theta) \rangle}}{\sum_{j=0}^{N} e^{\langle f(x, theta), f(\hat{x}_j, theta) \rangle}}$

Prediction by averaging: $y^{pred}(x) = \sum_i \hat{y}_i \cdot a_i(x, \hat{x}_i)$

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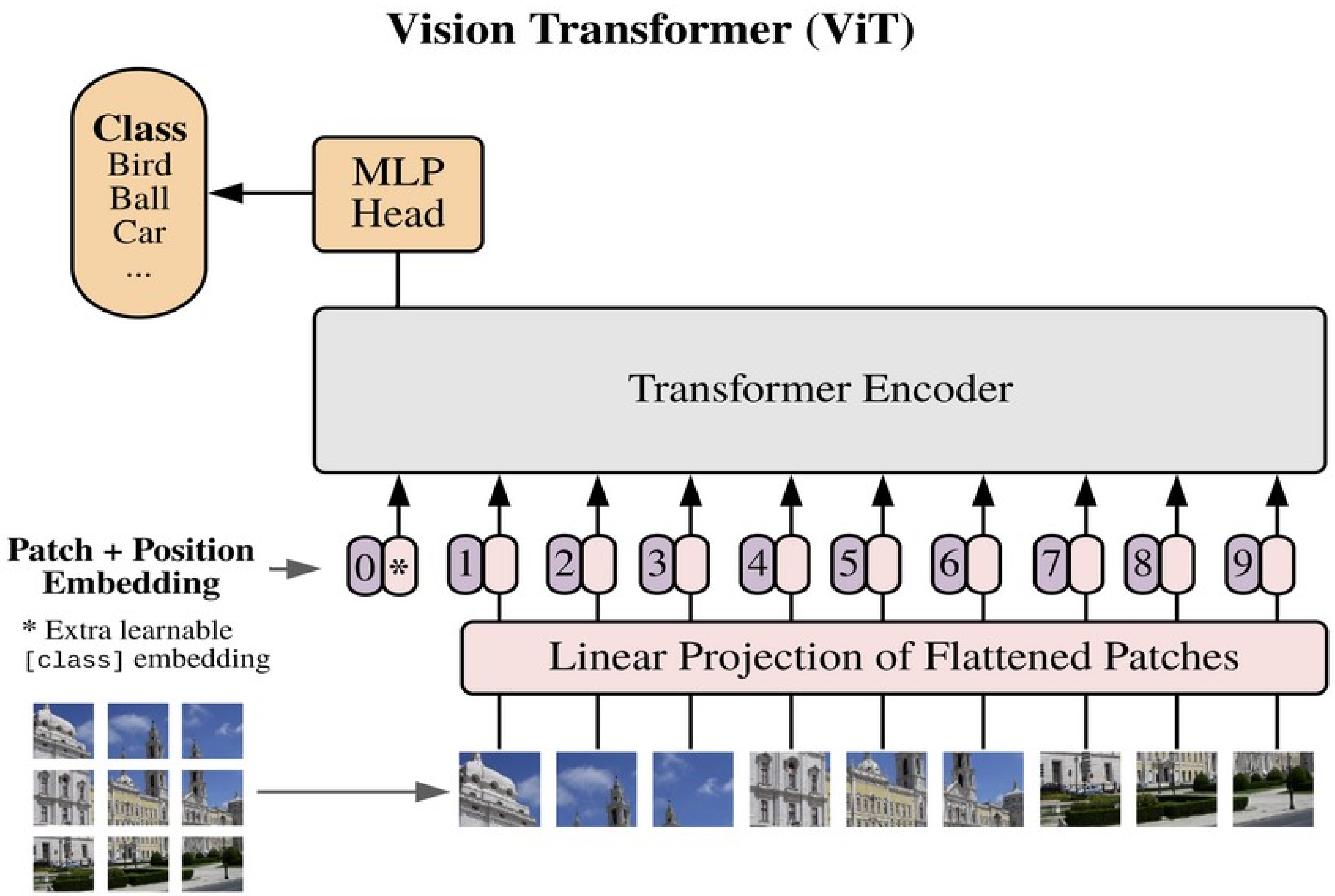
$$y^{pred}(x) = \sum_i \hat{y}_i \cdot a_i(x, \hat{x}_i)$$

Read more: KNN
arxiv.org/abs/1703.05175
arxiv.org/abs/1803.04765
arxiv.org/abs/1809.02847

Read more: Linear
arxiv.org/abs/1705.08078
arxiv.org/abs/1806.07538

Taking it to the extreme

Paper: https://arxiv.org/abs/2010.11929



Taking it to the extreme

Paper: https://arxiv.org/abs/2104.14294

View attention maps: https://epfml.github.io/attention-cnn/

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Types of uncertainty

example: binary classification

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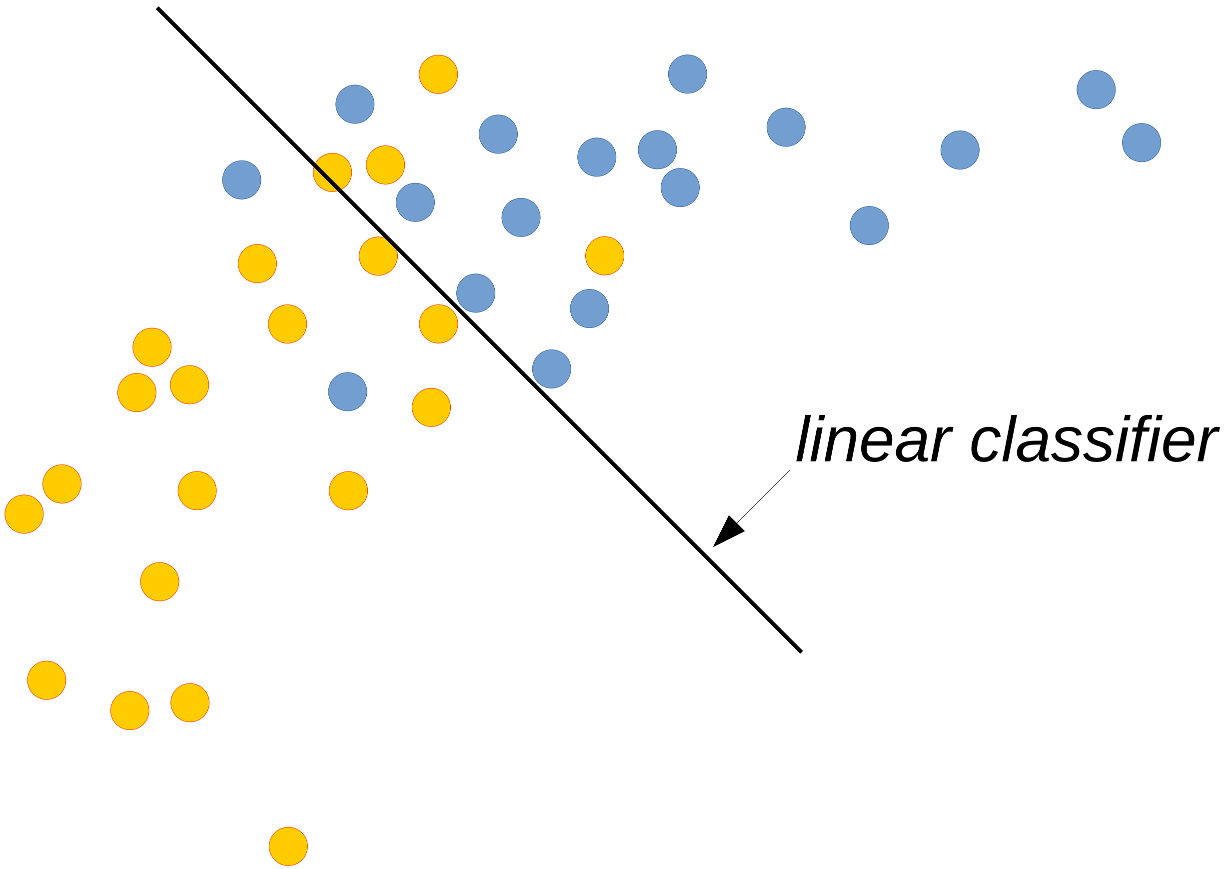
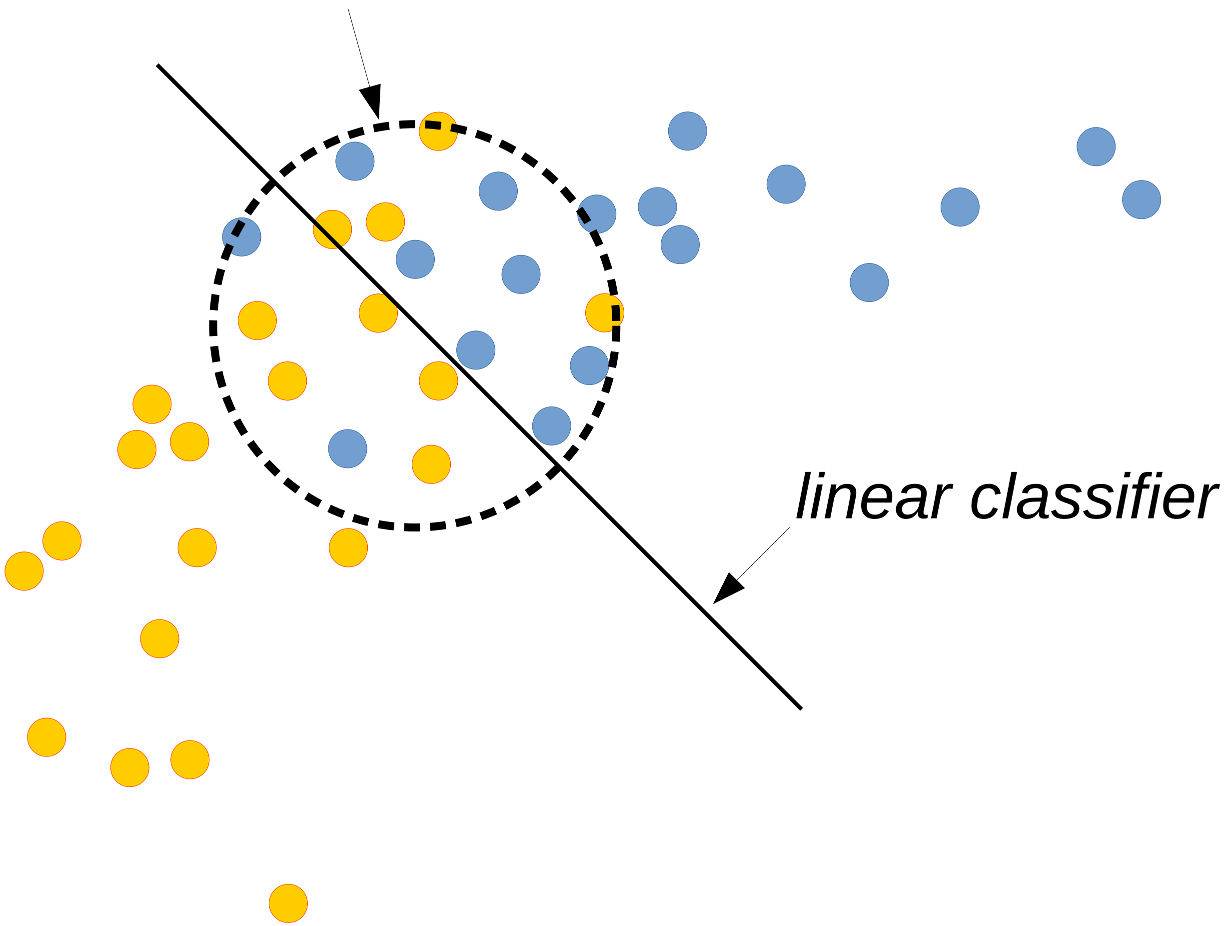


Types of uncertainty

Statistical (aleatoric) uncertainty
"I know there's randomness"



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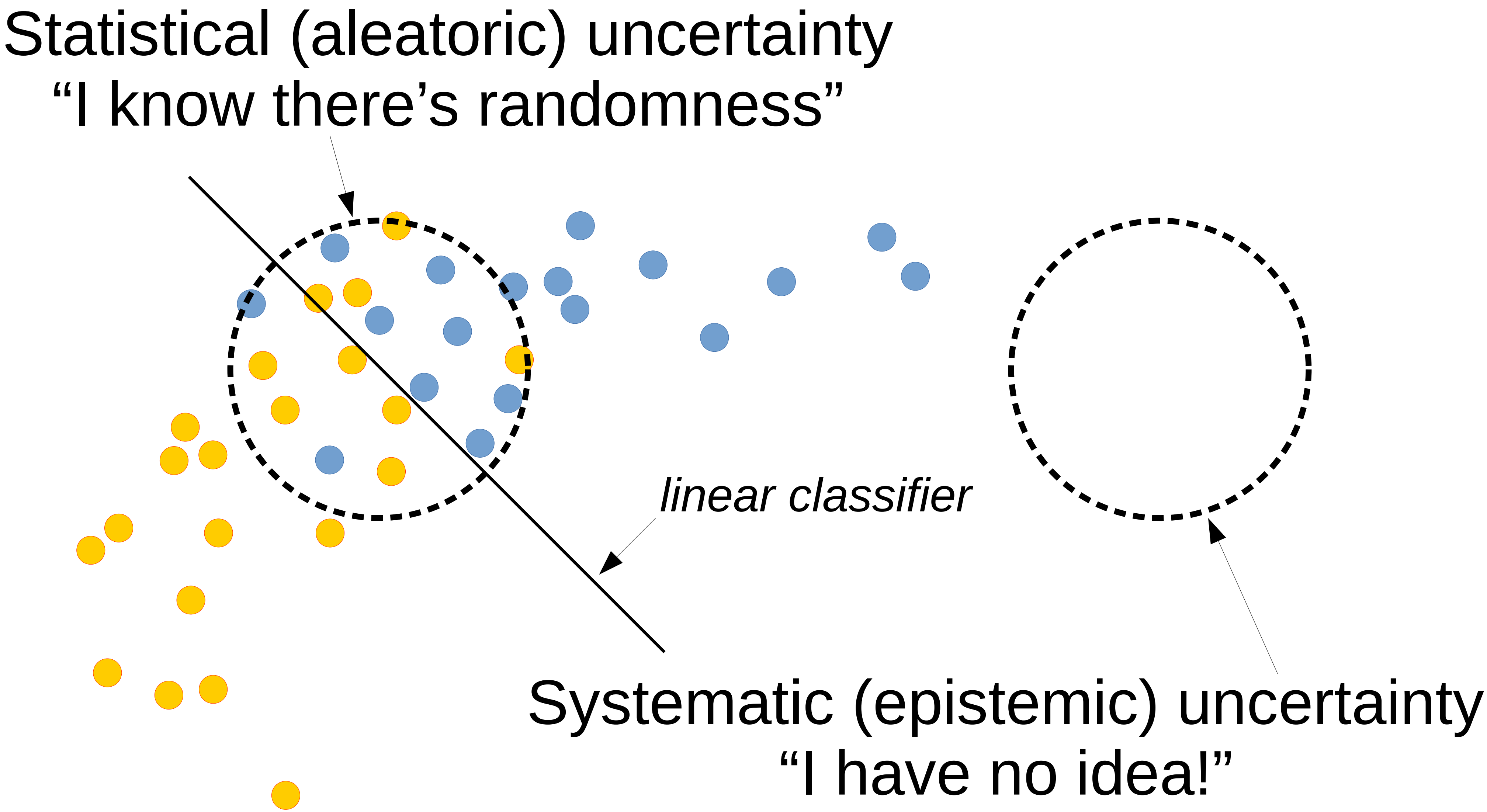

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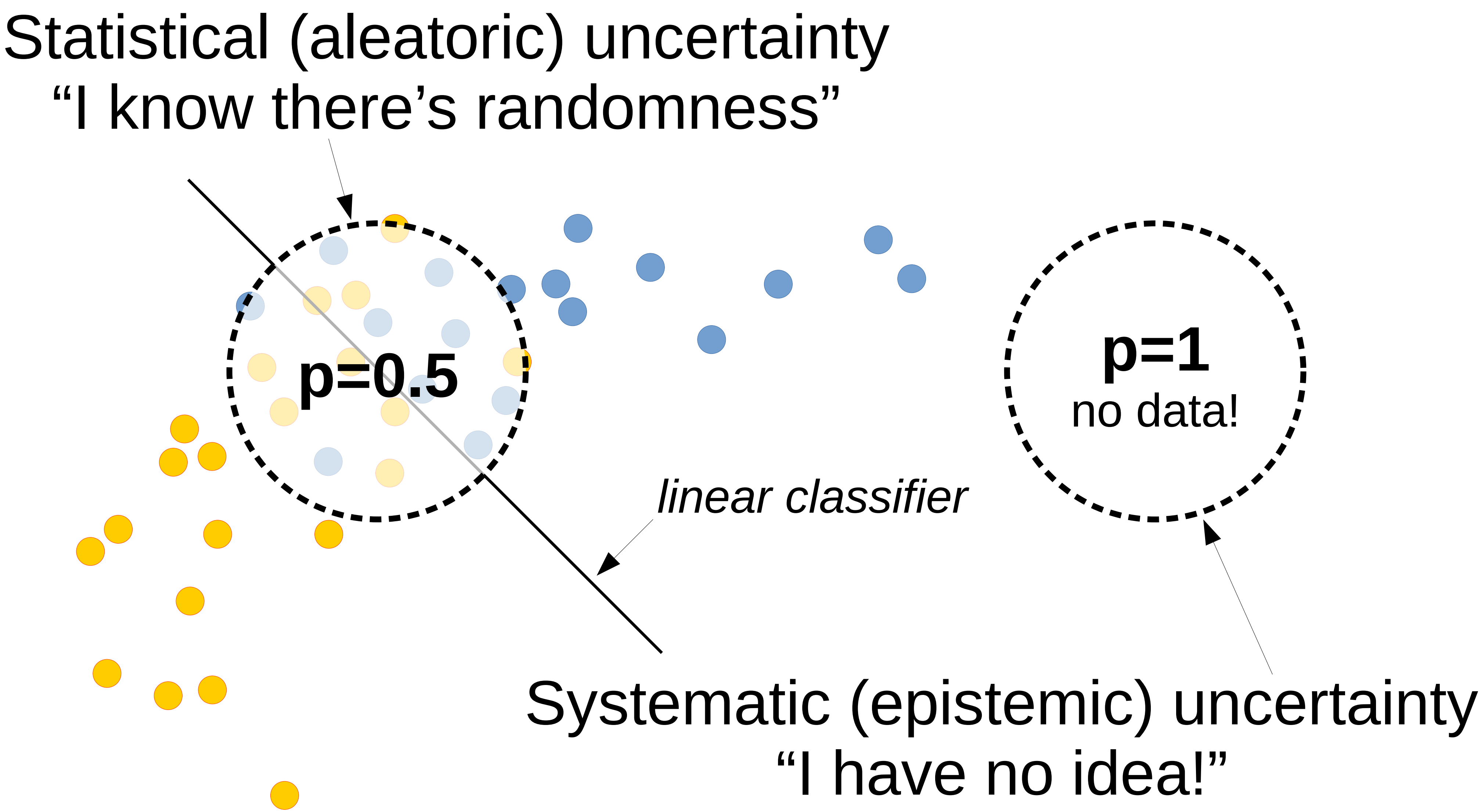
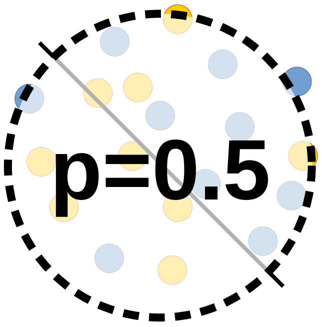


How to measure uncertainty

Aleatoric uncertainty: use predicted probability!
Exception: neural networks can be **overconfident**
Fix it by *calibrating* model predictions after the fact,
Read more: tinyurl.com/sklearn-calibration



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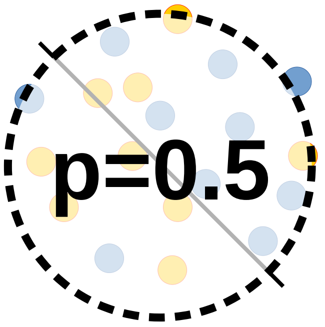

Epistemic (systematic) uncertainty: it gets tricky

Ideas?

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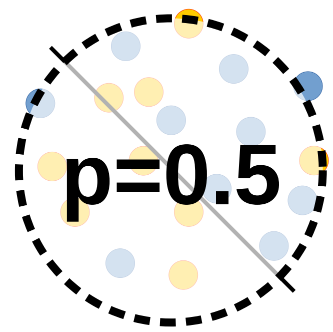
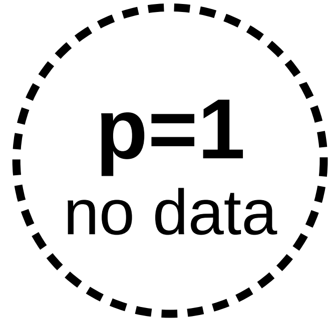


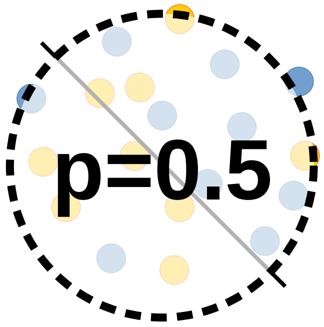
Epistemic (systematic) uncertainty: it gets tricky

Approach A: train *autoencoder* on input features
  Low reconstruction error = **certain or not?**
  High reconstruction error = **certain or not?**



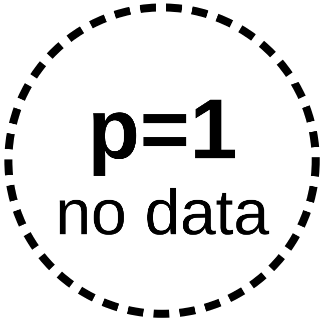
How to measure uncertainty

Aleatoric uncertainty: use predicted probability!
Exception: neural networks can be **overconfident**
Fix it by *calibrating* model predictions after the fact,
Read more: tinyurl.com/sklearn-calibration



Epistemic (systematic) uncertainty: it gets tricky

Approach A: train *autoencoder* on input features
  Low reconstruction error = familiar data
  High reconstruction error = unfamiliar data
    (*For NLP: use language models)*



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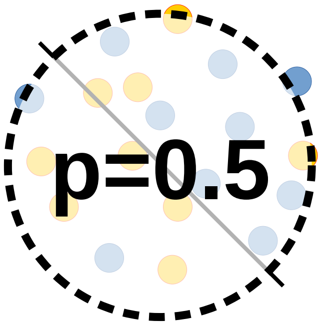
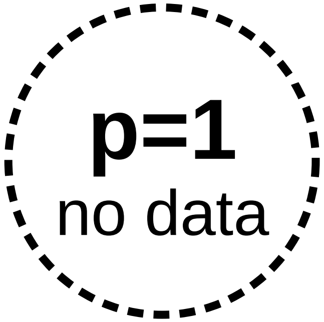


Epistemic (systematic) uncertainty: it gets tricky



Approach A: train *autoencoder* on input features
Low reconstruction error = familiar data
High reconstruction error = unfamiliar data

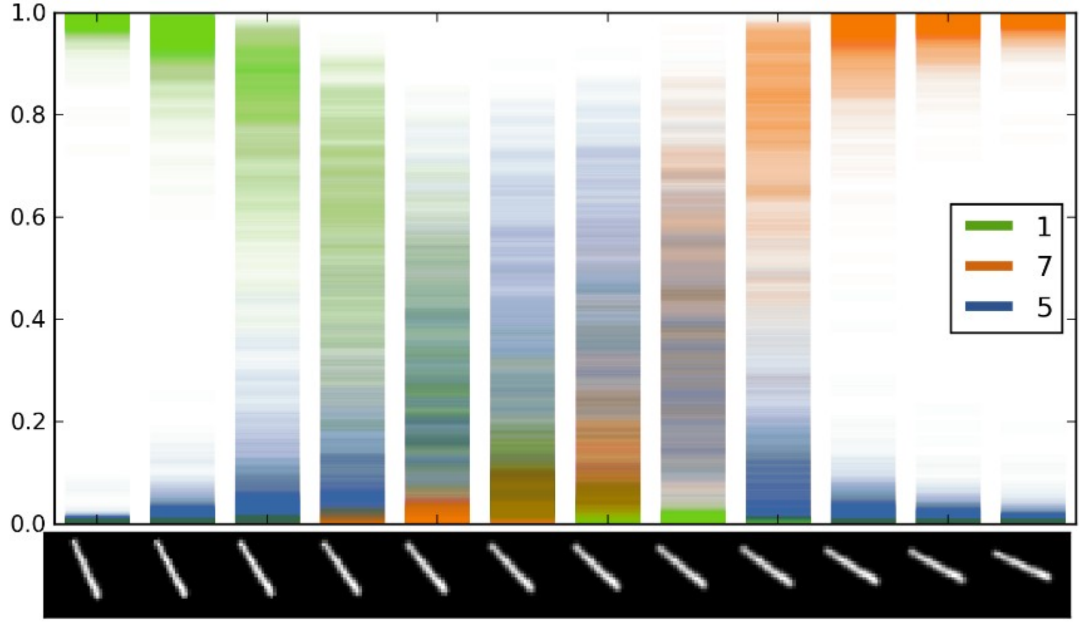
Approach B: train an *ensemble* of predictors
Predictors agree = familiar data
Predictors disagree = unfamiliar data

More: tinyurl.com/uncertainty-ensembles

Uncertainty from dropout

Idea:
measure how robust does your network perform under noise

Example (left):
use dropout and estimate variance



Systematic uncertainty for different input images, source: arXiv:1506.02142

Read more in the paper or in a blog post

Bayesian Neural Networks

Disclaimer: this is a hacker's guide to BNNs!

It does not cover all the philosophy and general cases.

Bayesian Neural Networks

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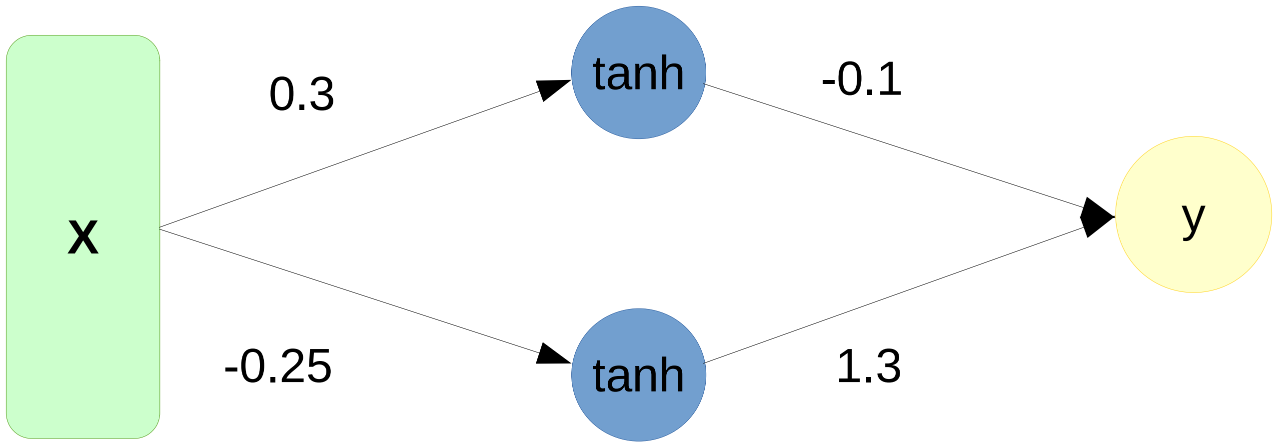
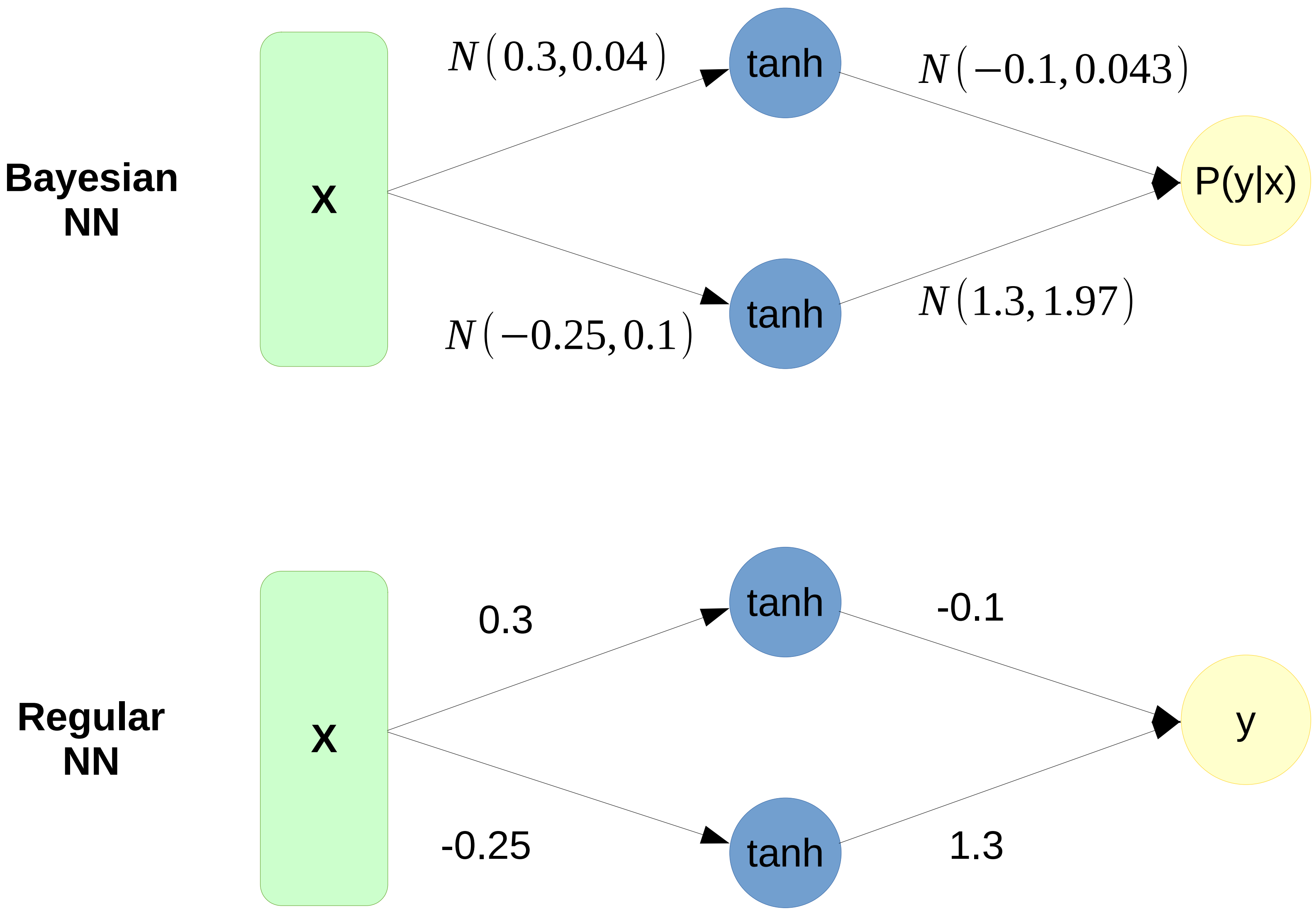
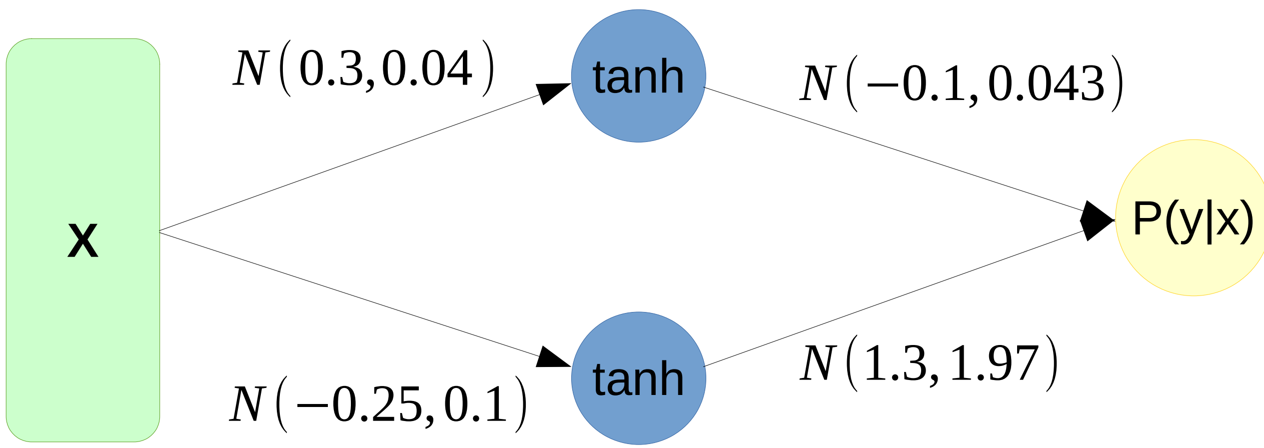
Regular NN



Bayesian Neural Networks



Bayesian Neural Networks



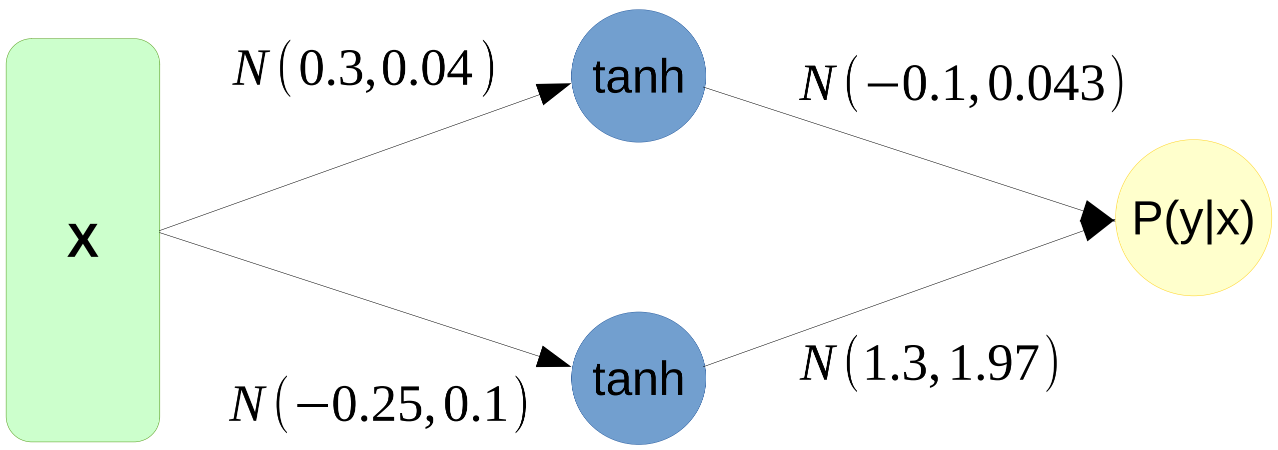
Idea:

- No explicit weights
  - Maintain parametric distribution on them instead!
    - Practical: fully-factorized normal or similar

$$q(\theta|\phi:[\mu,\sigma]) = \prod_i N(\theta_i|\mu_i,\sigma_i)$$

$$P(y|x) = E_{\theta\sim q(\theta|\phi)} P(y|x,\theta)$$

Bayesian Neural Networks



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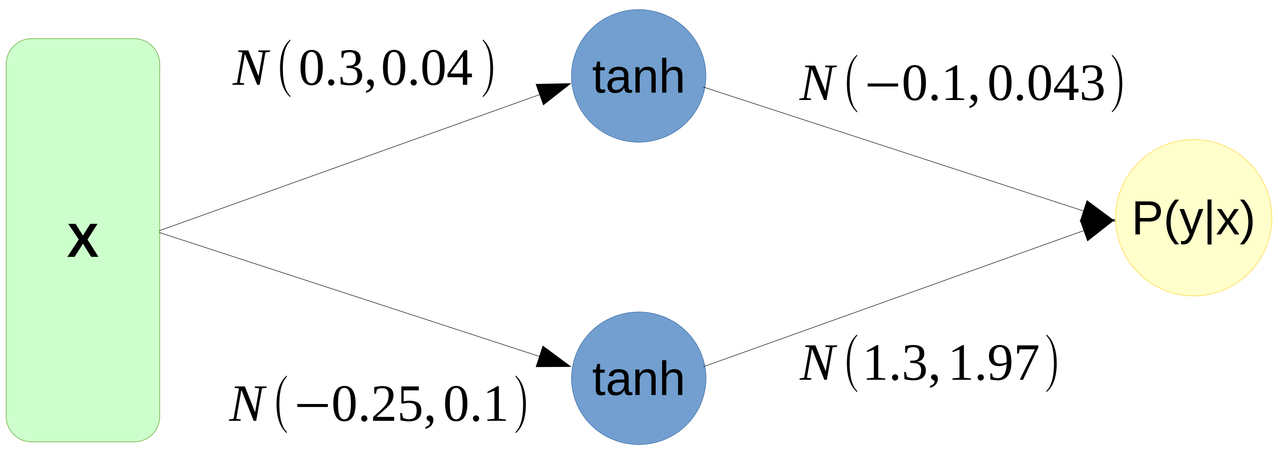
Bayesian Neural Networks



Idea:

- No explicit weights
- Inference: sample from weight distributions, predict 1 “sample”
- To get distribution, aggregate K samples (e.g. with histogram)
  - Yes, it means running network **multiple times per one X**

$$P(y|x) = E_{\theta \sim q(\theta|\phi)} P(y|x, \theta)$$

Bayesian Neural Networks

Idea:

- No explicit weights
  - Maintain parametric distribution on them instead!
    - Practical: fully-factorized normal or similar

$$q(\theta|\phi:[\mu,\sigma])=\prod_i N(\theta_i|\mu_i,\sigma_i)$$

$$P(y|x)=E_{\theta\sim q(\theta|\phi)}P(y|x,\theta)$$

- Learn parameters of that distribution (reparameterization trick)
  - Less variance: local reparameterization trick.

$$\mathring{\phi}=argmax_{\phi}E_{x_i,y_i\sim d}E_{\theta\sim q(\theta|\phi)}P(y_i|x_i,\theta)$$

wanna explicit formulae? *d = dataset*

Evidence Lower bound

d = dataset

$$-KL\left(q(\theta|\phi)\,||\,p(\theta|d)\right) = -\int_\theta q(\theta|\phi)\cdot\log\frac{q(\theta|\phi)}{p(\theta|d)}$$

$$-\int_\theta q(\theta|\phi)\cdot\log\frac{q(\theta|\phi)}{\left[\frac{p(d|\theta)\cdot p(\theta)}{p(d)}\right]} = -\int_\theta q(\theta|\phi)\cdot\log\frac{q(\theta|\phi)\cdot p(d)}{p(d|\theta)\cdot p(\theta)}$$

$$-\int_\theta q(\theta|\phi)\cdot\left[\log\frac{q(\theta|\phi)}{p(\theta)} - \log p(d|\theta) + \log p(d)\right]$$

$$\left[E_{\theta\sim q(\theta|\phi)}\log p(d|\theta)\right] - KL\left(q(\theta|\phi)\,||\,p(\theta)\right) + \log p(d)$$

loglikelihood **-distance to prior** **+const**

Evidence Lower bound

$$\phi = \underset{\phi}{argmax}\left(-KL\left(q\left(\theta|\phi\right)\|p\left(\theta|d\right)\right)\right)$$

$$\underset{\phi}{argmax}\left(\underbrace{\left[E_{\theta\sim q\left(\theta|\phi\right)}\log p\left(d|\theta\right)\right]}_{\textbf{fit to the data}}-KL\underbrace{\left(q\left(\theta|\phi\right)\|p\left(\theta\right)\right)\right)}_{\textbf{don't be too certain}}$$

Evidence Lower bound

$$\phi = \underset{\phi}{argmax}\left(-KL\left(q\left(\theta|\phi\right)\|p\left(\theta|d\right)\right)\right)$$

$$\underset{\phi}{argmax}\left(\left[E_{\theta\sim q\left(\theta|\phi\right)}\log p\left(d|\theta\right)\right]-KL\left(q\left(\theta|\phi\right)\|p\left(\theta\right)\right)\right)$$

Can we perform gradient ascent directly?

Reparameterization trick

$$\phi = \underset{\phi}{argmax}\left(-KL\left(q\left(\theta|\phi\right)||p\left(\theta|d\right)\right)\right)$$

$$\underset{\phi}{argmax}\left(\underbrace{\left[E_{\theta\sim q(\theta|\phi)}\log p\left(d|\theta\right)\right]}_{\text{Use reparameterization trick}}-\underbrace{KL\left(q\left(\theta|\phi\right)||p\left(\theta\right)\right)}_{\text{simple formula (for normal q)}}\right)$$

Use reparameterization trick

simple formula
(for normal q)

What does this log
P(d|...) mean?

BNN likelihood

$$E_{\theta\sim N(\theta|\mu_\phi,\sigma_\phi)}\log p\left(d|\theta\right)=E_{\psi\sim N(0,1)}\log p\left(d|\left(\mu_\phi+\sigma_\phi\cdot\psi\right)\right)$$

Reparameterization trick

$$\phi = \underset{\phi}{argmax}\left(-KL\left(q(\theta|\phi)\|p(\theta|d)\right)\right)$$

$$\underset{\phi}{argmax}\left(\left[E_{\theta\sim q(\theta|\phi)}\log p(d|\theta)\right]-KL\left(q(\theta|\phi)\|p(\theta)\right)\right)$$

In other words,
$\Sigma_{x,y\sim d}$ log p(y|x,μ+σψ)

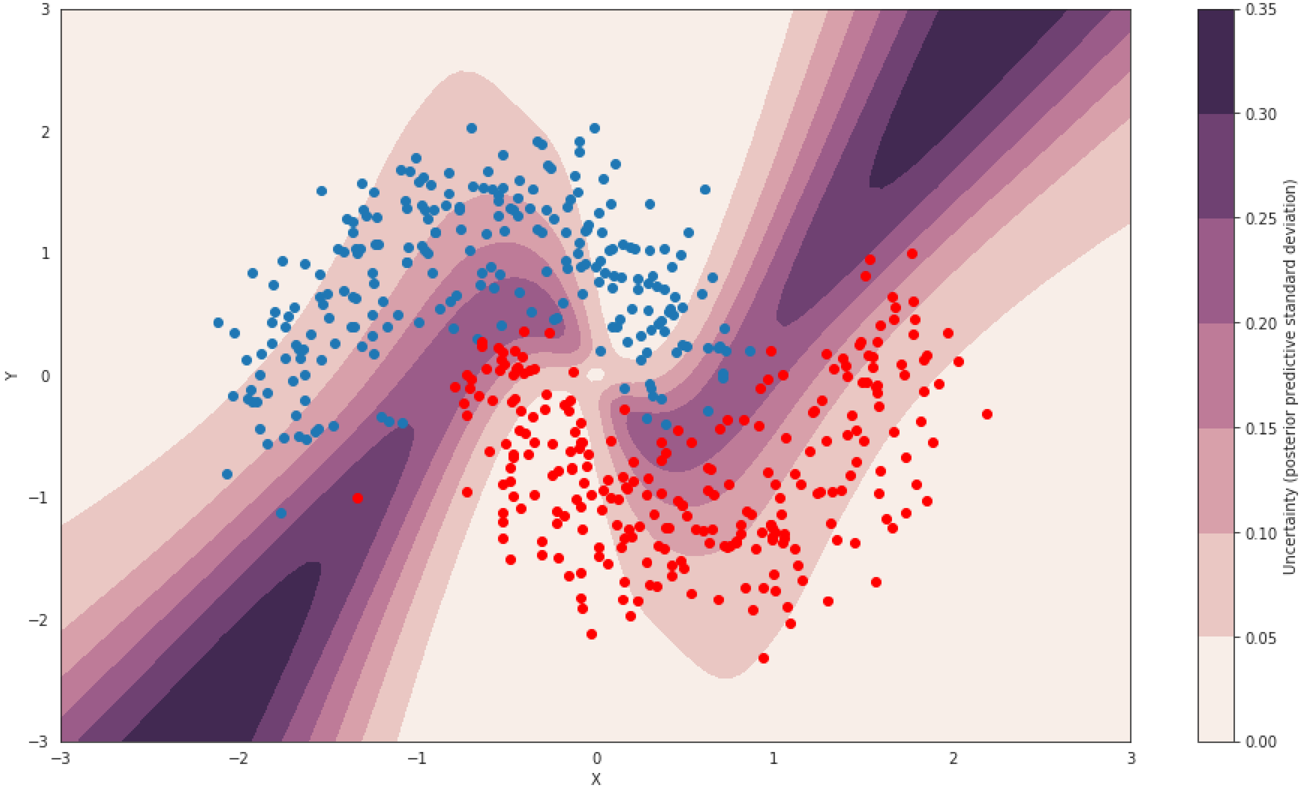
BNN likelihood

$$E_{\theta\sim N(\theta|\mu_\phi,\sigma_\phi)}\log p(d|\theta)=E_{\psi\sim N(0,1)}\log p\left(d|\left(\mu_\phi+\sigma_\phi\cdot\psi\right)\right)$$

Bayesian Neural Networks

Estimating uncertainty:

1. sample weights several times
2. predict by averaging outputs
3. uncertainty = standard deviation



Read more...

Papers on uncertainty

bayesian neural networks: blog post
prior networks: arxiv.org/abs/1802.10501
batchnorm: arxiv.org/abs/1802.04893
dropout: arxiv.org/abs/1506.02142
video stuff: youtube.com/watch?v=HRfDiqgh6CE

The question of trust

How can I explain my model’s prediction?
Why did it make this decision/mistake?
What features does it rely on?

Is my model certain about what it says?
Is there something wrong with this input?
Can I rely on this prediction?

Can I trust this data?
Is something missing?
Is there any bias?

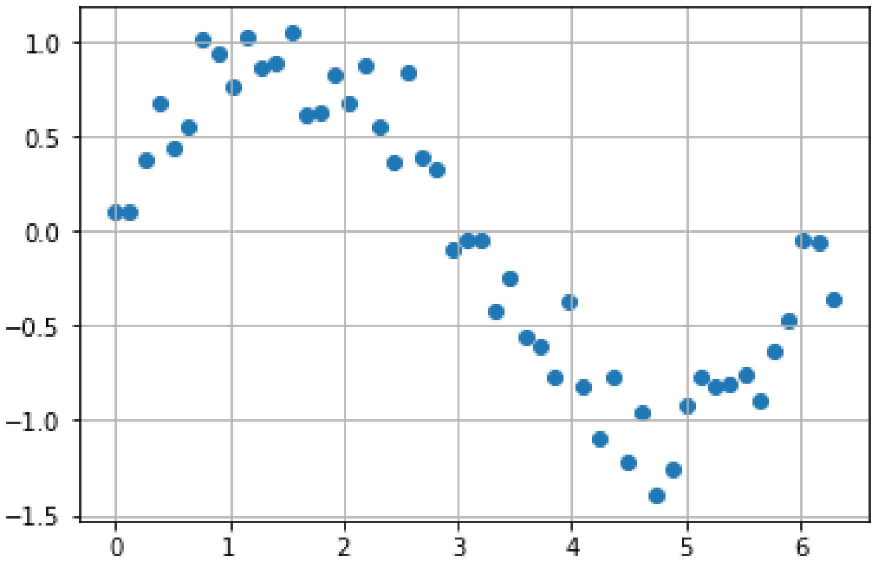
Exploratory data analysis

aka “seeing for yourself what’s in your data”

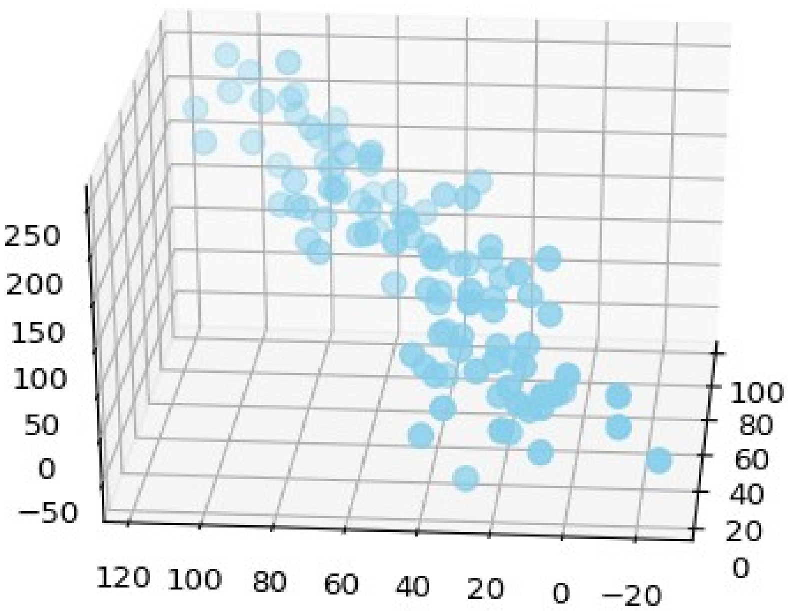
Q: How many dimensions can you show on a plot?

Exploratory data analysis

Q: How many dimensions can you show on a plot?



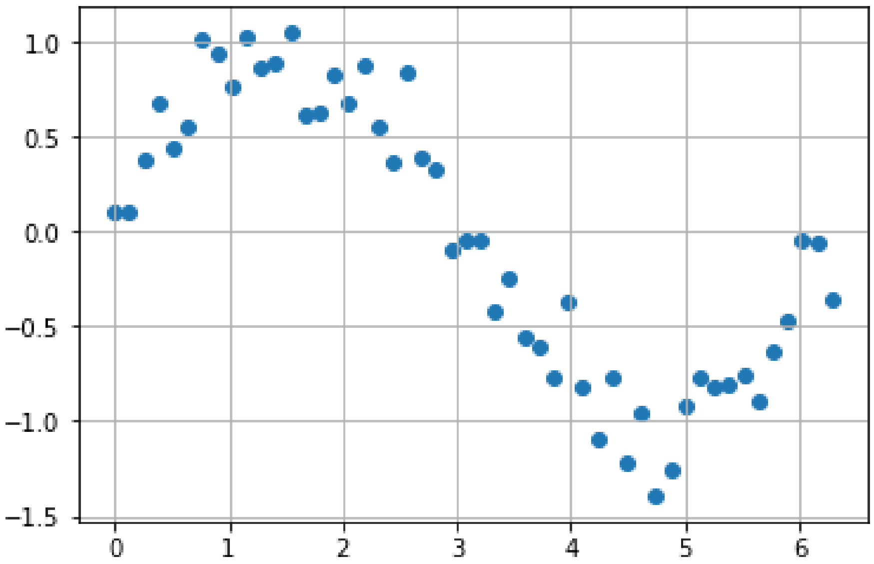
2d scatter-plot



3d scatter-plot

Exploratory data analysis

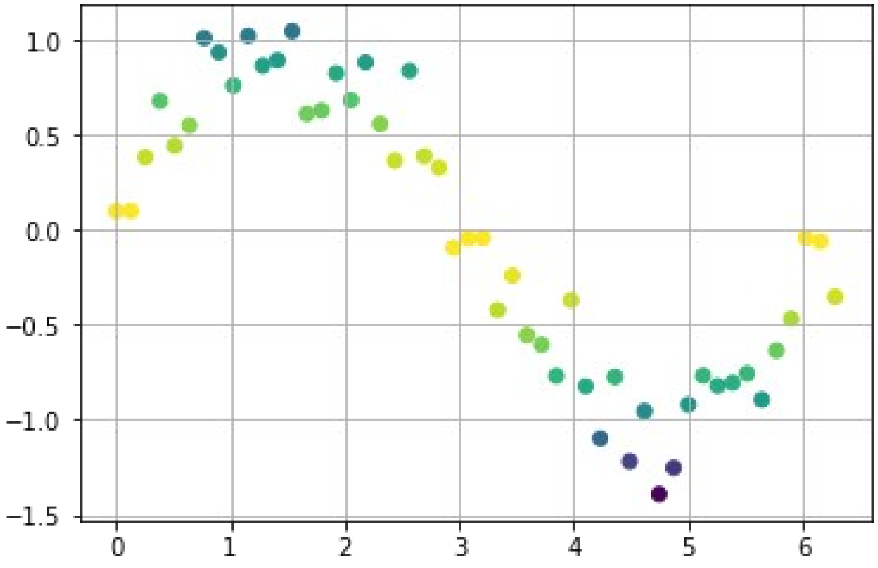
Q: How many dimensions can you show on a plot?



2 dimensions

Exploratory data analysis

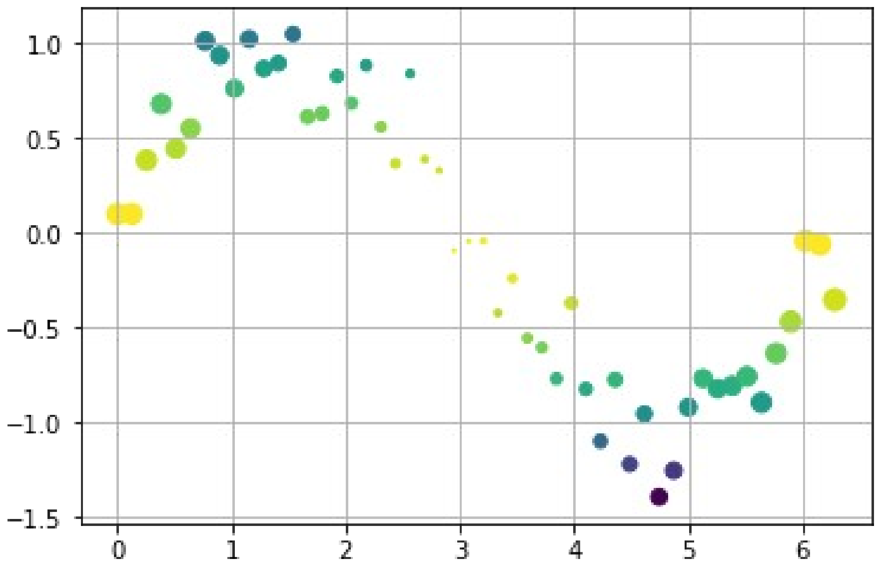
Q: How many dimensions can you show on a plot?



3 dimensions

Exploratory data analysis

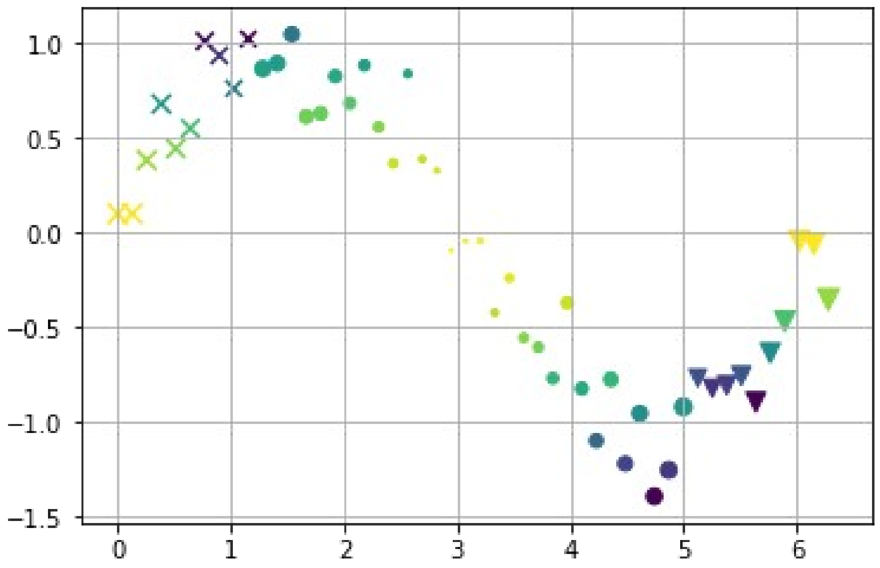
Q: How many dimensions can you show on a plot?



4 dimensions

Exploratory data analysis

Q: How many dimensions can you show on a plot?



5 dimensions

Exploratory data analysis

Q: How many dimensions can you show on a plot?

Your data has 200 dimensions...
any ideas?

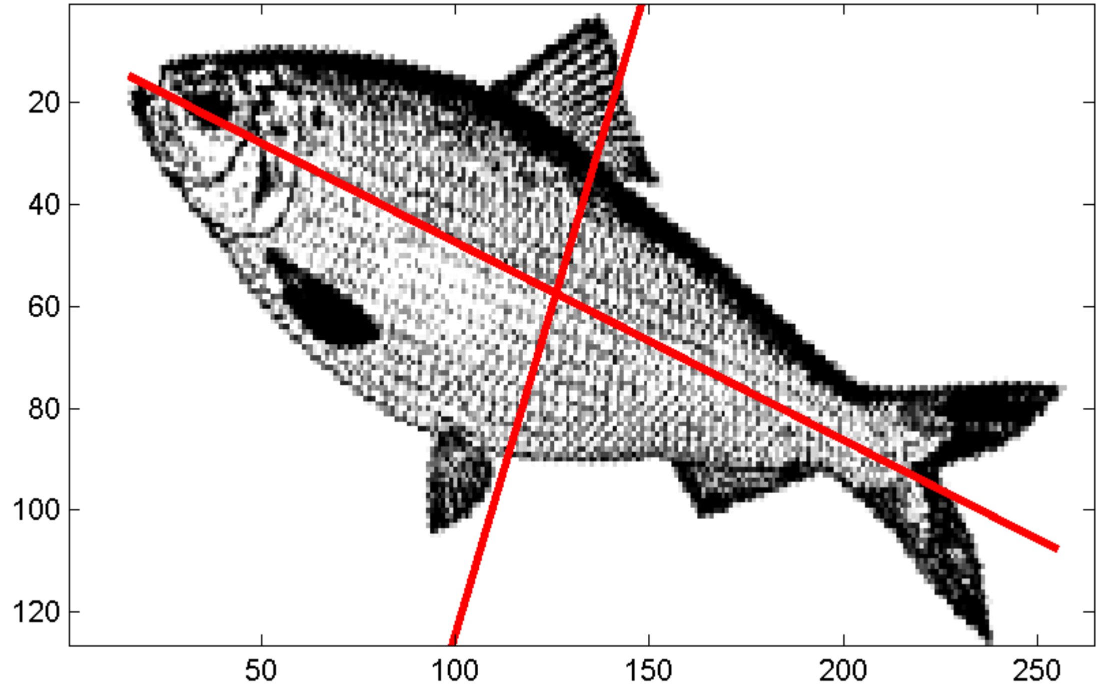
Recap: Principal Component Analysis

Idea:

- Linearly project data to lower-dim space

$$X \approx (X \times W_1) \times W_2$$

Minimize MSE

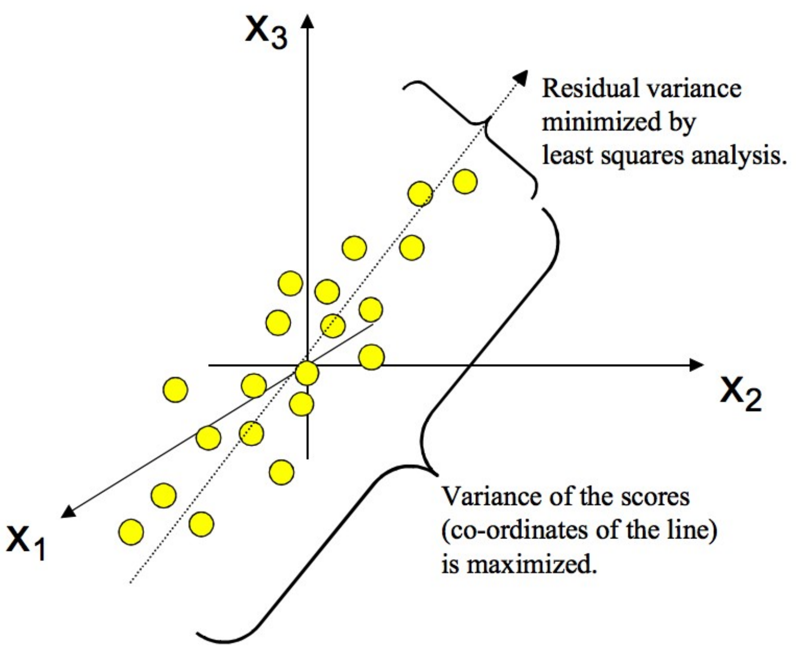


$$argmin_{W_1, W_2} \| X - (X \times W_1) \times W_2 \|$$

Recap: Principal Component Analysis

Idea:

- Linearly project data to lower-dim space
- Attempt to preserve as much variance as possible



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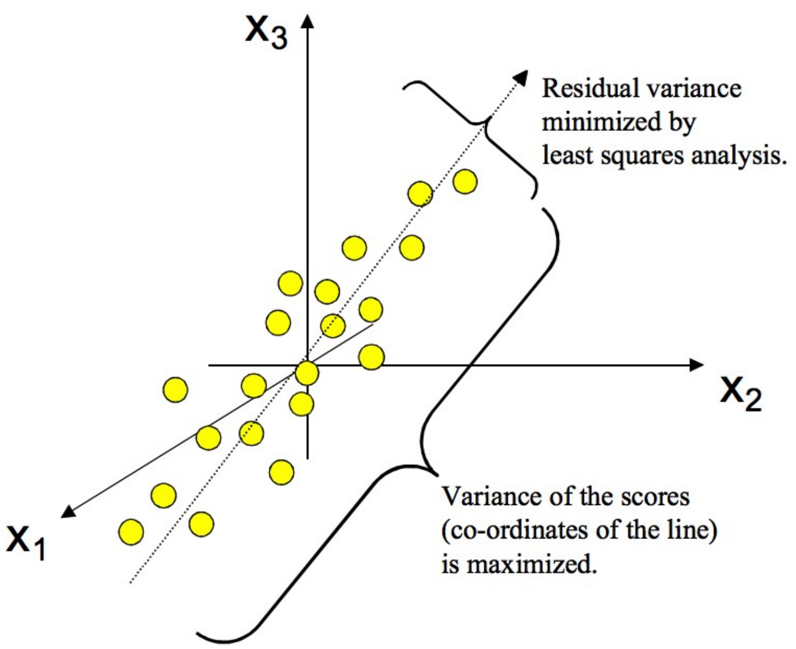
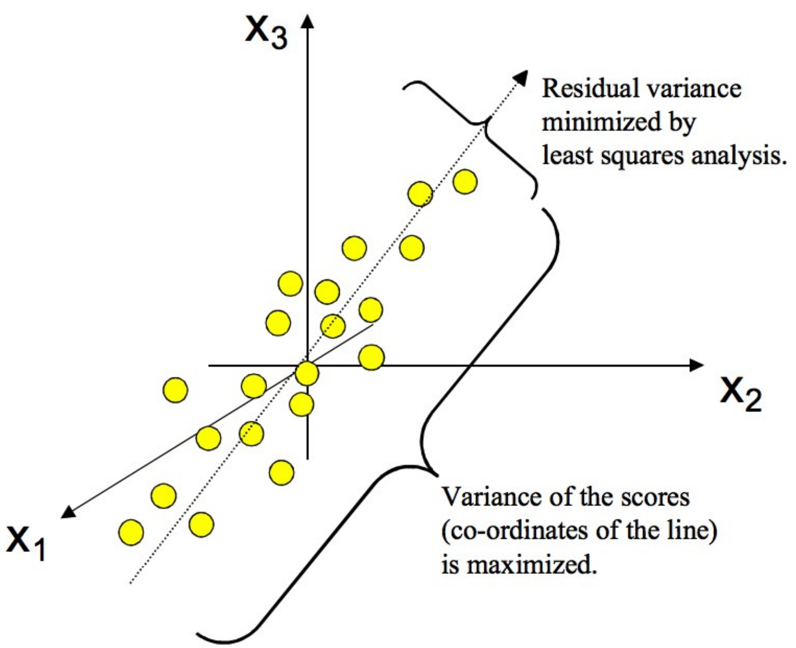


Q: What if linear projection is not enough?

Recap: Principal Component Analysis

Idea:

- Linearly project data to lower-dim space
- Attempt to preserve as much variance as possible



Q: What if linear projection is not enough?

deep autoencoders… or better

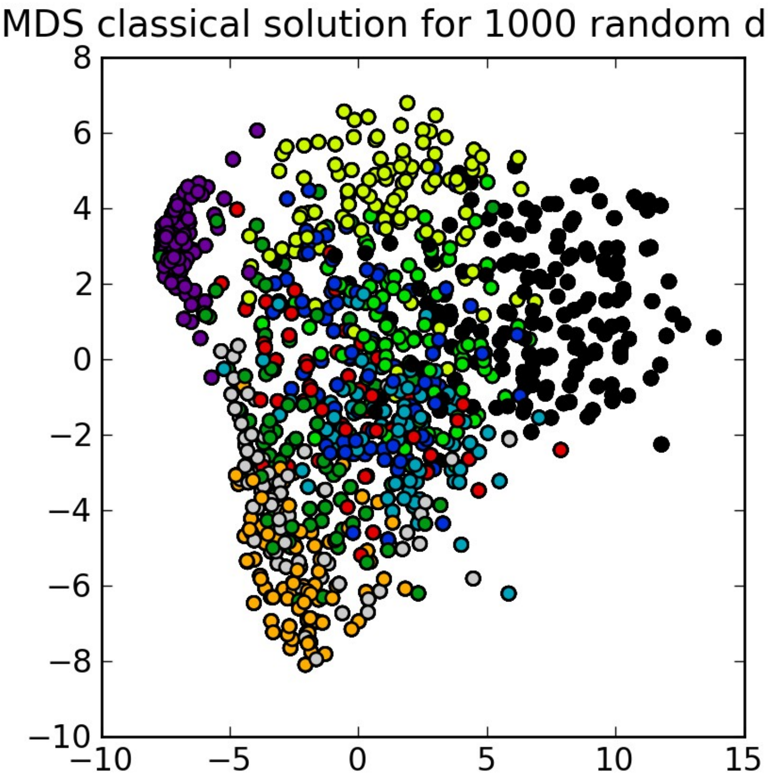
Manifold learning

Idea: let's directly "learn" 2d point coordinates

Multidimensional Scaling

preserve pairwise distances

$$\hat{x} = argmin_{\hat{x}} \frac{2}{N^2 - N} \sum_{i \neq j} \left(\|x_i - x_j\| - \|\hat{x}_i - \hat{x}_j\| \right)^2$$



Stochastic Neighborhood Embedding

preserve neighbor "probabilities"

$$P_{j|i} = \frac{e^{-\|x_i - x_j\|_2^2}}{\sum_k e^{-\|x_k - x_j\|_2^2}}$$

- large for nearest neighbors
- small for distant points
- adds up to 1

$$\hat{P}_{j|i} = \frac{e^{-\|\hat{x}_i - \hat{x}_j\|_2^2}}{\sum_k e^{-\|\hat{x}_k - \hat{x}_j\|_2^2}}$$

- same as P
- but in learned space

optimize crossentropy w.r.t. $\hat{x}$

$$\hat{x} = argmin_{\hat{x}} - \frac{1}{N} \sum_i \sum_j P_{j|i} \cdot \log \hat{P}_{j|i}$$

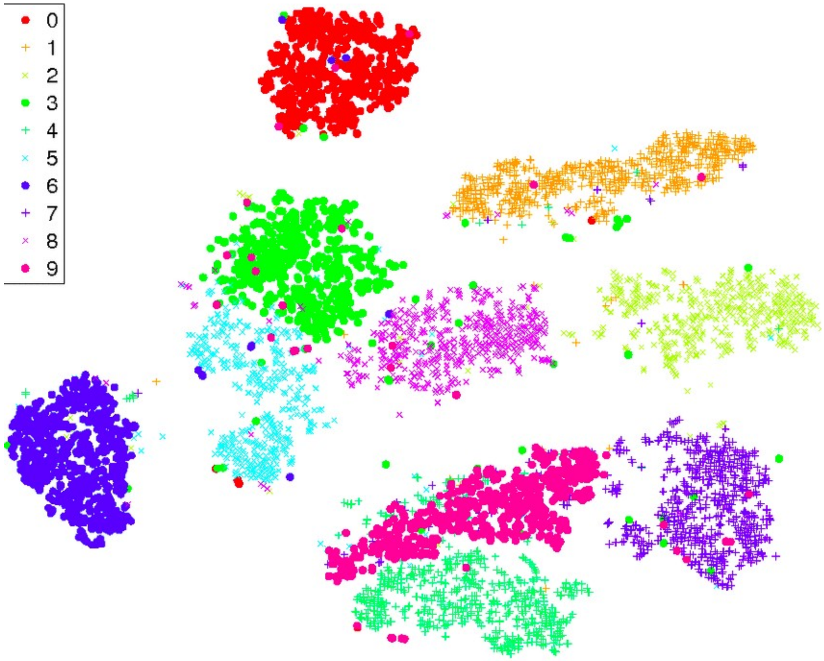
T-SNE

Like SNE from prev slide, but

- P is now *Student's t-distribution*

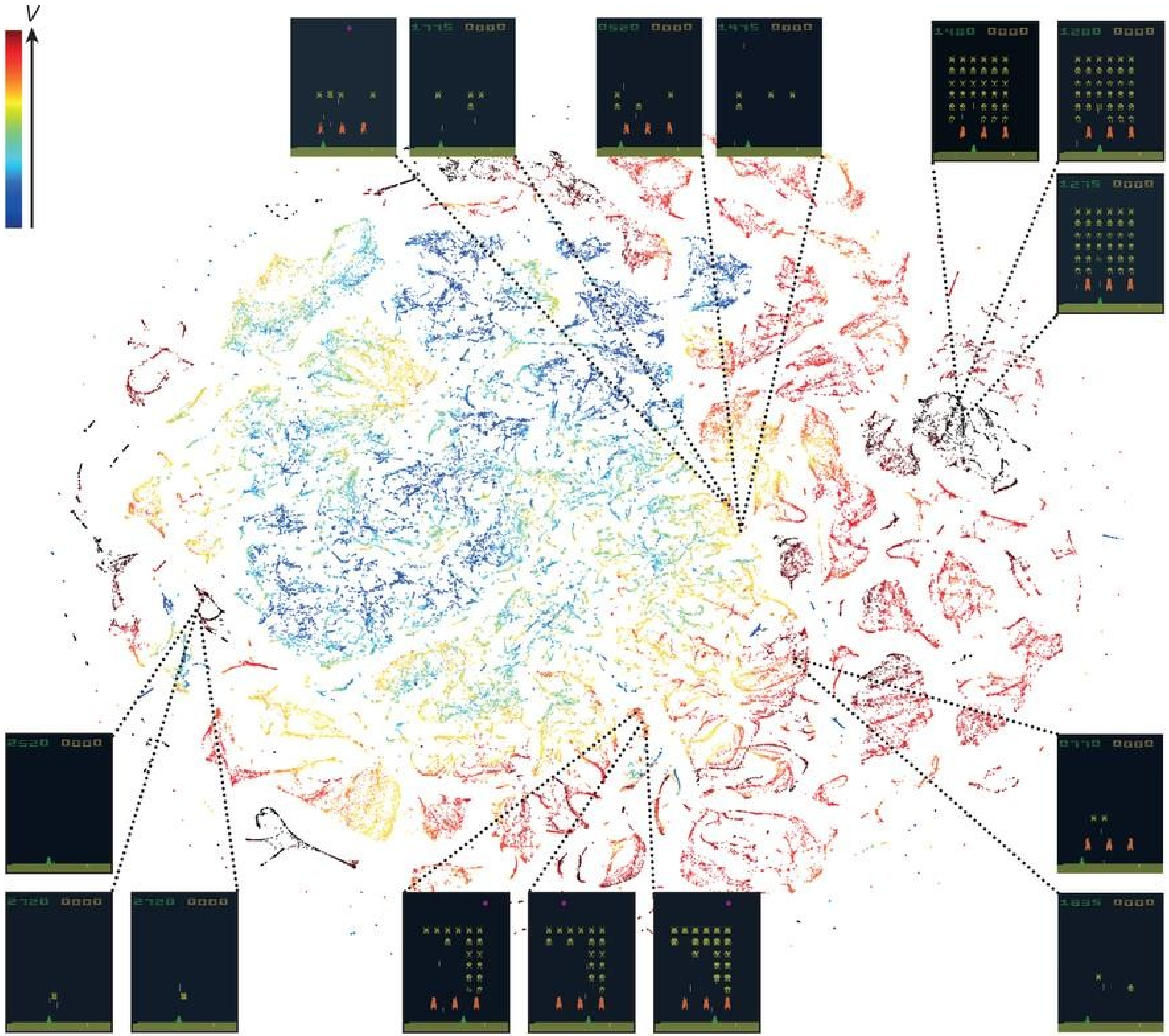
$$\hat{P}_{j|i} = \frac{\left(1 + \|\hat{x}_i - \hat{x}_j\|_2^2\right)^{-1}}{\sum_{k \neq l} \left(1 + \|\hat{x}_k - \hat{x}_l\|_2^2\right)^{-1}}$$

- A lot of optimization hacks
- By far the most popular method

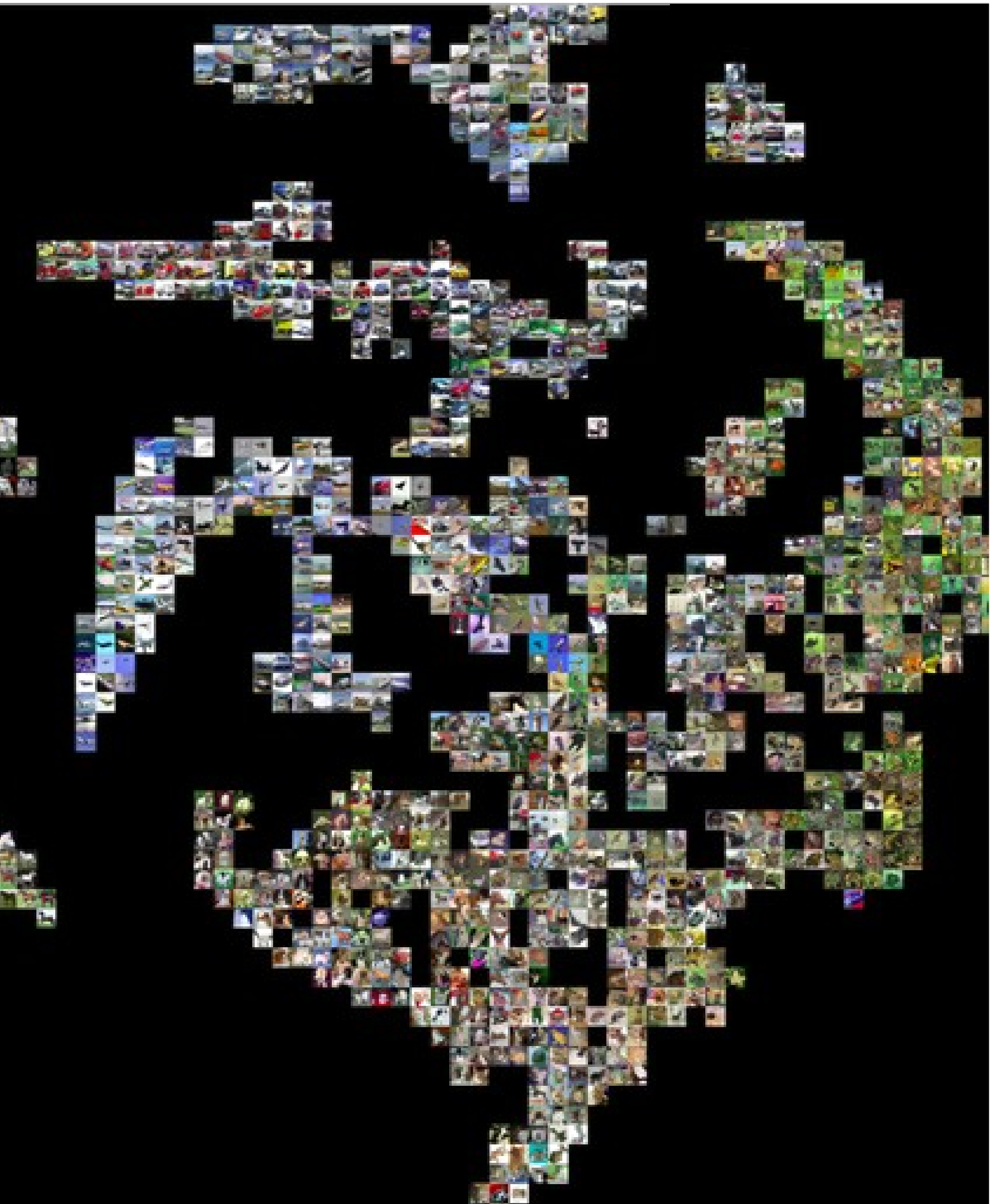


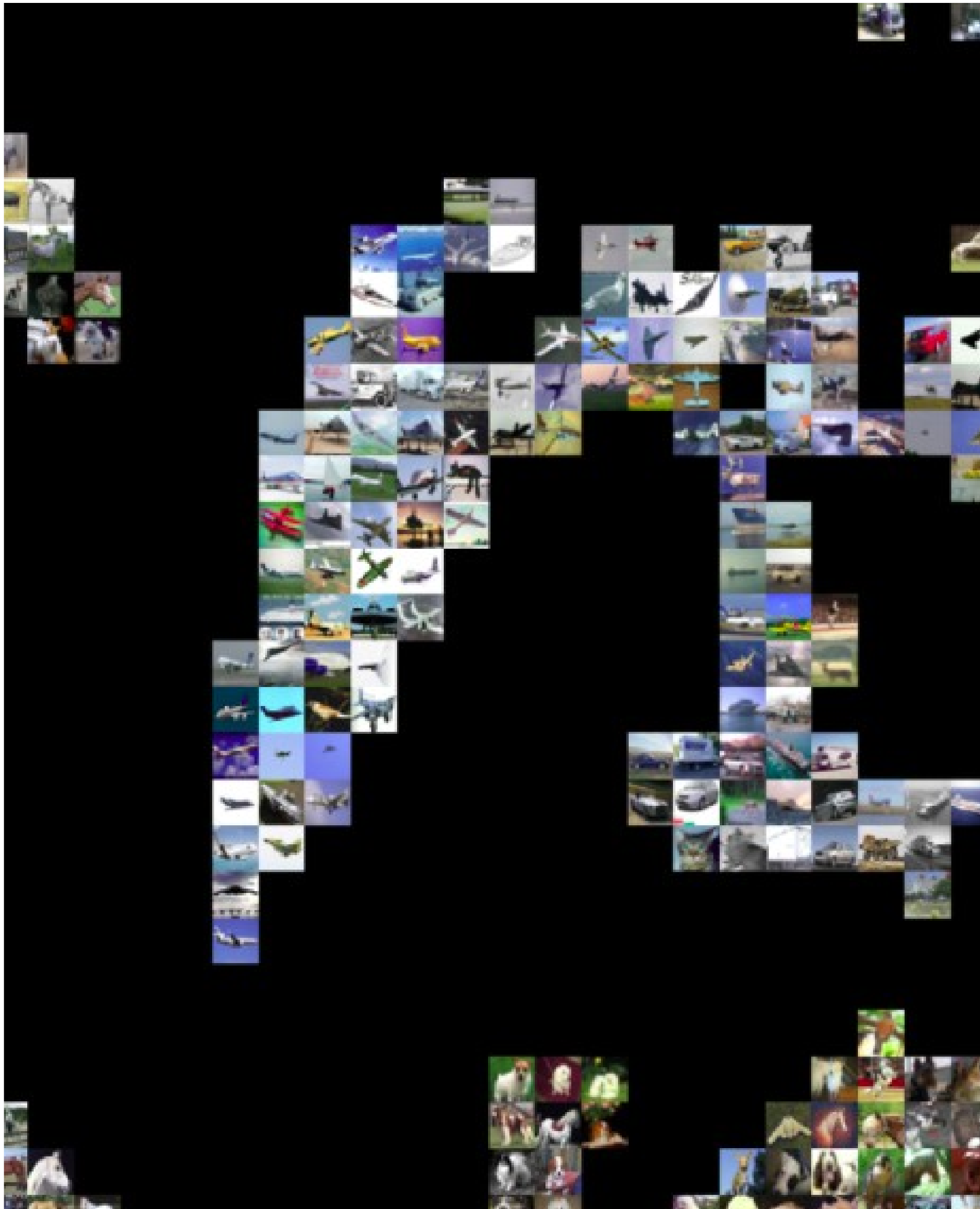
Read More:
Original paper
Interactive demo

T-SNE + deep encoder

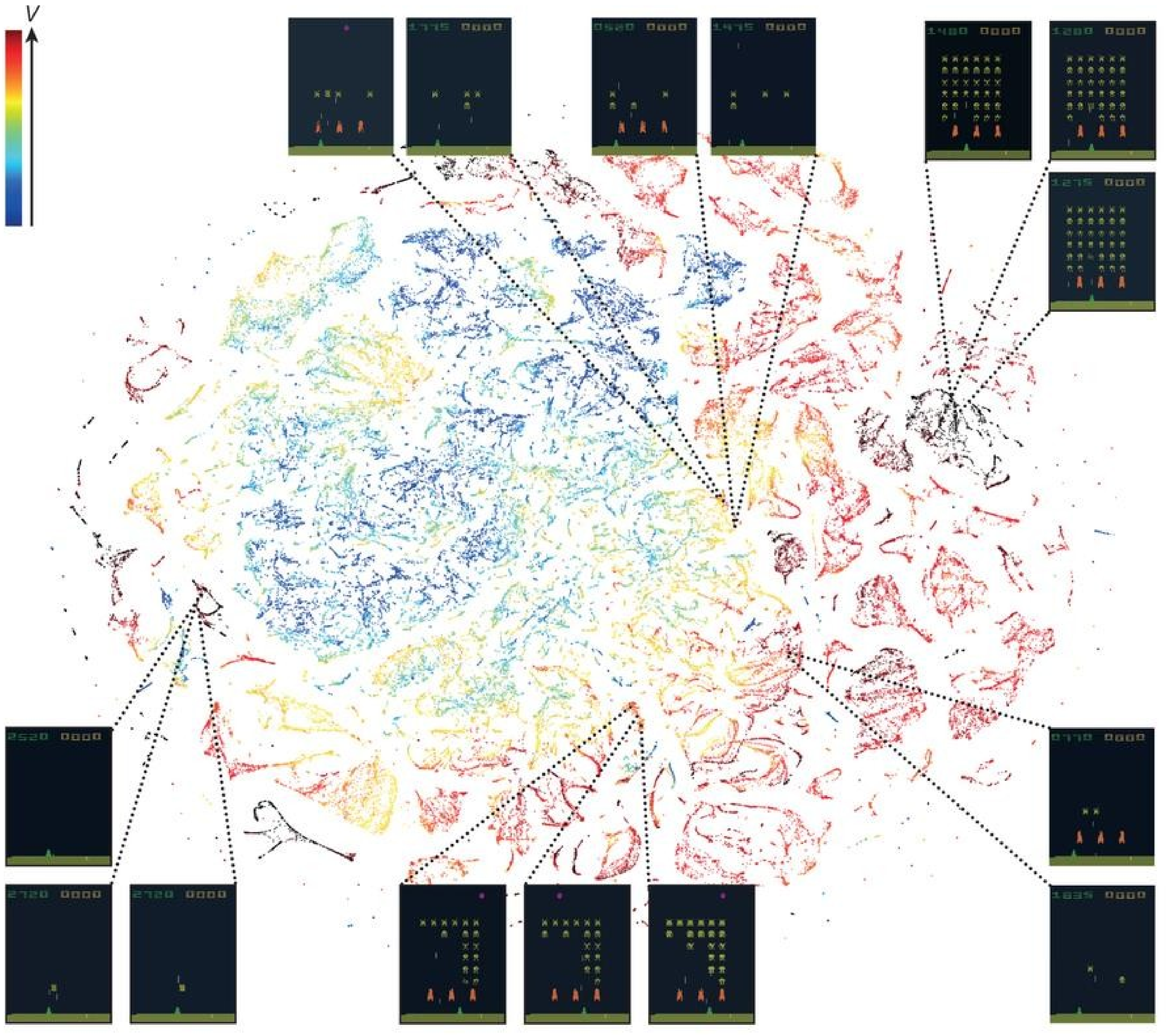


T-SNE + deep encoder (CIFAR10)





T-SNE + deep encoder (atari DQN)



Thank you

[question time!]

note 2self: if you reach this slide early, cover

- *https://arxiv.org/abs/2002.00937*
- *https://arxiv.org/abs/1812.02766*
- *https://arxiv.org/abs/2004.00345*
- *https://arxiv.org/abs/2103.09274*