NPFL099 Statistical Dialogue Systems
4. Training Neural Nets

http://ufal.cz/npfl099

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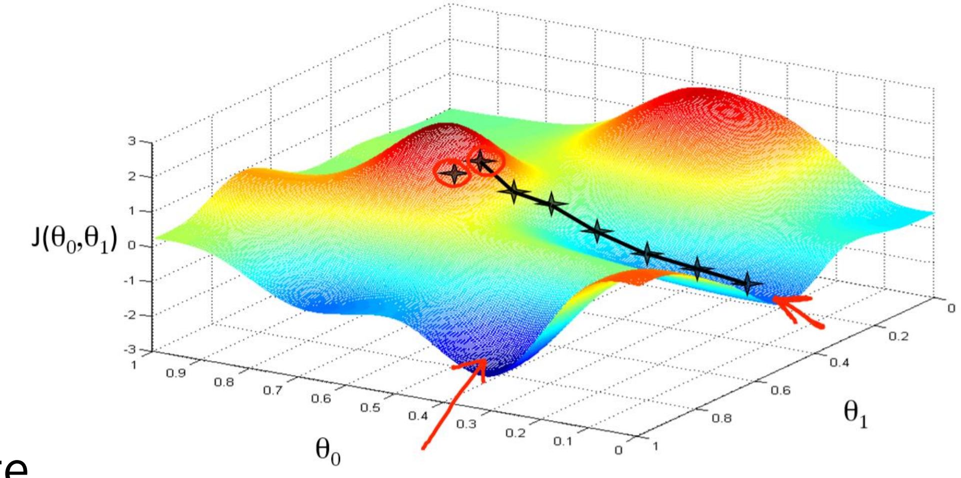
Recap: Neural Nets

- **complex functions, composed of simple functions** (=layers)
  - linear, ReLU, tanh, sigmoid, softmax
- **fully differentiable**
- different arrangements:
  - feed forward / multi-layer perceptron
  - CNNs
  - RNNs (LSTM/GRU)
  - attention
  - Transformer
- input: binary, float, embedding
- tasks/problems: classification, regression, structured (sequences/ranking)

Supervised Training: Gradient Descent

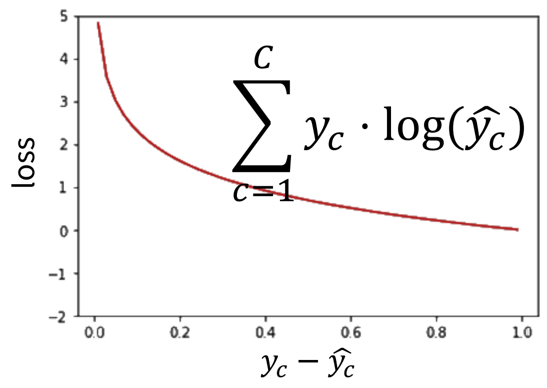
- supervised training– **gradient descent** methods
  - minimizing a **cost/loss function**
    (notion of error – given system output, how far off are we?)
  - calculus: derivative = steepness/slope
  - follow the slope to find the minimum – derivative gives the direction
  - **learning rate** = how fast we go (needs to be tuned)
- gradient typically computed (=averaged) over **mini-batches**
  - random bunches of a few training instances
  - not as erratic as using just 1 instance,
    not as slow as computing over whole data
  - **stochastic gradient descent**
  - batches may be accumulated to fit into memory
    - e.g. your GPU only fits one instance
      → compute forward pass multiple times, then do 1 update

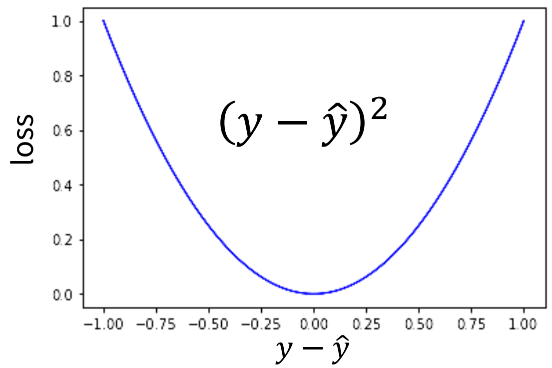


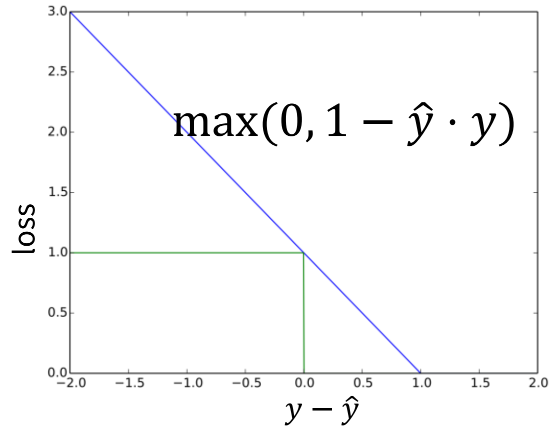
https://hackernoon.com/gradient-descent-aynk-7cbe95a778da

Cost/Loss Functions

- differ based on what we're trying to predict
- **logistic / log loss** ("cross entropy")
  - for classification / softmax – including **word prediction**
    - classes from the whole dictionary
  - pretty stupid for sequences, but works
    - sequence shifted by 1 ⇒ everything wrong
- **squared error loss** – for regression
  - forcing the predicted float value to be close to actual one
- **hinge loss** – for binary classification (SVMs), ranking
  - forcing the correct sign
- many others, variants







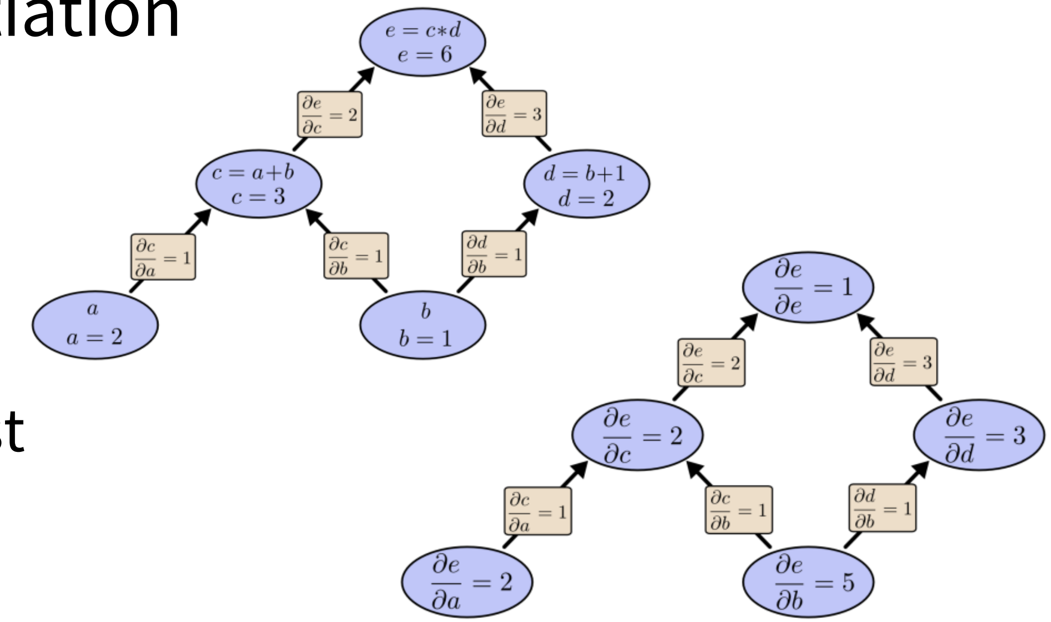
https://machinelearningmastery.com/loss-and-loss-functions-for-training-deep-learning-neural-networks/
https://medium.com/@risingdeveloper/visualization-of-some-loss-functions-for-deep-learning-with-tensorflow-9f60be9d09f9
https://en.wikipedia.org/wiki/Hinge_loss

Backpropagation

https://www.mathsisfun.com/calculus/derivatives-rules.html

Rules	Function	Derivative
Multiplication by constant	cf	cf′
Power Rule	x^n	nx^{n-1}
Sum Rule	f + g	f′ + g′
Difference Rule	f - g	f′ − g′
Product Rule	fg	f g′ + f′ g
Quotient Rule	f/g	$\frac{f' g - g' f}{g^2}$
Reciprocal Rule	1/f	$-f'/f^2$
Chain Rule (as "Composition of Functions")	f º g	(f′ º g) × g′

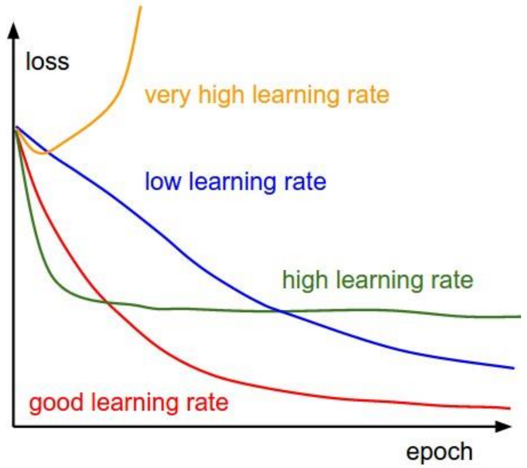
- network ~ computational graph
  - reflects function/layer composition
- composed function derivatives – simple rules
  - basically summing over different paths
  - factoring ~ merging paths at every node
- **backpropagation** = reverse-mode differentiation
  - going back from output to input
  - ~ how every node affects the output
  - output = cost function
  - → derivatives of all parameters w. r. t. cost
  - one pass through the network only → easy & fast
  - NN frameworks do this automatically



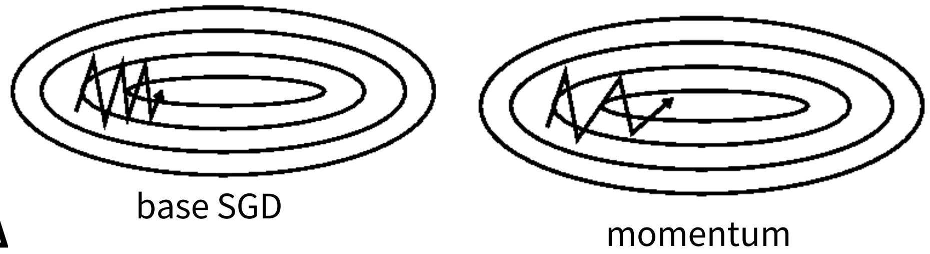
http://colah.github.io/posts/2015-08-Backprop/

Learning Rate (α) & Momentum

- α: **most important parameter** in (stochastic) gradient descent
- tricky to tune:
  - too high α = may not find optimum
  - too low α = may take forever
- **Learning rate decay**: start high, lower α gradually
  - make bigger steps (to speed learning)
  - slow down when you're almost there (to avoid overshooting)
  - linear, stepwise, exponential
  - **reduce-on-plateau** – check every now and then if we're still improving, reduce LR if not
- **Momentum**: moving average of gradients
  - make learning less erratic
  - $m = \beta \cdot m + (1 - \beta) \cdot \Delta$, update by m instead of Δ



http://cs231n.github.io/neural-networks-3/



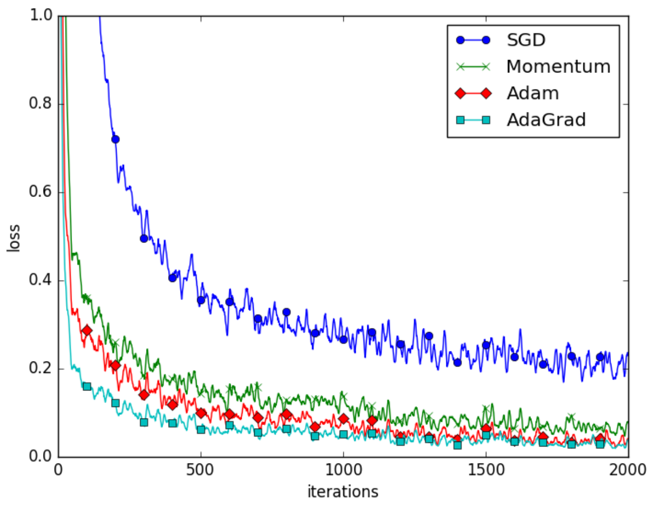
https://ruder.io/optimizing-gradient-descent/

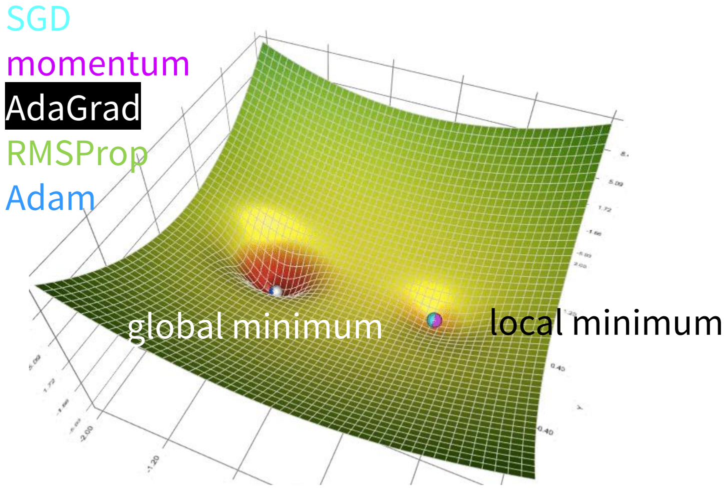
Optimizers

http://kaeken.hatenablog.com/entry/2016/11/10/203151

- Better LR management
  - change LR based on gradients
  - much less sensitive to user setting
- **AdaGrad** – all history
  - remember sum of total gradients squared: $\sum_t \Delta_t^2$
  - divide LR by $\sqrt{\sum \Delta_t^2}$
  - variants: **Adadelta**, **RMSProp** –slower LR drop
- **Adam** – per-parameter momentum (Kingma & Ba, 2015) https://arxiv.org/abs/1412.6980
  - moving averages for Δ & Δ^2:

    $m = \beta_1 \cdot m + (1-\beta_1)\Delta, v = \beta_2 \cdot v + (1-\beta_2)\Delta^2$
  - use m instead of Δ, divide LR by $\sqrt{v}$
  - used as default in most applications
  - variant: **AdamW** – decoupled LR drop (Loshchilov & Hutter, 2019) https://arxiv.org/abs/1711.05101



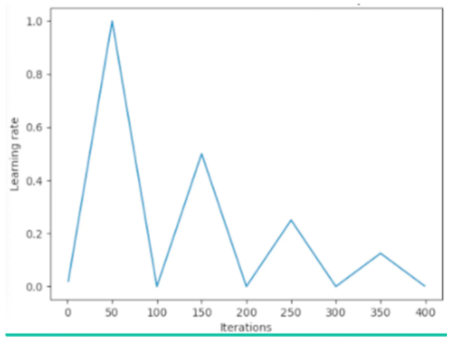


https://ruder.io/optimizing-gradient-descent/

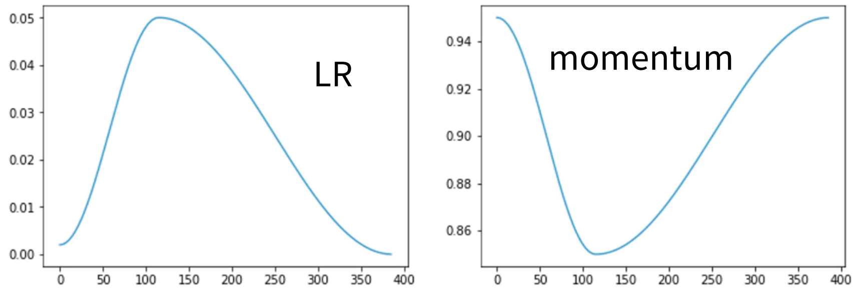
https://towardsdatascience.com/a-visual-explanation-of-gradient-descent-methods-momentum-adagrad-rmsprop-adam-f898b102325c

Schedulers

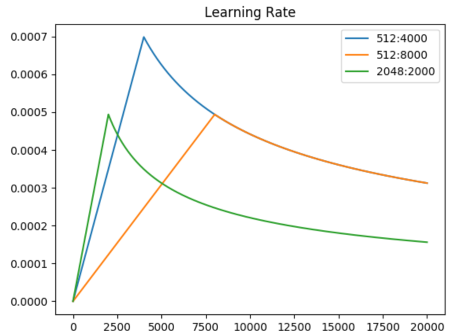
- more fiddling with LR – **warm-ups**
  - start learning slowly, then increase LR, then reduce again
  - may be repeated (warm restarts), with lowered maximum LR
    - allow to diverge slightly – work around local minima
- multiple options:
  - cyclical – linear, cosine annealing
  - **one cycle** – same, just don’
  - **Noam scheduler** – linear warm-up, decay by $\sqrt{\text{steps}}$
- combine with base SGD or Adam/Adadelta etc.
  - momentum updated inversely to LR
  - may have less effect with optimizers
    - trade-off: speed vs. sensitivity to parameter settings



cyclical scheduler (warm restarts)



one cycle with cosine annealing

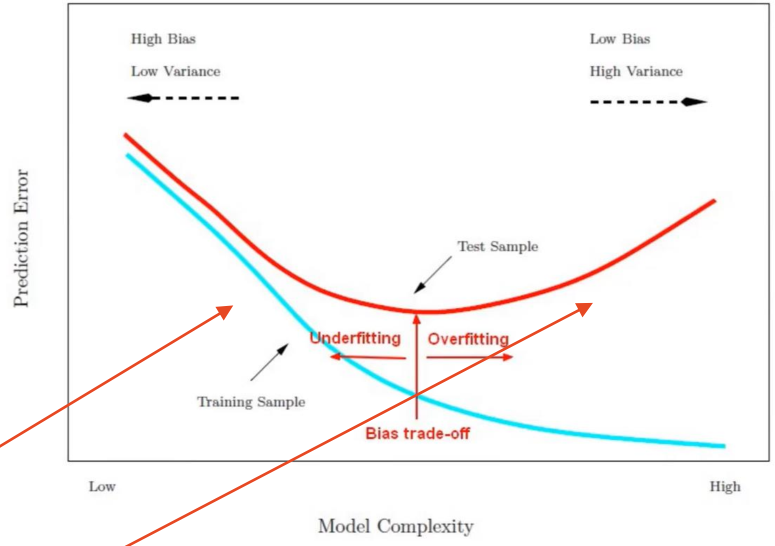


Noam scheduler with different parameters

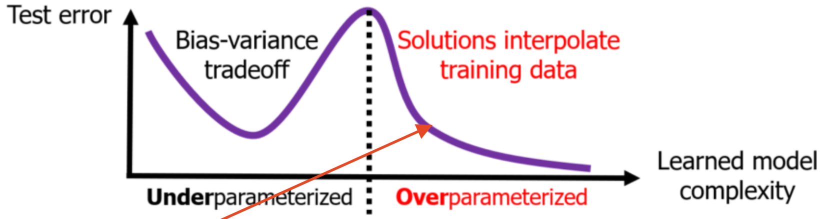
https://spell.ml/blog/lr-schedulers-and-adaptive-optimizers-YHmwMhAAACYADm6F
https://nn.labml.ai/optimizers/noam.html

When to stop training

https://www.andreaperlato.com/theorypost/bias-variance-trade-off/



- generally, when cost stops improving
  - despite all the LR fiddling
- problem: **overfitting**
  - cost is low on training set, high on validation set
  - network essentially memorized the training set
  - → check on validation set after each epoch (pass through data)
  - stop when cost goes up on validation set
  - regularization (see →) helps delay overfitting
- **bias-variance** trade-off
  - smaller models may underfit (high bias, low variance = not flexible enough)
  - larger models likely to overfit (too flexible, memorize data)
  - XXL models: overfit soo much they actually interpolate data → good (🤔?)

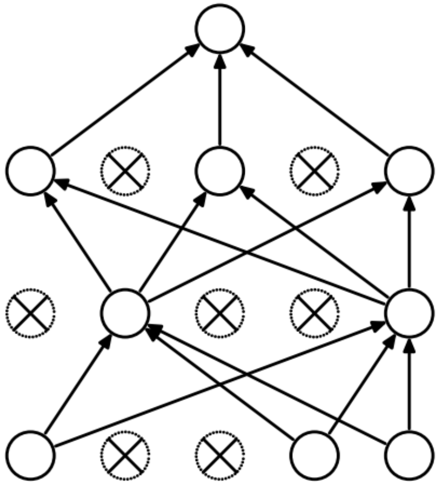


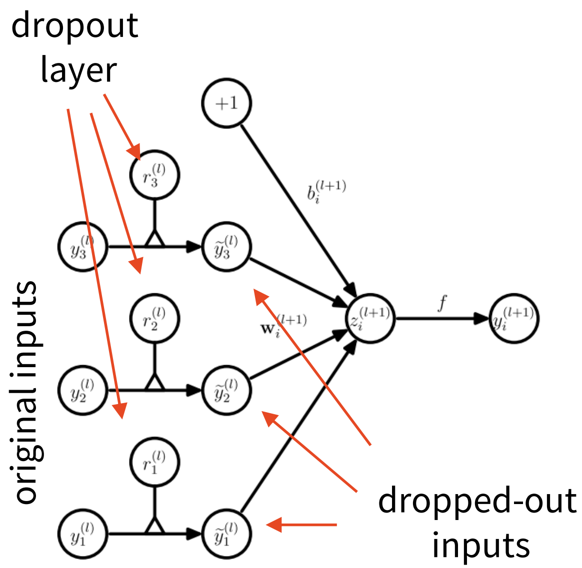
(Dar et al., 2021) https://arxiv.org/abs/2109.02355

Regularization: Dropout

(Srivastava et al., 2014)
http://jmlr.org/papers/v15/srivastava14a.html

- regularization: preventing overfitting
  - making it harder for the network to learn, adding noise
- **Dropout** – simple regularization technique
  - more effective than e.g. weight decay (L2)
  - **zero out some neurons/connections** in the network at random
  - technically: multiply by dropout layer
    - 0/1 with some probability (typically 0.5–0.8)
  - at training time only – full network for prediction
  - weights scaled down after training
    - they end up larger than normal because there's fewer nodes
    - done by libraries automatically
  - may need larger networks to compensate



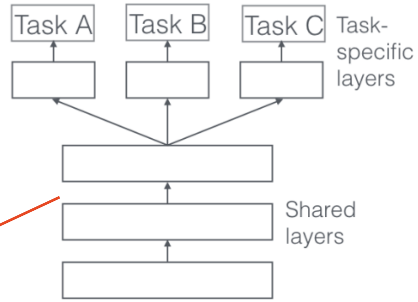


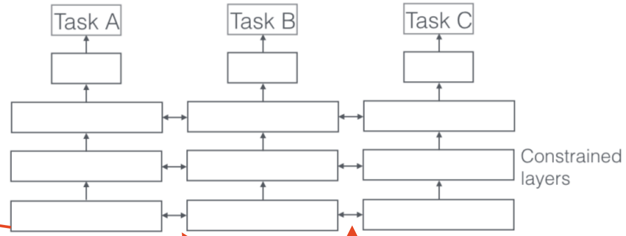
(b) Dropout network

Regularization: Multi-task Learning

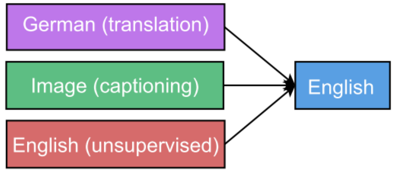
(Ruder, 2017) http://arxiv.org/abs/1706.05098
(Fan et al., 2017) http://arxiv.org/abs/1706.04326
(Luong et al., 2016) http://arxiv.org/abs/1511.06114

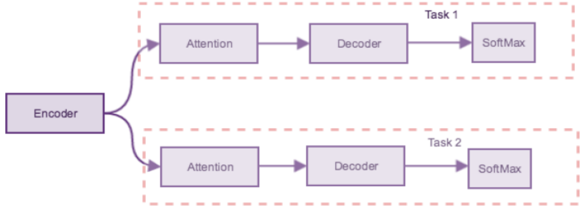
- achieve better generalization by **learning more things at once**
  - a form of regularization
  - implicit data augmentation
  - biasing/focusing the model
    - e.g. by explicitly training for an important subtask
- parts of network shared, parts task-specific
  - hard sharing = parameters truly shared (most common)
  - soft sharing = regularization by parameter distance
  - different approaches w. r. t. what to share
- training – alternating between tasks
  - so the network doesn't "forget"

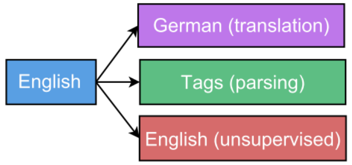


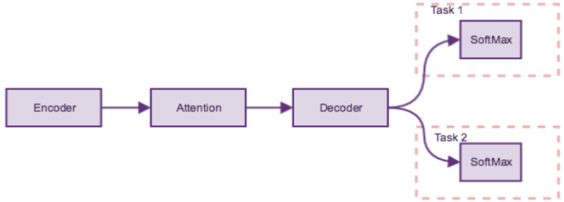


e.g. L2 on distance









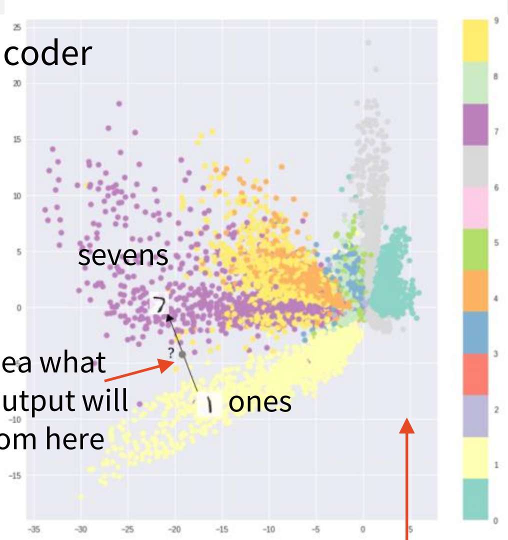
Self-supervised training

- train supervised, but **don't provide labels**
  - use naturally occurring labels
  - create labels automatically somehow
    - corrupt data & learn to fix them
    - learn from rule-based annotation (not ideal!)
  - use specific tasks that don't require manually created labels
- good to train on huge amounts of data
  - language modelling
    - next-word prediction
    - MLM – masked word prediction (~like word2vec)
  - **autoencoding**: predict your own input (see →)
- good to **pretrain** the network for a final task
- unsupervised, but with supervised approaches

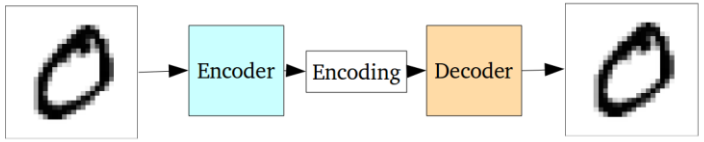
https://ai.stackexchange.com/questions/10623/what-is-self-supervised-learning-in-machine-learning

Autoencoders

MNIST digits autoencoder latent space



- Using NNs as **generative models**
  - more than just classification – modelling the whole distribution
    - (of e.g. possible texts, images)
  - generate new instances that look similar to training data
- **Autoencoder**: input → encoding → input
  - encoding ~ "embedding" in latent space (i.e. some vector)
  - trained by reconstruction loss
  - problem: can't easily get valid embeddings for generating new outputs
    - parts of embedding space might be unused – will generate weird stuff
    - no easy interpretation of embeddings – no idea what the model will generate

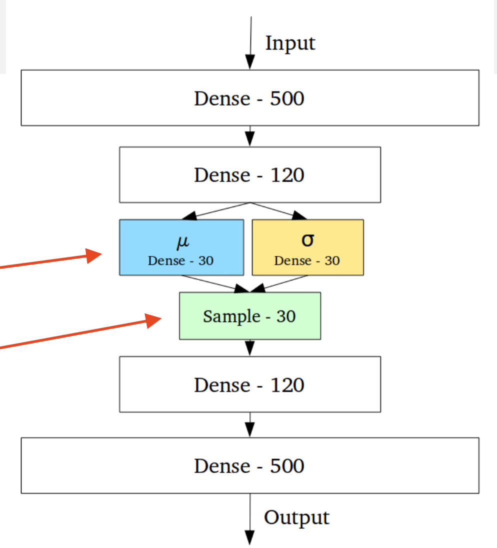


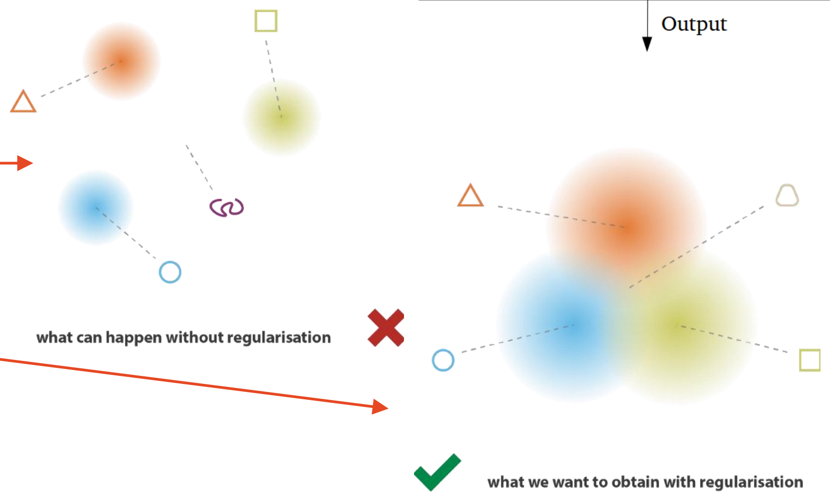
- extension – **denoising autoencoder**:
  - add noise to inputs, train to generate clean outputs
  - use in multi-task learning, representations for use in downstream tasks

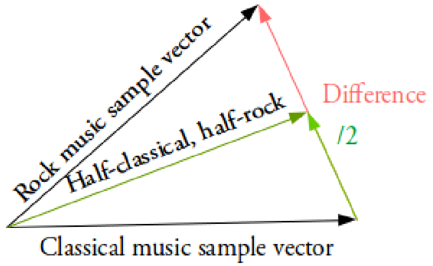
https://towardsdatascience.com/intuitively-understanding-variational-autoencoders-1bfe67eb5daf

Variational Autoencoders

- Making the encoding latent space more useful
  - using **Gaussians** – continuous space by design
  - encoding input into vectors of means μ & std. deviations σ
  - sampling encodings from $N(\mu, \sigma)$ for generation
    - samples vary a bit even for the same input
    - decoder learns to be more robust
  - model can degenerate into normal AE ($\sigma \rightarrow 0$)
    - we need to encourage some σ, smoothness, overlap ($\mu \sim 0$)
    - add **2nd loss: KL divergence** from $N(0,1)$
    - VAE learns a trade-off between
      using unit Gaussians & reconstructing inputs
- Problem: still not too much control of the embeddings
  - we can only guess what kind of output the model will generate







https://towardsdatascience.com/intuitively-understanding-variational-autoencoders-1bfe67eb5daf
https://towardsdatascience.com/understanding-variational-autoencoders-vaes-f70510919f73
http://kvfrans.com/variational-autoencoders-explained/

VAE details

- VAE objective:
  - “AE” **reconstruction loss** (maximizing $p(x|z)$ in the decoder), MLE as per usual
  - “V” **latent loss** (KL-divergence from ideal $p(z) \sim \mathcal{N}(0,1)$ in the encoder)

$$\mathcal{L} = -\mathbb{E}_q[\log p(x|z)] + KL[q(z|x)||p(z)]$$

- This is equivalent to maximizing true $\log p(x)$ with some error
  - i.e. maximizing **evidence lower bound** (ELBO) / variational lower bound:

$$\mathbb{E}_q[\log p(x|z)] - KL[q(z|x)||p(z)] = \underbrace{\underbrace{\log p(x)}_{\text{“evidence” (i.e. data)}} - KL[q(z|x)||p(z|x)]}_{\text{ELBO}}$$

error incurred by using q instead of true distribution p

Normal noise

- Sidestepping sampling – **reparameterization trick**
  - $z \sim \mu + \sigma \cdot \mathcal{N}(0,1)$, then differentiate w. r. t. μ and σ
    - differentiating w. r. t. μ & σ still works, no hard sampling on that path

https://wiseodd.github.io/techblog/2016/12/10/variational-autoencoder/

Discrete VAE: Gumbel-Softmax

(Jang et al., 2017)
https://arxiv.org/abs/1611.01144

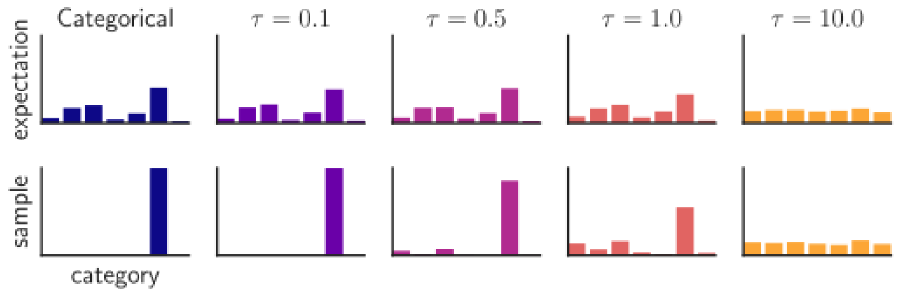
- “reparameterization trick for discrete distributions”
  - same idea, just with a **discrete/categorial distribution**
  - this makes the latent space better interpretable
- **Gumbel-max trick**:
  - categorial distribution π with probabilities π_i
  - sampling from π: $z = \text{onehot}(\arg\max_i(\log \pi_i + g_i))$
- Swap argmax for softmax with temperature τ
  - differs from π if $\tau > 0$, but may be close
  - approx. sample of the true distribution
  - fully differentiable
  - g_i bypassed in differentiation, same as $\mathcal{N}(0,1)$ in Gaussian sampling

Gumbel noise:
$g_i = -\log(-\log(\text{Uniform}(0,1)))$

$$y_i = \frac{\exp\left(\frac{\log(\pi_i) + g_i}{\tau}\right)}{\sum_{j=1}^{N} \exp\left(\frac{\log(\pi_j) + g_j}{\tau}\right)}$$

$\tau \to 0$: more like one-hot

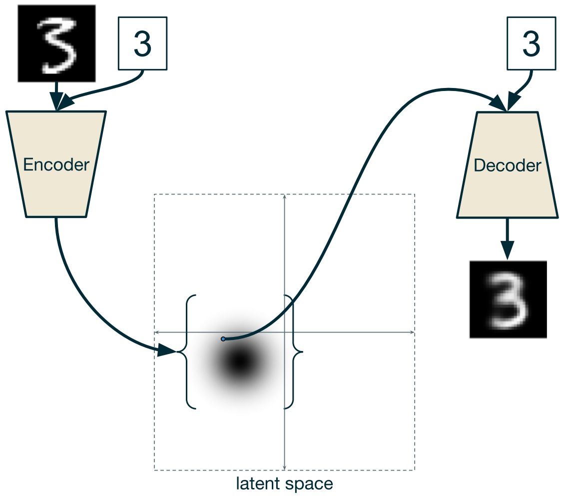
$\tau \to \infty$: more like uniform



https://anotherdatum.com/gumbel-gan.html

Conditional Variational Autoencoders

- Direct control over types of things to generate
- Additional conditioning on a given label/type/class c
  - c can be anything (discrete, continuous…)
    - image class: MNIST digit
    - sentiment
    - “is this a good reply?”
    - coherence level
  - just concatenate to input
  - given to both encoder & decoder at training time
- Generation – need to provide c
  - CVAE will generate a sample of type c
  - Latent space is partitioned by c
    - same latent input with different c will give different results



Pretraining & Finetuning

- 2-step training:
  1. **Pretrain** a model on a huge dataset (**self-supervised**, language-based tasks)
  2. **Fine-tune** for your own task on your smaller data (**supervised**)
- ~pretrained embeddings, many variants
  - mostly Transformer architecture
  - pretraining tasks vary and make a difference
- **BERT** + variants: multilingual, **RoBERTa** (optimized)
- **GPT**(**-2**/**-3**): Transformer decoder only, next-word prediction
- **BART**: BERT as denoising autoencoder (more below)
- **T5**: generalization, many variants
- a lot of pretrained models released plug-and-play
  - you only need to finetune (and sometimes, not even that)

(Devlin et al., 2019) https://www.aclweb.org/anthology/N19-1423 https://github.com/google-research/bert

(Rogers et al., 2020) http://arxiv.org/abs/2002.12327

(Liu et al., 2019) http://arxiv.org/abs/1907.11692

(Radford et al., 2019) https://openai.com/blog/better-language-models/

(Brown et al., 2020) http://arxiv.org/abs/2005.14165

(Lewis et al., 2019) http://arxiv.org/abs/1910.13461

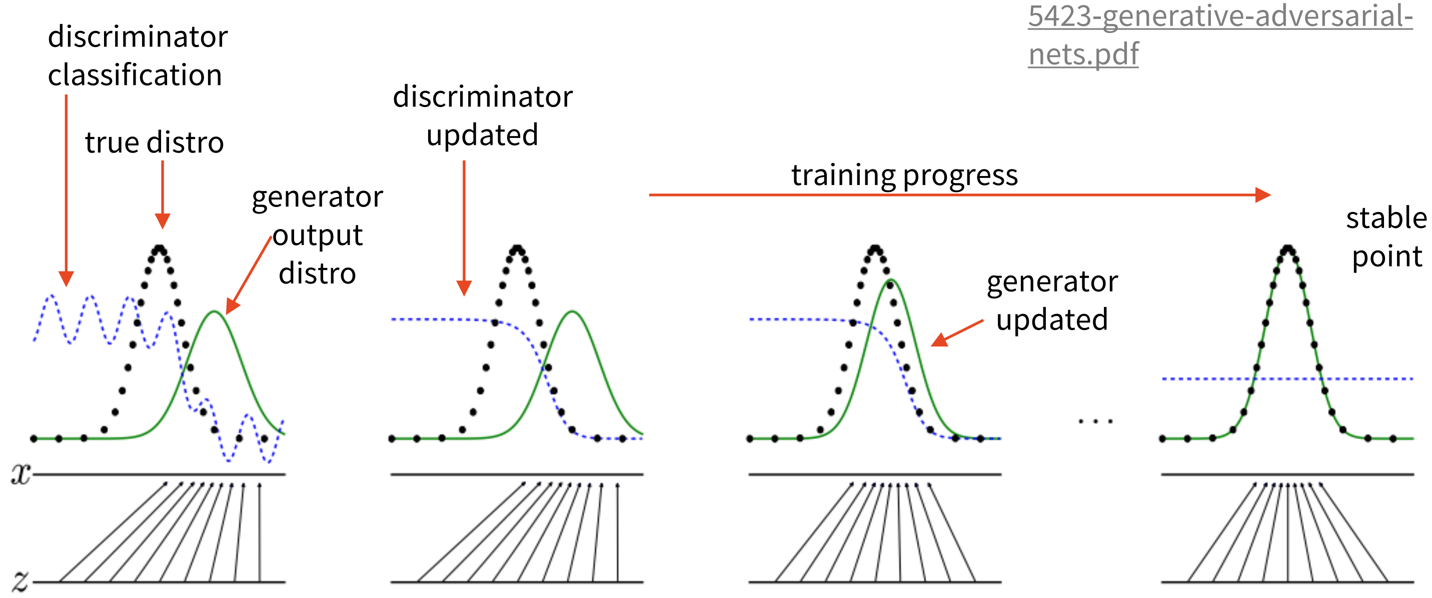
(Raffel et al., 2019) http://arxiv.org/abs/1910.10683

https://github.com/huggingface/transformers

Generative Adversarial Nets

- Training generative models to generate **believable** outputs
  - to do so, they necessarily get a better grasp on the distribution
- Getting loss from a 2nd model:
  - **discriminator** $\boldsymbol{D}$ – "adversary" classifying real vs. generated samples
  - **generator** $\boldsymbol{G}$ – trained to fool the discriminator
    - the best chance to fool the discriminator is to generate likely outputs
- Training iteratively (EM style)
  - generate some outputs
  - classify + update discriminator
  - update generator based on classification
  - this will reach a stable point

(Goodfellow et al, 2014)
http://papers.nips.cc/paper/5423-generative-adversarial-nets.pdf

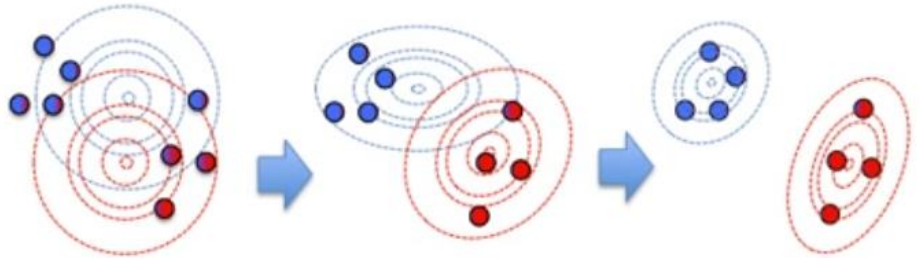


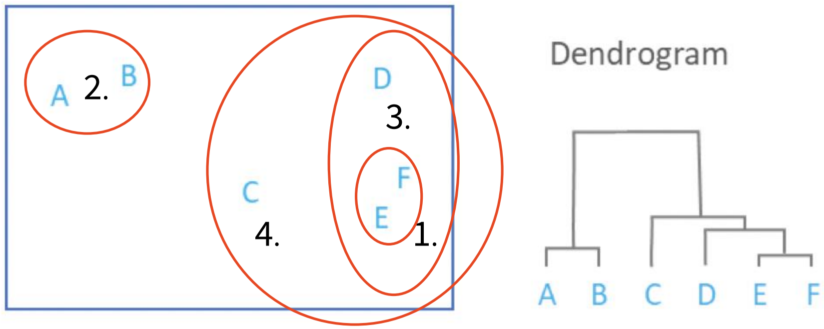
Clustering

https://en.wikipedia.org/wiki/K-means_clustering
https://www.displayr.com/what-is-hierarchical-clustering/
https://towardsdatascience.com/gaussian-mixture-models-d13a5e915c8e

- Unsupervised, finding similarities in data
- basic algorithms
  - **k-means**: assign into k clusters randomly, iterate:
    - compute means (centroids)
    - reassign to nearest centroid
  - **Gaussian mixture**: similar, but soft & variance
    - clusters = multivariate Gaussian distributions
    - estimating probabilities of belonging to each cluster
    - cluster mean/variance based on data weighted by probabilities
  - **hierarchical** (bottom up):
    start with one cluster per instance, iterate:
    - merge 2 closest clusters
    - end when you have k clusters / distance is too big
  - hierarchical top-down (reversed ↵)
- distance metrics & features decide what ends up together

https://www.youtube.com/watch?v=9YA2t78Ha68

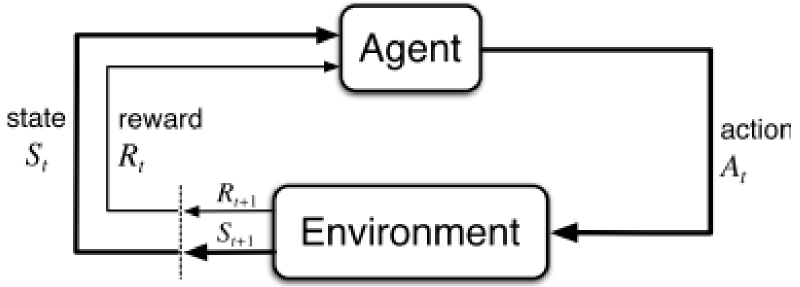




Reinforcement Learning

- Learning from **weaker supervision**
  - only get feedback once in a while, not for every output
  - good for globally optimizing sequence generation
    - you know if the whole sequence is good
    - you don't know if step X is good
  - sequence = e.g. sentence, dialogue
- Framing the problem as **states & actions & rewards**
  - "robot moving in space", but works for dialogue too
  - state = generation so far (sentence, dialogue state)
  - action = one generation output (word, system dialogue act)
  - defining rewards might be an issue
- Training: **maximizing long-term reward**
  - via state/action values (Q function)
  - directly – optimizing policy

your model



(Sutton & Barto, 2018)

some definition of rewards

Summary

- Supervised training
  - cost function
  - stochastic **gradient descent** – minibatches
  - backpropagation
  - **learning rate** tricks – optimizers (Adam), schedulers
  - regularization: dropout, multi-task training
- Self-supervised learning (~kinda unsupervised)
  - autoencoders, denoising, variational autoencoders
  - (masked) language models
- Unsupervised
  - generative adversarial nets
  - clustering
- Reinforcement learning (more to come later)

Thanks

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Troja N230/231/233 (by agreement)

Labs in 10 mins
Next Monday 15:40

Get the slides here:

http://ufal.cz/npfl099

References/Further:

Goodfellow et al. (2016): Deep Learning, MIT Press (http://www.deeplearningbook.org)
Kim et al. (2018): Tutorial on Deep Latent Variable Models of Natural Language (http://arxiv.org/abs/1812.06834)
Milan Straka's Deep Learning slides: http://ufal.mff.cuni.cz/courses/npfl114/1819-summer

Neural nets tutorials:

- https://codelabs.developers.google.com/codelabs/cloud-tensorflow-mnist/#0
- https://minitorch.github.io/index.html
- https://objax.readthedocs.io/en/latest/