Advanced Machine Learning
Lecture 20

Wrapping Up

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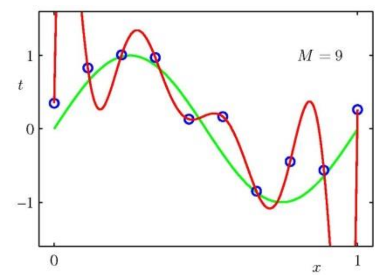
Announcements

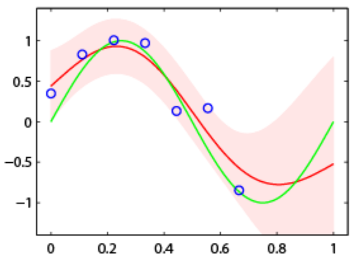
- Last lecture next Thursday: Repetition
  - Summary of all topics in the lecture
  - "Big picture" and current research directions
  - Opportunity to ask questions
  - *Please use this opportunity and prepare questions!*
- Exam format
  - Exams will be oral
  - Duration: 30 minutes
  - I will give you 4 questions and expect you to answer 3 of them.
    - Each such question will cover material from ~1-2 lecture slots

This Lecture: *Advanced Machine Learning*

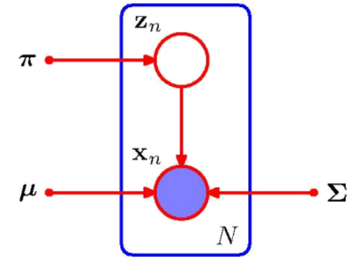
$$f : \mathcal{X} \to \mathbb{R}$$

- Regression Approaches
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Gaussian Processes

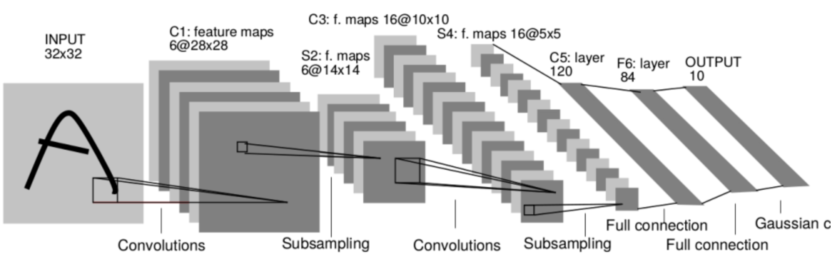




- Learning with Latent Variables
  - Prob. Distributions & Approx. Inference
  - Mixture Models
  - EM and Generalizations



- Deep Learning
  - Linear Discriminants
  - Neural Networks
  - Backpropagation & Optimization
  - CNNs, RNNs, RBMs, etc.



Topics of This Lecture

- Recap: Restricted Boltzmann Machines
  - Energy based Models
  - RBMs
  - Deep Belief Networks
- Initialization Revisited
  - Analysis
  - Glorot Initialization
  - Extension to ReLU
- Outlook
  - Reinforcement Learning

Recap: Energy Based Models (EBM)

- **Energy Based Probabilistic Models**
  - Define the joint probability over a set of variables $\mathbf{x}$ through an energy function

$$p(\mathbf{x}) = \frac{1}{Z} e^{-E(\mathbf{x})}$$

where the normalization factor Z is called the partition function

$$Z = \sum_{\mathbf{x}} e^{-E(\mathbf{x})}$$

  - An EBM can be learned by performing (stochastic) gradient descent on the negative log-likelihood of the training data

$$\mathcal{L}(\theta, \mathcal{D}) = \frac{1}{N} \sum_{x_n \in \mathcal{D}} \log p(x_n)$$

using the stochastic gradient $-\frac{\partial \log p(x_n)}{\partial \theta}$

Recap: EBMs with Hidden Units

- Expressing the gradient
  - Free energy for a model with hidden variables $\mathbf{h}$

$$\mathcal{F}(\mathbf{x}) = -\log \sum_{\mathbf{h}} e^{-E(\mathbf{x},\mathbf{h})}$$

  - Free energy formulation of the joint probability

$$p(\mathbf{x}) = \frac{e^{-\mathcal{F}(\mathbf{x})}}{Z} \qquad \text{with} \qquad Z = \sum_{\mathbf{x}} e^{-\mathcal{F}(\mathbf{x})}.$$

  - The negative log-likelihood gradient then takes the following form, which is difficult to determine analytically

$$-\frac{\partial \log p(\mathbf{x})}{\partial \theta} = \underbrace{\frac{\partial \mathcal{F}(\mathbf{x})}{\partial \theta}}_{\text{Positive phase}} - \underbrace{\sum_{\tilde{\mathbf{x}}} p(\tilde{\mathbf{x}}) \frac{\partial \mathcal{F}(\tilde{\mathbf{x}})}{\partial \theta}}_{\text{Negative phase}}.$$

Positive phase

Negative phase

Recap: Steps Towards a Solution...

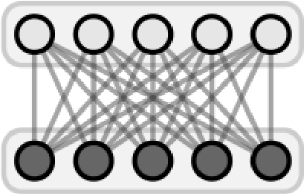
- **Monte Carlo approximation**
  - Estimate the expectation using a fixed number of model samples for the negative phase gradient ("negative particles")

$$-\frac{\partial \log p(\mathbf{x})}{\partial \theta} \approx \underbrace{\frac{\partial \mathcal{F}(\mathbf{x})}{\partial \theta}}_{\text{free energy at current point}} - \underbrace{\frac{1}{|\mathcal{N}|} \sum_{\tilde{\mathbf{x}} \in \mathcal{N}} \frac{\partial \mathcal{F}(\tilde{\mathbf{x}})}{\partial \theta}}_{\text{avg. free energy for all other points}}.$$

  - With this, we almost have a practical stochastic algorithm for learning an EBM.
  - We just need to define how to extract the negative particles $\mathcal{N}$.
    - Many sampling approaches can be used here.
    - MCMC methods are especially well-suited.

And this is where all parts of the lecture finally come together...

Recap: Restricted Boltzmann Machines



- Properties
  - Energy Function of an RBM

$$E(\mathbf{v},\mathbf{h}) = -\sum_i b_i v_i - \sum_j c_j h_j - \sum_{i,j} w_{ij} v_i h_j$$

  - This translates to a free energy formula

$$\mathcal{F}(\mathbf{v}) = -\mathbf{b}^\top \mathbf{v} - \sum_i \log \sum_{h_i} e^{h_i(c_i + W_i \mathbf{v})}.$$

  - Factorization property

$$p(\mathbf{h}|\mathbf{v}) = \prod_i p(h_i|\mathbf{v})$$

$$p(\mathbf{v}|\mathbf{h}) = \prod_j p(v_j|\mathbf{h}).$$

  - RBMs can be seen as a product of experts specializing on different areas and detecting *negative constraints*.

Recap: RBMs with Binary Units

- Binary units
  - Free energy

$$\mathcal{F}(\mathbf{v}) = -\mathbf{b}^\top \mathbf{v} - \sum_i \log\left(1 + e^{(c_i + W_i \mathbf{v})}\right).$$

  - This results in the iterative update equations for the gradient log-likelihoods

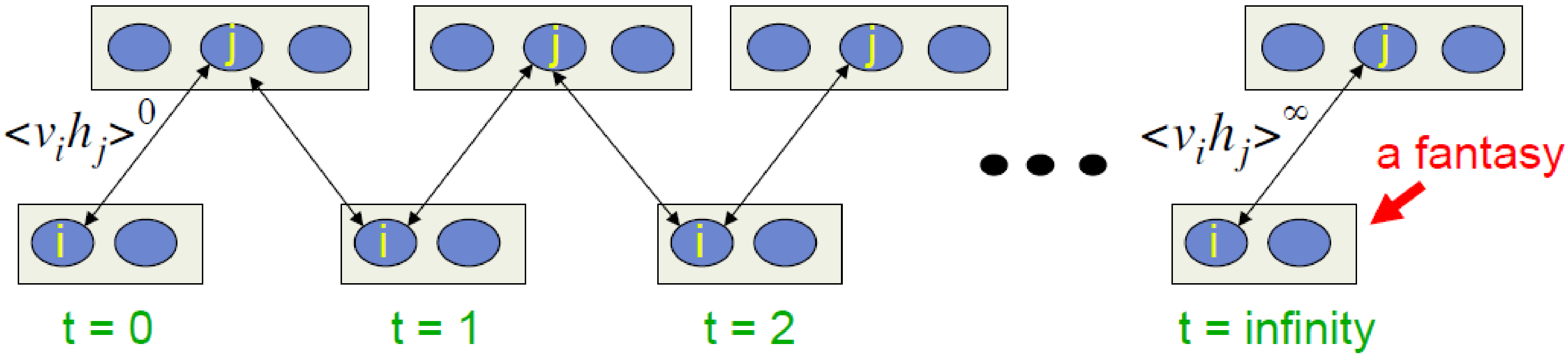
$$-\frac{\partial \log p(\mathbf{v})}{\partial W_{ij}} = \mathbb{E}_{\mathbf{v}}\left[p(h_i|\mathbf{v}) \cdot v_j\right] - v_j^{(t)} \cdot \sigma(W_i \cdot \mathbf{v}^{(t)} + c_i)$$

$$-\frac{\partial \log p(\mathbf{v})}{\partial c_i} = \mathbb{E}_{\mathbf{v}}[p(h_i|\mathbf{v})] - sigm(W_i \cdot \mathbf{v}^{(t)})$$

$$-\frac{\partial \log p(\mathbf{v})}{\partial b_j} = \mathbb{E}_{\mathbf{v}}[p(v_j|\mathbf{h})] - \mathbf{v}_j^{(t)}$$

Recap: RBM Learning (Slow)

- Iterative approach

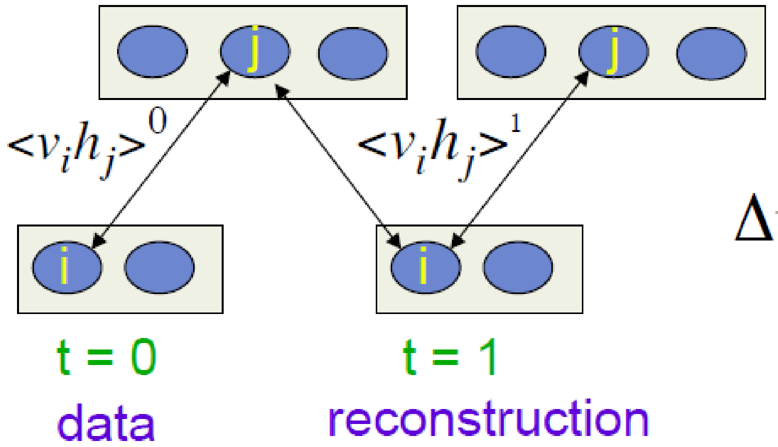


  - Start with a training vector on the visible units. Then alternate between updating all the hidden units in parallel and updating all the visible units in parallel.
  - This implements a Markov chain that we use to approximate the gradient

$$\frac{\partial \log p(\mathbf{v})}{\partial w_{ij}} = < v_i, h_j >^0 - < v_i, h_j >^\infty$$

  - Better method in practice: Contrastive Divergence

Recap: Contrastive Divergence (Fast)



$$\Delta w_{ij} = \varepsilon \, (<v_i h_j>^0 - <v_i h_j>^1)$$

- **A surprising shortcut**
  - **Start with a training vector on the visible units.**
  - **Update all the hidden units in parallel.**
  - **Update the all visible units in parallel to get a "reconstruction".**
  - **Update the hidden units again (no further iterations).**

  - **This does not follow the gradient of the log likelihood. But it works well [Hinton].**

Historical Perspective

- Training deep networks is difficult
  - Major difficulty: getting the gradient to propagate to the lower layers, so that the weights there can be learned
  - Initialization of the weights plays a major role
    - Weights too small ⇒ Signal shrinks from layer to layer
    - Weights too large ⇒ Signal grows until it is too massive

  ⇒ Vanishing and exploding gradient problems known from RNNs

- How can we arrive at a good initialization?

Deep Belief Networks (DBN)

- **DBN as stacked RBMs**
  - **RBM:** $p(\mathbf{v}, \mathbf{h}) = \dfrac{e^{-E(\mathbf{x},\mathbf{h})}}{Z}$

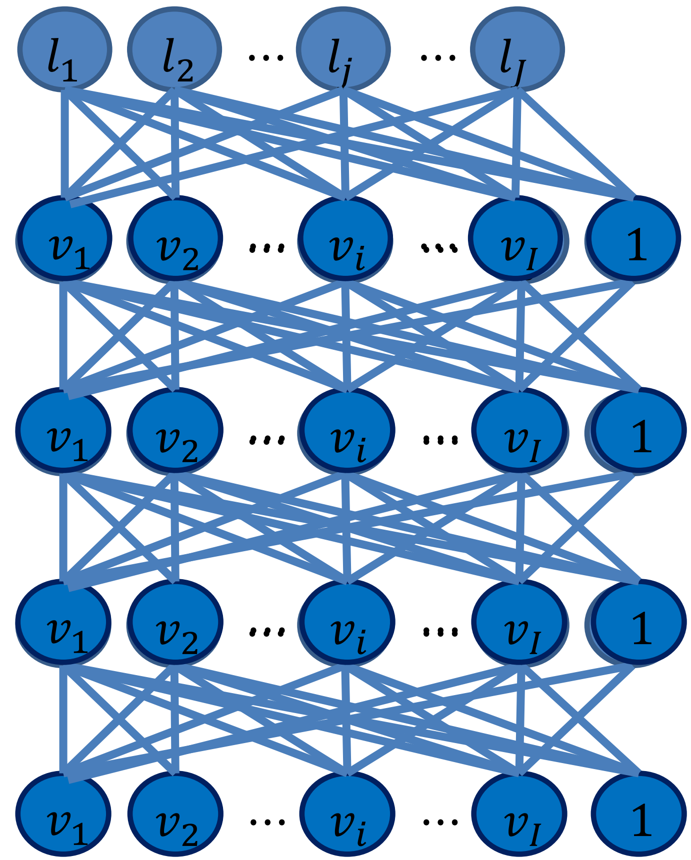
$$E(\mathbf{v}, \mathbf{h}) = -\mathbf{b}^\top \mathbf{v} - \mathbf{c}^\top \mathbf{h} - \mathbf{v}^\top W \mathbf{h}$$

$$p(\mathbf{h}|\mathbf{v}) = \prod_i p(h_i|\mathbf{v})$$

$$p(h_i = 1|\mathbf{v}) = \sigma(c_i + \mathbf{v}^\top W_i)$$

  - **Pre-train each layer from bottom up by considering each pair of layers as an RBM.**
  - **Jointly fine-tune all layers using back-propagation algorithm**

⇒ Layer-by-layer unsupervised training



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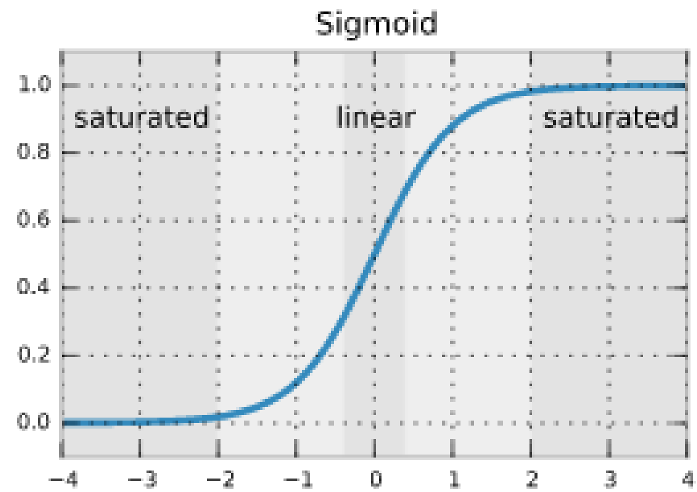
  - Extension to ReLU
- Outlook
  - Reinforcement Learning

Glorot Initialization

- Breakthrough results
  - In 2010, Xavier Glorot published an analysis of what went wrong in the initialization and derived a method for automatic initialization.
  - This new initialization massively improved results and made direct learning of deep networks possible overnight.
  - Let's look at his analysis in more detail...

X. Glorot, Y. Bengio, Understanding the Difficulty of Training Deep Feedforward Neural Networks, AISTATS 2010.

Effect of Sigmoid Nonlinearities



- Effects of sigmoid/tanh function
  - Linear behavior around 0
  - Saturation for large inputs
- If all parameters are too small
  - Variance of activations will drop in each layer
  - Sigmoids are approximately linear close to 0
  - Good for passing gradients through, but...
  - Gradual loss of the nonlinearity
  - ⇒ No benefit of having multiple layers
- If activations become larger and larger
  - They will saturate and gradient will become zero

Image source: http://deepdish.io/2015/02/24/network-initialization/

Analysis

- **Variance of neuron activations**
  - Suppose we have an input X with n components and a linear neuron with random weights W that spits out a number Y.
  - What is the variance of Y?

$$Y = W_1 X_1 + W_2 X_2 + \cdots + W_n X_n$$

  - If inputs and outputs have both mean 0, the variance is

$$\text{Var}(W_i X_i) = E[X_i]^2 \text{Var}(W_i) + E[W_i]^2 \text{Var}(X_i) + \text{Var}(W_i)\text{Var}(i_i)$$

$$= \text{Var}(W_i)\text{Var}(X_i)$$

  - If the X_i and W_i are all i.i.d, then

$$\text{Var}(Y) = \text{Var}(W_1 X_1 + W_2 X_2 + \cdots + W_n X_n) = n\text{Var}(W_i)\text{Var}(X_i)$$

$\Rightarrow$ The variance of the output is the variance of the input, but scaled by $n \ \text{Var}(W_i)$.

Analysis (cont'd)

- **Variance of neuron activations**
  - if we *want the variance of the input and output of a unit to be the same*, then $n\,\mathrm{Var}(W_i)$ should be 1. This means

$$\mathrm{Var}(W_i) = \frac{1}{n} = \frac{1}{n_{\mathrm{in}}}$$

  - If we do the same for the backpropagated gradient, we get

$$\mathrm{Var}(W_i) = \frac{1}{n_{\mathrm{out}}}$$

  - As a compromise, Glorot & Bengio propose to use

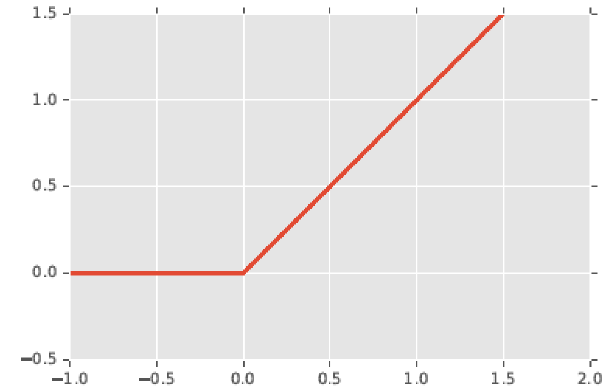
$$\mathrm{Var}(W) = \frac{2}{n_{\mathrm{in}} + n_{\mathrm{out}}}$$

$\Rightarrow$ Randomly sample the weights with this variance. That's it.

Extension to ReLU

- Another improvement for learning deep models
  - Use Rectified Linear Units (ReLU)

$$g(a) = \max\{0, a\}$$



  - Effect: gradient is propagated with a constant factor

$$\frac{\partial g(a)}{\partial a} = \begin{cases} 1, & a > 0 \\ 0, & \text{else} \end{cases}$$

- We can also improve them with proper initialization
  - However, the Glorot derivation was based on tanh units, linearity assumption around zero does not hold for ReLU.
  - He et al. made the derivations, proposed to use instead

$$\mathrm{Var}(W) = \frac{2}{n_{\mathrm{in}}}$$

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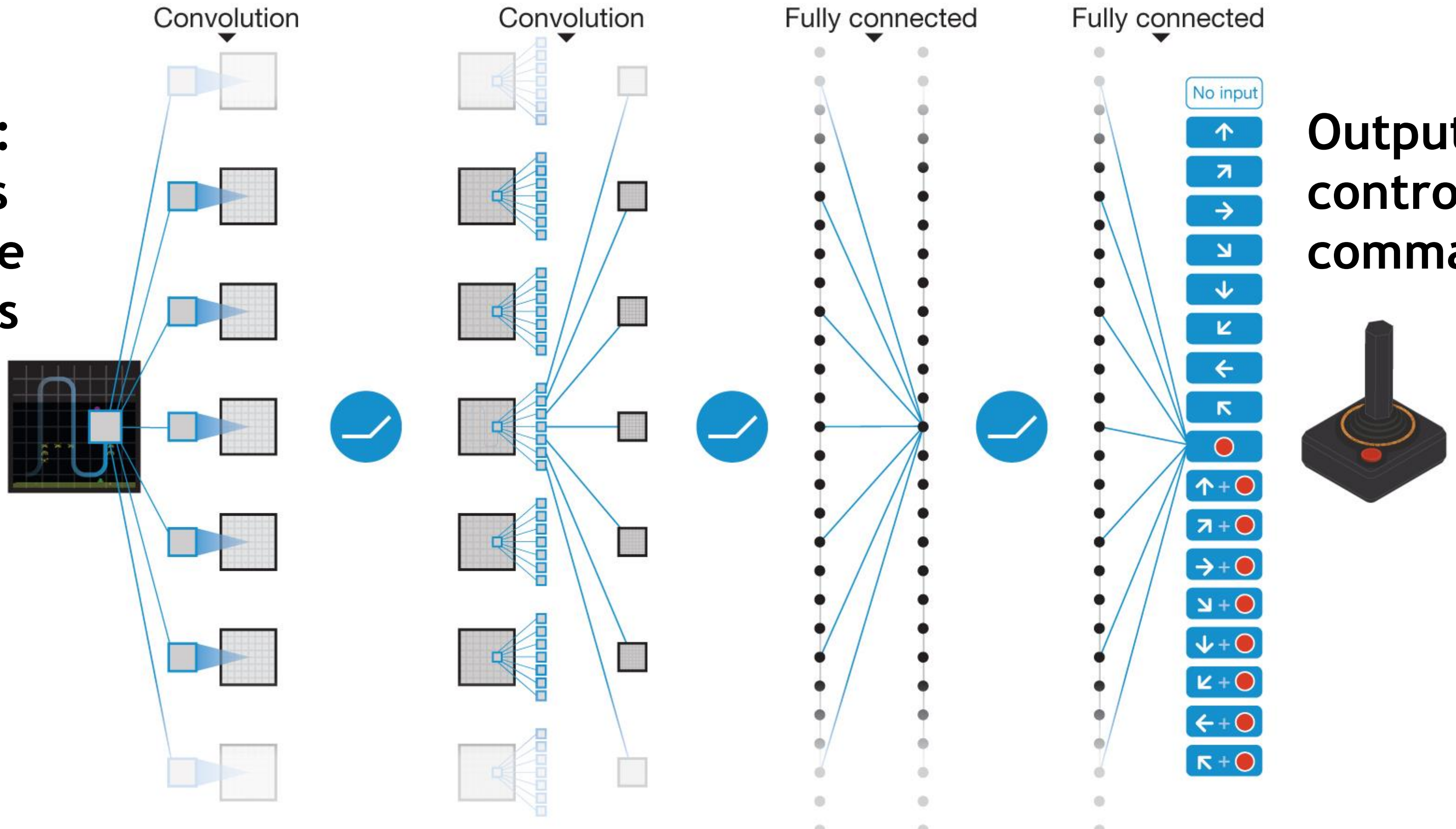
- **Outlook**
  - **Reinforcement Learning**

Outlook: Reinforcement Learning

- Learning to play computer games

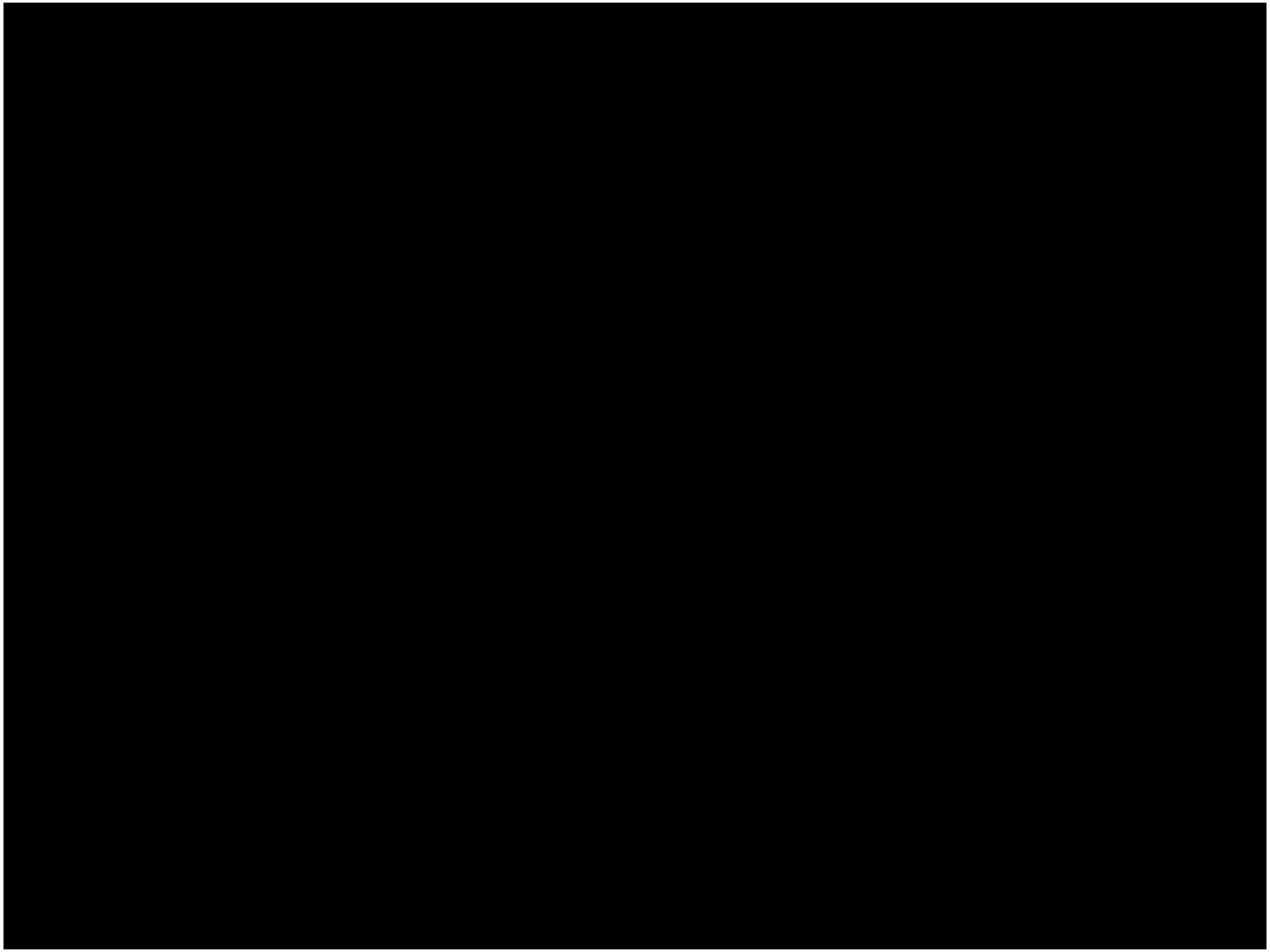
Input: pixels +game scores



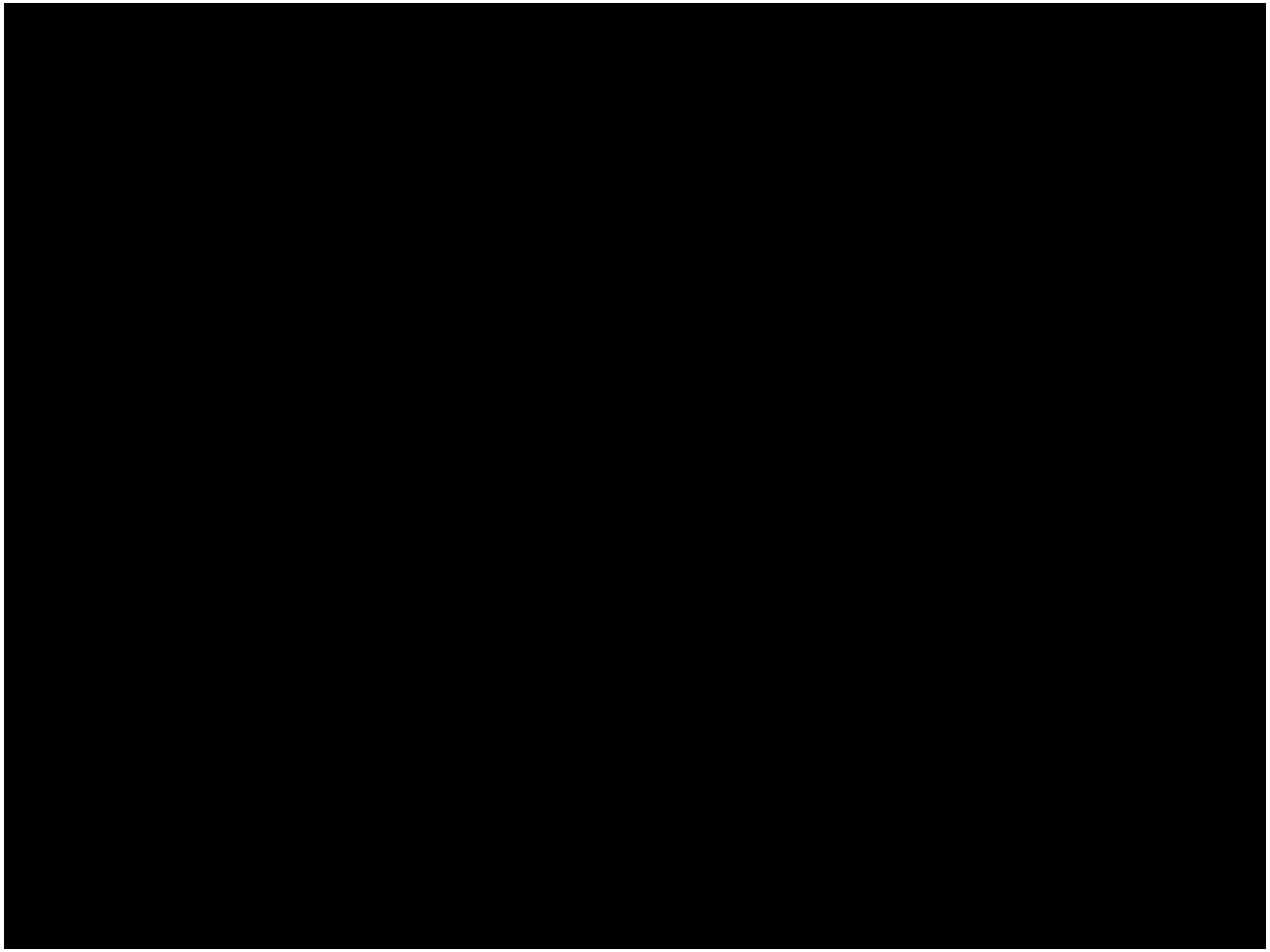
Output: control commands

V. Mnih et al., Human-level control through deep reinforcement learning, Nature Vol. 518, pp. 529-533, 2015

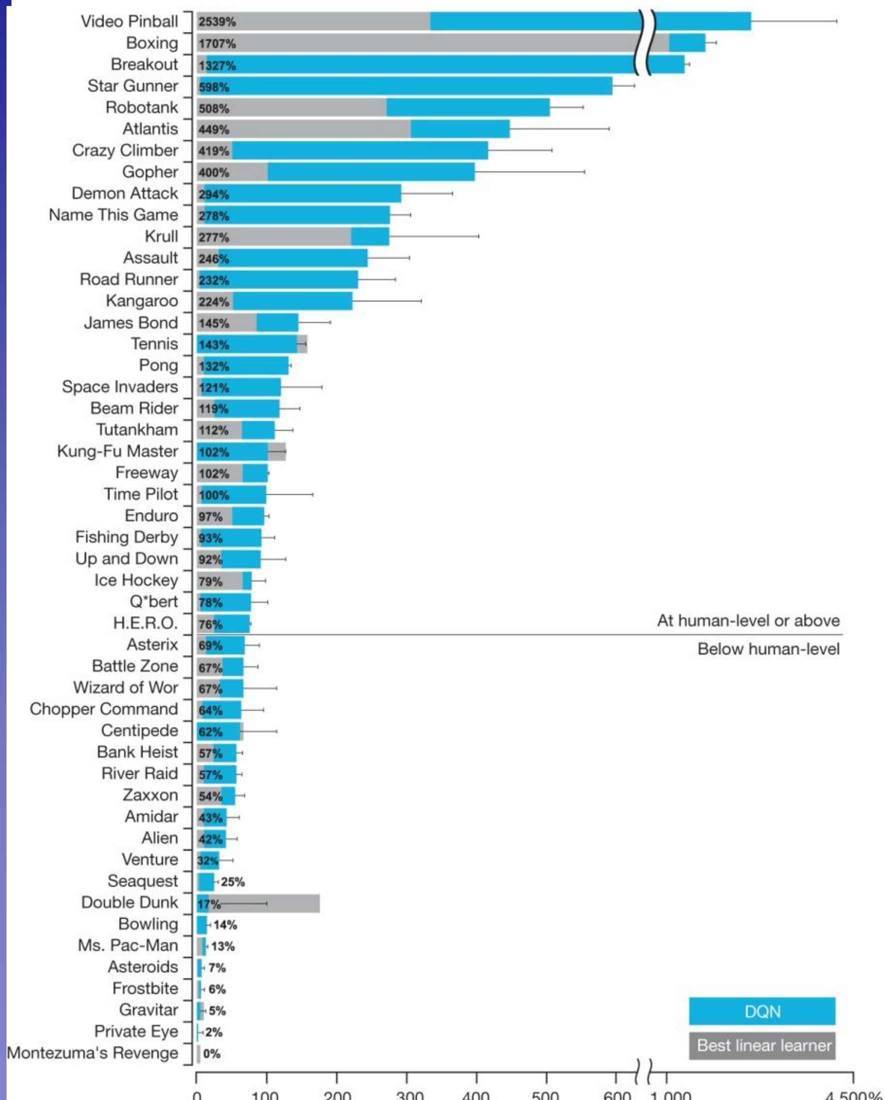
Results: Space Invaders

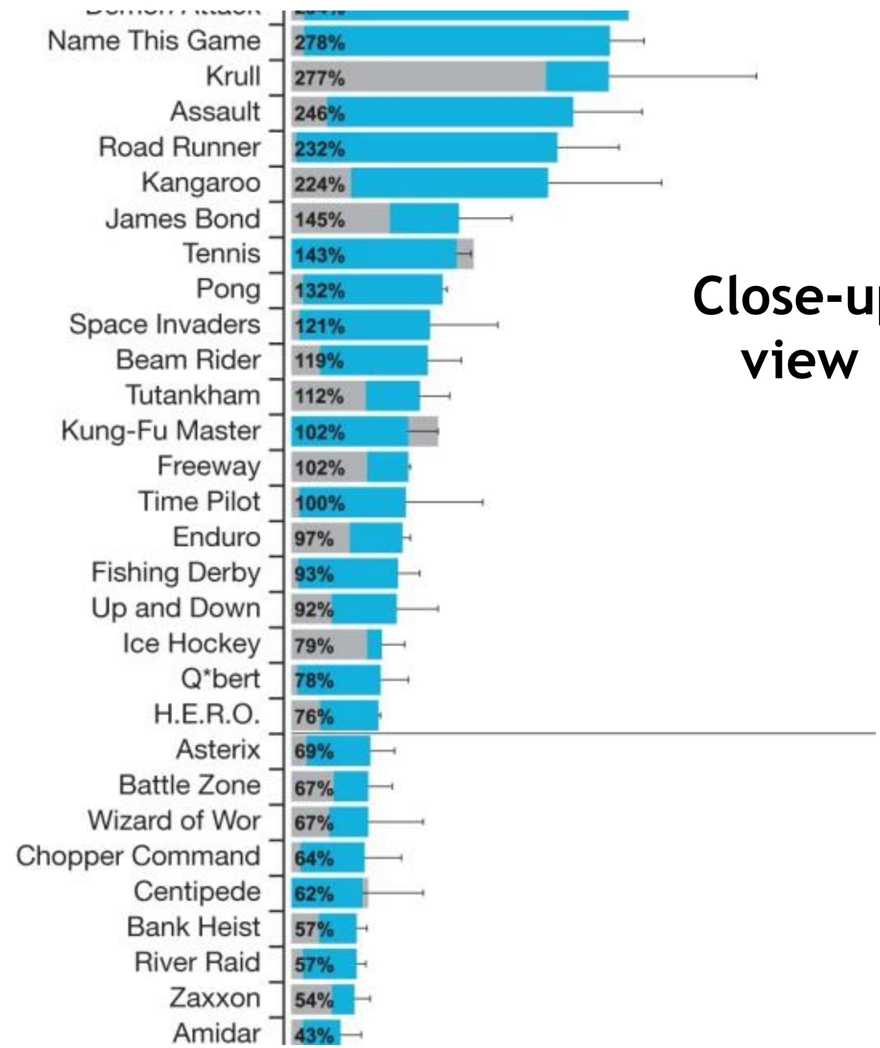


Results: Breakout



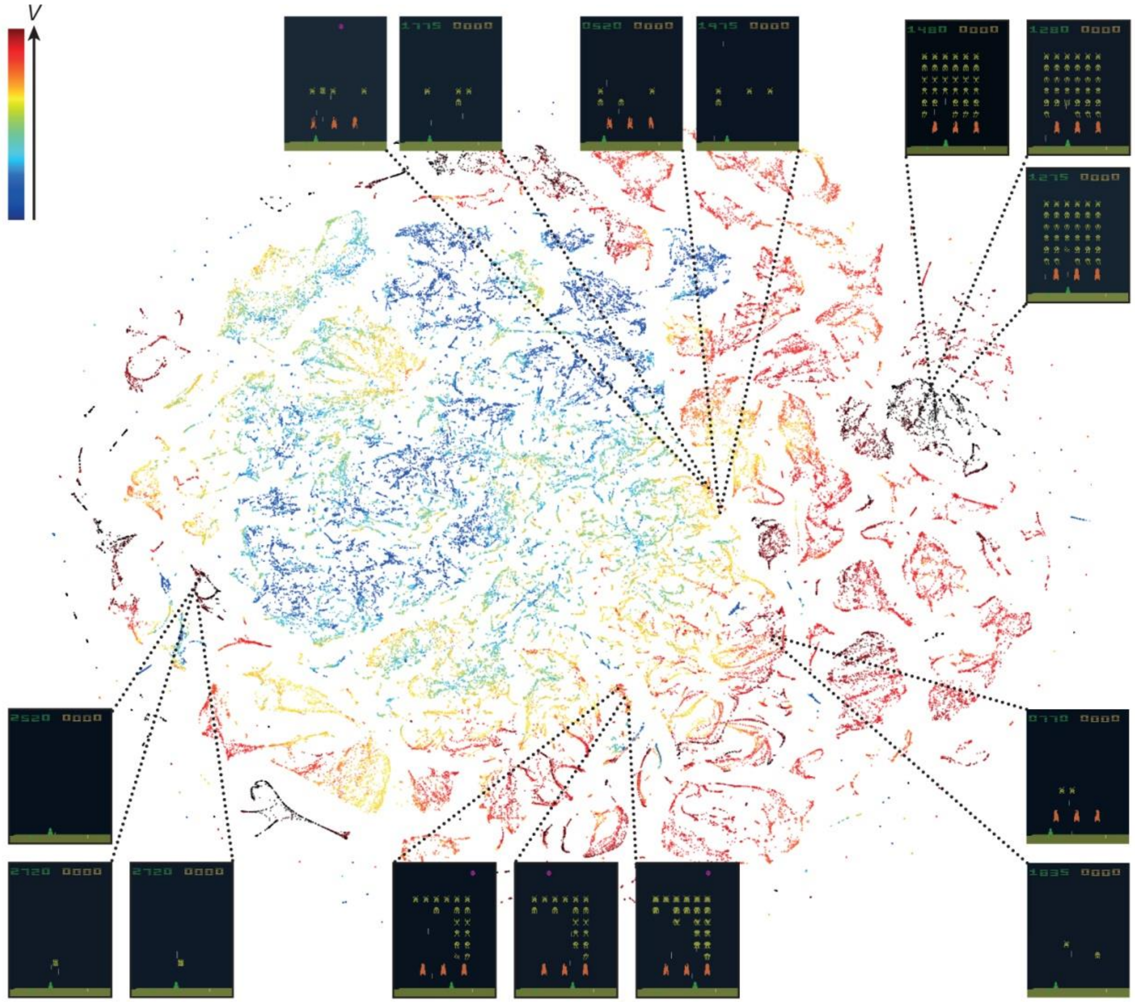
Comparison with Human Performance





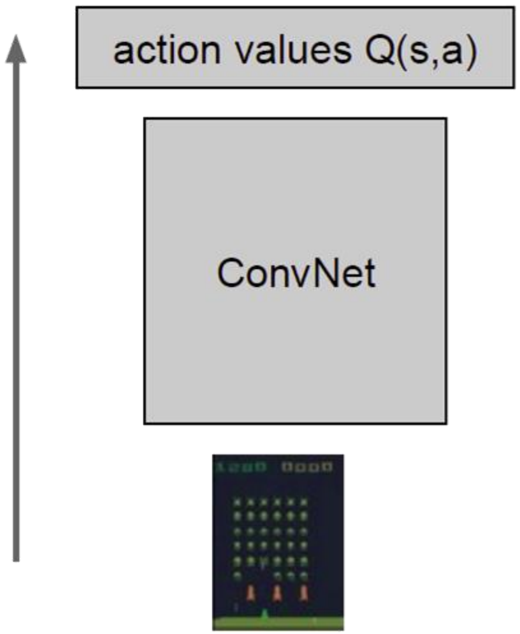
Close-up view

Learned Representation



- **t-SNE embedding of DQN last hidden layer (Space Inv.)**

Idea Behind the Model



- Interpretation
  - Assume finite number of actions
  - Each number here is a real-valued quantity that represents the "Q function" in Reinforcement Learning
- Collect experience dataset:
  - Set of tuples {(s,a,s',r), … }
  - (State, Action taken, New state, Reward received
- L2 Regression Loss

target value predicted value

$$L_i(\theta_i) = \mathbb{E}_{(s,a,r,s')\sim \mathrm{U}(D)}\left[\left(r + \gamma \max_{a'} Q(s',a';\theta_i^-) - Q(s,a;\theta_i)\right)^2\right]$$

Current reward + estimate of future reward, discounted by γ

References and Further Reading

- Initialization
  - X. Glorot, Y. Bengio, Understanding the difficulty of training deep feedforward neural networks, AISTATS 2010.
  - K. He, X. Zhang, S. Ren, J. Sun, Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification, arXiv 1502.01852, 2015.
- ReLu
  - X. Glorot, A. Bordes, Y. Bengio, Deep sparse rectifier neural networks, AISTATS 2011.