Lecture 5 - Training & Regularizing Neural Networks

DD2424

April 5, 2017

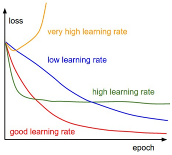
Baby sitting the training process

Training neural networks not completely trivial

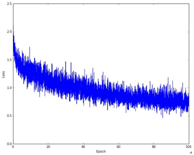
- Several **hyper-parameters** affect the quality of your training.
- These include
  - learning rate
  - degree of regularization
  - network architecture
  - hyper-parameters controlling weight initialization
- If these (potentially correlated) hyper-parameters are not appropriately set $\implies$ you will not learn an **effective** network.
- Multiple quantities you should monitor during training.
- These quantities indicate
  - a reasonable hyper-parameter setting and/or
  - how hyper-parameters setting could be changed for the better.

What to monitor during training

Monitor & Visualize the loss/cost curve

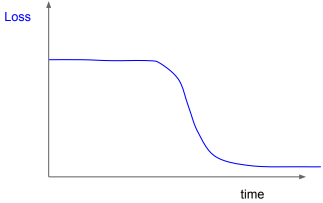


Evolution of your training loss
is telling you something!

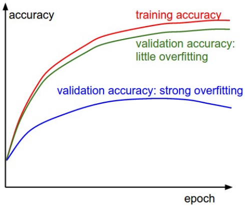


Typical training loss over time

Telltale sign of a bad initialization



Monitor & visualize the accuracy

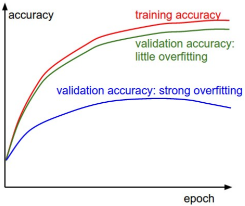


Gap between training and validation accuracy indicates amount of over-fitting.

Over-fitting $\Longrightarrow$ should increase regularization during training:

- increase the degree of L_2 regularization
- more dropout
- use more training data.

Monitor & visualize the accuracy



Gap between training and validation accuracy indicates amount of over-fitting.

Under-fitting $\Longrightarrow$ model capacity not high enough:

- increase the size of the network

Track the ratio of weight updates to weight magnitudes

- Track the **ratio** of the magnitude of the update vector to the magnitude of the parameter vector.
- So for a weight matrix, W, and vanilla SGD updates:

$$r = \frac{\| -\eta \nabla_W J \|}{\|W\|}$$

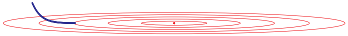
- A rough heuristic is that $r \sim .001$.
- If $r \ll .001 \implies$ learning rate might be too low.
- If $r \gg .001 \implies$ learning rate might be too high.

Parameter Updates: Variations of Stochastic Gradient Descent

One weakness of SGD

- SGD can be very slow......
- **Example**: Use SGD to find the optimum of

$$f(\mathbf{x}) = -\exp(-.5\mathbf{x}^T \Sigma \mathbf{x})$$



150 iterations, $\eta = .01$

Curves show the iso-contours of $f(\mathbf{x})$

- Speed up optimization by increasing the learning rate?

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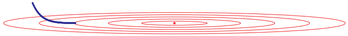
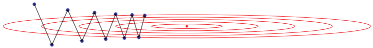


150 iterations, $\eta = .01$

Curves show the iso-contours of $f(\mathbf{x})$

- Speed up optimization by increasing the learning rate?

One weakness of SGD



10 iterations, $\eta = .5$
(ridiculous learning rate to visualize effect)

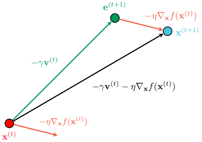
- SGD has trouble navigating ravines with high learning rates
  - SGD oscillates across the slopes of the ravine.
  - Makes slow progress along the bottom towards the local optimum.
- Unfortunately, ravines are common around local optima.

Solution: SGD with momentum

- Introduce **momentum** vector as well as the gradient vector.
- Let $\gamma \in [0, 1]$ and $\mathbf{v}$ is the momentum vector

$$\mathbf{v}^{(t+1)} = \gamma\, \mathbf{v}^{(t)} + \eta\, \nabla_{\mathbf{x}} f(\mathbf{x}^{(t)}) \quad \leftarrow \text{update vector}$$
$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \mathbf{v}^{(t+1)}$$

Typically γ set to .9.



How and why momentum helps

How?

- Momentum helps accelerate SGD in the appropriate direction.
- Momentum dampens the oscillations of default SGD.
  $\Longrightarrow$ **Faster convergence**.

($\gamma = .9$, $\eta = .01$, 150 iterations)

Why?

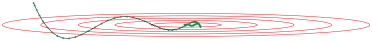
- For dimensions whose gradient is constantly changing then their entries in the update vector are damped.
- For dimensions whose gradient is **approx. constant** then their entries in the update vector are **not damped**.

Momentum not the complete answer

- When using momentum

$\Longrightarrow$ can pick up too much speed in one direction.

$\Longrightarrow$ can overshoot the local optimum.



($\gamma = .9$, $\eta = .03$)

Solution: Nesterov accelerated gradient (NAG)

- Look and measure ahead.
- Use gradient at an estimate of the parameters at the next iteration.
- Let $\gamma \in [0, 1]$ then

$$\mathbf{e}^{(t+1)} = \mathbf{x}^{(t)} - \gamma \mathbf{v}^{(t)} \quad \leftarrow \text{estimate of } \mathbf{x}^{(t+1)}$$
$$\mathbf{v}^{(t+1)} = \gamma\, \mathbf{v}^{(t)} + \eta\, \nabla_{\mathbf{x}} f(\mathbf{e}^{(t+1)}) \quad \leftarrow \text{update vector}$$
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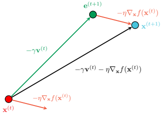
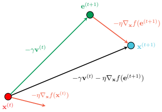


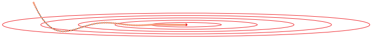
Momentum update



NAG update

How and why NAG helps

- The anticipatory update prevents the algorithm having too large updates and overshooting.
- Algorithm has increased responsiveness to the landscape of f.



($\gamma = .9$, $\eta = .01$, 150 iterations)

Note:
NAG shown to greatly increase the ability to train RNNs:

Bengio, Y., Boulanger-Lewandowski, N. & Pascanu, R. *Advances in Optimizing Recurrent Networks, (2012).*

http://arxiv.org/abs/1212.0901

More convenient form of NAG update

- Let $\gamma \in [0, 1]$ then

$$\mathbf{e}^{(t+1)} = \mathbf{x}^{(t)} - \gamma \mathbf{v}^{(t)} \quad \leftarrow \text{estimate of } \mathbf{x}^{(t+1)}$$
$$\mathbf{v}^{(t+1)} = \gamma\, \mathbf{v}^{(t)} + \eta\, \nabla_{\mathbf{x}} f(\mathbf{e}^{(t+1)}) \quad \leftarrow \text{update vector}$$
$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \mathbf{v}^{(t+1)}$$

- Form of update inconvenient as usually have $\mathbf{x}^{(t)}, \nabla_{\mathbf{x}} f(\mathbf{x}^{(t)})$.
  - Can make a variable transformation

$$\mathbf{m}^{(t)} = \mathbf{x}^{(t)} - \gamma \mathbf{v}^{(t)} \quad \left(\equiv \mathbf{e}^{(t+1)}\right)$$

  - Can write $\mathbf{x}^{(t+1)}$ as

$$\mathbf{x}^{(t+1)} = \mathbf{m}^{(t+1)} + \gamma \mathbf{v}^{(t+1)} = \mathbf{x}^{(t)} - \mathbf{v}^{(t+1)}$$

$\Longrightarrow$

$$\mathbf{m}^{(t+1)} = \mathbf{x}^{(t)} - (1+\gamma)\mathbf{v}^{(t+1)}$$
$$= \mathbf{m}^{(t)} + \gamma \mathbf{v}^{(t)} - (1+\gamma)\mathbf{v}^{(t+1)}$$

where

$$\mathbf{v}^{(t+1)} = \gamma\, \mathbf{v}^{(t)} + \eta\, \nabla_{\mathbf{x}} f(\mathbf{m}^{(t)})$$

Improvements to NAG

- Want to adapt the updates to each individual parameter.
- Perform larger or smaller updates depending on the landscape of the cost function.
- Family of algorithms with **adaptive learning rates**
  - AdaGrad
  - AdaDelta
  - RMSProp
  - Adam

AdaGrad

- Fora cleaner statement introduce some notation:

$$\mathbf{g}_t = \nabla_{\mathbf{x}} f(\mathbf{x}^{(t)}) \quad \text{and } \mathbf{g}_t = (g_{t,1}, \ldots, g_{t,d})^T.$$

- Keep a record of the sum of the squares of the gradients w.r.t. each x_i up to time t:

$$G_{t,i} = \sum_{j=1}^{t} g_{j,i}^2$$

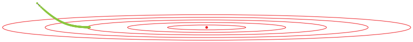
- The AdaGrad update step for each dimension is

$$x_i^{(t+1)} = x_i^{(t)} - \frac{\eta}{\sqrt{G_{t,i} + \epsilon}} \, g_{t,i}$$

- Usually set $\epsilon = 1e-8$ and $\eta = .01$.

J. Duchi, E. Hazan & Y. Singer, *Adaptive Subgradient Methods for Online Learning and Stochastic Optimization*, Journal of Machine Learning Research, 2011.

Adagrad's convergence on our toy problem



($\epsilon = 1e-8$, $\eta = .01$, 150 iterations)

Big weakness of AdaGrad

- Each $g_{t,i}^2$ is positive.

$\Longrightarrow$ Each $G_{t,i} = \sum_{j=1}^{t} g_{j,i}^2$ keeps growing during training.

$\Longrightarrow$ the effective learning rate $\eta/(\sqrt{G_{t,i} + \epsilon})$ shrinks and eventually $\longrightarrow 0$.

$\Longrightarrow$ updates of $\mathbf{x}^{(t)}$ stop.

AdaDelta

- Devised as an improvement to AdaGrad.
- Tackles AdaGrad's convergence to zero of the learning rate as t increases.
- AdaDelta's two central ideas
  - scale learning rate based on the previous gradient values (like AdaGrad) but only using a recent time window,
  - include an acceleration term (like momentum) by accumulating prior updates.

M. Zeiler, *ADADELTA: An Adaptive Learning Rate Method*, 2012. `http://arxiv.org/abs/1212.5701`

Technical details of AdaDelta

- Compute gradient vector $\mathbf{g}_t$ at current estimate $\mathbf{x}^{(t)}$.
- Update average of previous squared gradients (AdaGrad-like step)
$$\tilde{G}_{t,i} = \rho \, \tilde{G}_{t-1,i} + (1-\rho) \, g_{t,i}^2$$
- Compute the update vector
$$u_{t,i} = \frac{\sqrt{U_{t-1,i} + \epsilon}}{\sqrt{\tilde{G}_{t,i} + \epsilon}} \, g_{t,i}$$
- Compute exponentially decaying average of updates (momentum-like step)
$$U_{t,i} = \rho \, U_{t-1,i} + (1-\rho) \, u_{t,i}^2$$
- The AdaDelta update step:
$$x_i^{(t+1)} = x_i^{(t)} - u_{t,i}$$

RMSProp

Also addresses AdaGrad's radically diminishing learning rate:

- RMSProp an **adaptive learning rate** method proposed by Geoff Hinton in *Lecture 6e of his Coursera Class*.
- Stores an exponentially decaying average of the square of the gradient vector:
$$E\left[\mathbf{g}_{t+1}^2\right] = \gamma \; E\left[\mathbf{g}_t^2\right] + (1-\gamma) \, \mathbf{g}_{t+1}^2$$
- The RMSProp update rule:
$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \frac{\eta}{\sqrt{E\left[\mathbf{g}_{t+1}^2\right] + \epsilon}} \, \mathbf{g}_{t+1}$$
- Typically set $\gamma = .9$ and $\eta = 0.001$.

Adaptive Moment Estimation (Adam)

- Computes **adaptive learning rates** for each parameter.
- How?
  - Stores an **exponentially decaying average** of
    - ⋆ past gradients $\mathbf{m}^{(t)}$ and
    - ⋆ past squared gradients $\mathbf{v}^{(t)}$
  - $\mathbf{m}^{(t)}$ and $\mathbf{v}^{(t)}$ estimate the mean and variance of the sequence of computed gradients in each dimension.
  - Uses the variance estimate to
    - ⋆ damp the update in dimensions varying alot and
    - ⋆ increase the update in dimensions with low variation.

D. P. Kingma & J. L. Ba, *Adam: a Method for Stochastic Optimization*, International Conference on Learning Representations, 2015.

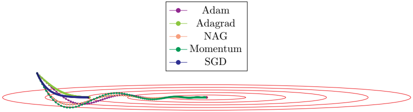
Update equations for Adam

- Let $\mathbf{g}_t = \nabla_{\mathbf{x}} f(\mathbf{x}^{(t)})$
$$\mathbf{m}^{(t+1)} = \beta_1 \mathbf{m}^{(t)} + (1-\beta_1) \, \mathbf{g}_t$$
$$\mathbf{v}^{(t+1)} = \beta_2 \mathbf{v}^{(t)} + (1-\beta_2) \, \mathbf{g}_t \; .* \; \mathbf{g}_t$$
- Set $\mathbf{m}^{(0)} = \mathbf{v}^{(0)} = \mathbf{0} \implies \mathbf{m}^{(t)}$ and $\mathbf{v}^{(t)}$ are biased towards zero (especially during the initial time-steps).
- Counter these biases by setting:
$$\hat{\mathbf{m}}^{(t+1)} = \frac{\mathbf{m}^{(t+1)}}{1-\beta_1^t}, \qquad \hat{\mathbf{v}}^{(t+1)} = \frac{\mathbf{v}^{(t+1)}}{1-\beta_2^t}$$
- The Adam update rule:
$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \frac{\eta}{\sqrt{\hat{\mathbf{v}}^{(t+1)}} + \epsilon} \, \hat{\mathbf{m}}^{(t+1)}$$
- Suggested default values $\beta_1 = .9, \beta_2 = .999, \epsilon = 10^{-8}$.

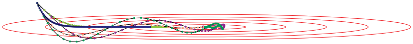
Adam's performance on our toy problem

(default parameter settings, 150 iterations)

Comparison of different algorithms on our toy problem



($\epsilon = 1e-8$, $\gamma = .9$, $\eta = .01$, 150 iterations)



($\epsilon = 1e-8$, $\gamma = .9$, $\eta = .03$, 150 iterations)

Comparison of different algorithms

Comparison of different algorithms at a saddle point

Which optimizer to use?

- Data sparse $\implies$ likely to achieve best results using one of the adaptive learning-rate methods.
- Using the adaptive learning-rate methods $\implies$ won't need to tune the learning rate (much!).
- RMSprop, AdaDelta, and Adam are very similar algorithms that do well in similar circumstances.
- Adam slightly outperforms RMSProp near the end of optimization.
- Adam might be the best overall choice.
- But vanilla SGD (without momentum) and a simple learning rate annealing schedule may be sufficient. But time until finding a local minimum may be long....

Annealing the learning rate

Useful to anneal the learning rate

- When training deep networks, usually helpful to anneal the learning rate over time.
- **Why?**
  - Stops the parameter vector from bouncing around too widely.
  - $\implies$ can reach into deeper, but narrower parts of the loss function.
- But knowing when to decay the learning rate is tricky!
- Decay too slowly $\implies$ waste computations bouncing around chaotically with little improvement.
- Decay too aggressively $\implies$ system unable to reach the best position it can.

Common approaches to learning rate decay

- **Step decay**:
  After every nth epoch set
  $$\eta = \alpha\eta$$
  where $\alpha \in (0, 1)$. (Instead sometimes people monitor the validation loss and reduce the learning rate when this loss stops improving.)
- **Exponential decay**:
  $$\eta = \eta_0 e^{-kt}$$
  where t is iteration number (either w.r.t. number of update steps or epochs). Then η_0 and k are hyper-parameters.
- $1/t$ **decay**:
  $$\eta = \frac{\eta_0}{1 + kt}$$

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Step decay most common. Better to decay conservatively and train for longer.

Optimization of the training hyper-parameters

Hyperparameters to adjust

- Initial learning rate.
- Learning rate decay schedule.
- Regularization strength
  - L_2 penalty
  - Dropout strength

Cross-validation strategy

- Do a **coarse** $\rightarrow$ **fine** cross-validation in stages.
- **Stage 0**: Identify the range of feasible learning rates & regularization penalties. (usually done interactively and train only for a few updates.)
- **Stage 1**: Broad search. Goal is to narrow the search range. Only run training for a few epochs.
- **Stage 2**: Finer search. Increase training times.
- **Stage ...**: Repeat Stage 2 as necessary.

Use performance on the **validation set** to identify good hyper-parameter settings.

Hyper-parameter ranges

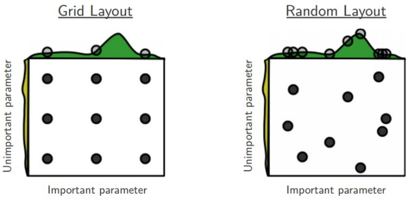
- Search for the **learning-rate** and **regularization** hyperparameters on a log scale.

Example:
Generate a potential learning rate with

$$\alpha = \mathsf{uniform}(-6, 1)$$
$$\eta = 10^{\alpha}$$

Evaluation: Model Ensembles

Prefer random search to grid search



"*randomly chosen trials are more efficient for hyper-parameter optimization than trials on a grid*"
Random Search for Hyper-Parameter Optimization, Bergstra and Bengio, 2012

Model Ensembles

- Train multiple independent models (same hyper-parameter settings, different initializations). ($\sim$ 5 models)
- At test time apply each model and average their results.

Model Ensemble on the cheap

- Can also get a small boost from averaging multiple model checkpoints of a single model.
- At test time apply each model and average their results.

Estimating Test Error

(just so that everyone knows what is acceptable and what's not)

Measuring the performance of a classifier

- Have learnt a classification $f(\cdot \mid \hat{\boldsymbol{\theta}})$ from the training data $\mathcal{D}$
- How well does $f(\cdot \mid \hat{\boldsymbol{\theta}})$ **generalize** to unseen examples?
- Does $f(\mathbf{x}_{\text{new}} \mid \hat{\boldsymbol{\theta}}) = y_{\text{new}}$ for a large number of $(\mathbf{x}_{\text{new}}, y_{\text{new}})$?

Estimating the Generalization Ability

- To measure accuracy of $f(\cdot \mid \hat{\boldsymbol{\theta}})$ ideally would compute the **Expected loss**:

$$\mathrm{E}\left[l(Y, f(\mathbf{X} \mid \hat{\boldsymbol{\theta}})\right] = \int_{\mathbf{x}} \int_{y} l\left(y, f(\mathbf{x} \mid \hat{\boldsymbol{\theta}})\right) p_{\mathbf{X},Y}(\mathbf{x}, y)\, d\mathbf{x}\, dy$$

  where
  - $l(y, f(\mathbf{x} \mid \hat{\boldsymbol{\theta}}))$ measures how well $f(\mathbf{x} \mid \hat{\boldsymbol{\theta}})$ predicts labels y.

Estimating the Error rate

- Usually don't know the distribution $p_{\mathbf{X},Y}(\mathbf{x}, y)$.

  $\Rightarrow$ cannot compute the Expected loss

- Instead maybe one could consider the **Training Error**:

$$\frac{1}{|\mathcal{D}|} \sum_{(\mathbf{x},y)\in\mathcal{D}} l\left(y, f(\mathbf{x} \mid \hat{\boldsymbol{\theta}})\right)$$

- Training error frequently not a good proxy for the test performance.

- Especially if $\hat{\theta}$ has been estimated from $\mathcal{D}$ (and some parameter tuning has occurred).

- What is the standard thing to do then?

Estimating the Error rate

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- What is the standard thing to do then?

For a data-rich situation

Randomly divide the dataset into 2 parts: $\mathcal{D} = \mathcal{D}_{\text{train}} \cup \mathcal{D}_{\text{test}}$.

Common split ratio 75%, 25%

- Use $\mathcal{D}_{\text{train}}$ to estimate f's parameters $\hat{\boldsymbol{\theta}}$.

- Use $\mathcal{D}_{\text{test}}$ to compute the **test loss** for $f(\cdot \mid \hat{\boldsymbol{\theta}})$:

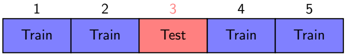
$$\text{Err} = \frac{1}{|\mathcal{D}_{\text{test}}|} \sum_{(\mathbf{x},y)\in\mathcal{D}_{\text{test}}} l\left(y, f(\mathbf{x} \mid \hat{\boldsymbol{\theta}})\right)$$

  an estimate of the expected loss.

However, if labelled data is scarce then your test set may be small and not so representative.

When labelled data is scarce: K-Fold Cross-Validation

General Approach



- Partition the data into K roughly equal-size subsets

$$\mathcal{D} = \mathcal{D}_1 \cup \mathcal{D}_2 \cup \cdots \cup \mathcal{D}_K$$

- Use $\mathcal{D}_k$ to estimate the test loss of f where $\hat{\boldsymbol{\theta}}$ is calculated from $\mathcal{D} \setminus \mathcal{D}_k$.

- Do this for $k = 1, 2, \ldots, K$ and average the K estimates of the expected loss. The is the cross validation (CV) error.

- The cross validation error $CV(f)$ is an estimate of the test loss.

K-Fold Cross-validation: Detailed description

- The mapping $\kappa : \{1, \ldots, n\} \to \{1, \ldots, K\}$ indicates example i belongs to partition $\kappa(i)$.

- Denote estimate of the parameters using data $\mathcal{D} \setminus \mathcal{D}_k$ by $\hat{\boldsymbol{\theta}}^{-k}$.

- **Cross-validation** estimate of the test loss is:

$$\boxed{\mathrm{CV}(f) = \frac{1}{n} \sum_{i=1}^{n} l\left(y_i, f(x_i \mid \hat{\boldsymbol{\theta}}^{-\kappa(i)})\right)}$$

- Typical choices for K are 5 or 10.

- The case $K = n$ is known as leave-one-out cross-validation.

Model/Classifier Selection

Selecting between different classifiers

You can generate different classifiers $f_1, \ldots, f_m$ because you

1. Investigate different types of classifiers
   - Random forest,
   - Linear SVM,
   - Bayesian classifier, ...
2. Have same type of classifier but different architectures
   - Random forest but depth of trees differs,
   - Neural networks but number of nodes and layers differ,
   - Bayesian classifier with different class likelihoods, ...
3. Have same type of classifier but different tuning parameters
   - Linear SVMs but C parameter differs,
   - Neural networks with different # of training iterations,
   - Kernel SVMs with different kernel parameters, ...
4. Any mixture of the above.

How do we choose the best classifier?

For a data-rich situation

Randomly divide the dataset into 3 parts: $\mathcal{D} = \mathcal{D}_{\text{train}} \cup \mathcal{D}_{\text{val}} \cup \mathcal{D}_{\text{test}}$.

Train	Validation	Test

Common split ratio 50%, 25%, 25%.

Model Selection

- Use **training set**, $\mathcal{D}_{\text{train}}$, to estimate $\hat{\boldsymbol{\theta}}_j$ for each f_j.

- Use **validation set**, $\mathcal{D}_{\text{val}}$, to estimate the test loss for each f_j.

- Choose f_{j^*} as the f_j with the lowest test loss estimate.

Assessment of the chosen model

- Use $\mathcal{D}_{\text{train}} \cup \mathcal{D}_{\text{val}}$ to estimate $\hat{\boldsymbol{\theta}}_{j^*}$ for f_{j^*}.

- Use **test set** $\mathcal{D}_{\text{test}}$ - unseen till now - to estimate f_{j^*}'s test loss.

When labelled data is scarce: K-Fold Cross-Validation

General Approach

1	2	3	4	5
Train	Train	Validation	Train	Train

- Partition the data into K roughly equal-size subsets

$$\mathcal{D} = \mathcal{D}_1 \cup \mathcal{D}_2 \cup \cdots \cup \mathcal{D}_K$$

- Use the $\mathcal{D}_k$ to estimate the expected loss of f_j where $\hat{\boldsymbol{\theta}}_j$ is calculated from $\mathcal{D} \setminus \mathcal{D}_k$.

- Do this for $k = 1, 2, \ldots, K$ and average the K estimates of the expected loss. Compute the cross-validation error $CV(f_j)$ for each classifier.

- Select the classifier, f_{j^*}, with lowest cross validation error.

Cross-Validation for Model Selection **&** Model Assessment

Option 1

- For each classifier f_j compute its K-fold cross-validation error $CV(f_j)$

- Choose the classifier f_{j^*} such that

$$j^* = \arg\min_{1 \leq j \leq m} \; CV(f_j)$$

- The estimate of the test error of the best classifier is given by

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You may have some concerns.

Have used the same training data for

- model selection **and**
- model assessment.

$\Longrightarrow$ Chance you have over-estimated generalization ability of selected model.

Option 2: Nested CV

Measures the performance of your model selection process.

1. Partition the data into K_0 folds $\mathcal{D} = \mathcal{D}_1 \cup \mathcal{D}_2 \cup \cdots \cup \mathcal{D}_{K_0}$.

2. for $k = 1, \ldots, K_0$
   - Set $\mathcal{E} = \mathcal{D} \setminus \mathcal{D}_k$
   - Perform K_1-fold cross-validation using $\mathcal{E}$ to select the best classifier $f_{j_k^*}$.
   - Compute the average loss of this classifier on $\mathcal{D}_k$

$$\text{Err}_k = \frac{1}{|\mathcal{D}_k|} \sum_{(\mathbf{x},y)\in\mathcal{D}_k} l\left(y, f_{j_k^*}(\mathbf{x}; \hat{\boldsymbol{\theta}}_{j_k^*})\right)$$

3. The cross-validation score for the model selection process is

$$CV(\text{model selection process}) = \frac{1}{K_0} \sum_{k=1}^{K_0} \text{Err}_k$$

And for deep neural network hyper-parameter tuning.

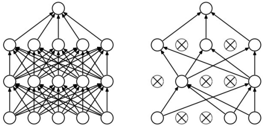
One validation set

- Usually have one validation fold as opposed to cross-validation.
- Simplifies the code base
- Makes things computationally feasible.

Regularization Via **Dropout**

Dropout

- **Randomly set some activations to zero in forward pass**



(a) Standard Neural Net (b) After applying dropout.

[Srivastava et al.]

- Training practice introduced by Hinton.

- **Note**: Each training sample in the mini-batch has its own random dropout mask.

Training with Dropout

Set $p \in (0, 1]$ $\leftarrow$ probability of keeping an activation active.

The Forward Pass (for a 2-layer network)

1. Compute the first set of activation values:

$$\mathbf{x}^{(1)} = \max(0, W_1\mathbf{x}^{(0)} + \mathbf{b}_1)$$

2. Randomly choose which entries of $\mathbf{x}^{(1)}$ to switch off

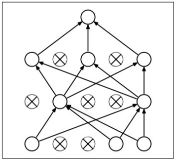
$$\mathbf{u}_1 = \text{rand}(\text{size}(\mathbf{x}^{(1)})) < p \quad \text{(Matlab notation)}$$
$$\mathbf{x}^{(1)} = \mathbf{x}^{(1)} .* \mathbf{u}_1$$

3. Repeat the process for the next layer

$$\mathbf{x}^{(2)} = \max(0, W_2\mathbf{x}^{(1)} + \mathbf{b}_2)$$
$$\mathbf{u}_2 = \text{rand}(\text{size}(\mathbf{x}^{(2)})) < p \quad \text{(Matlab notation)}$$
$$\mathbf{x}^{(2)} = \mathbf{x}^{(2)} .* \mathbf{u}_2$$

4. Output: $\mathbf{x}^{(3)} = \text{SoftMax}(W_3\mathbf{x}^{(2)} + \mathbf{b}_3)$

Why is this a good idea?



- Forces the network to have a redundant representation.
- **Another interpretation**
  - Dropout is training a large ensemble of models.
  - Each binary mask is one model, gets trained on only ∼one datapoint.

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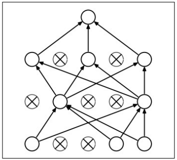

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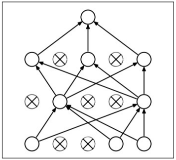
At test time

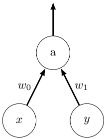


- **Ideally**: Want to integrate out all the noise.
- **Monte Carlo approximation**
  - Do many forward passes with different dropout masks.
  - Average all the predictions.

At test time

- Can do this with a single forward pass (approximately).
- Leave all the activations turned on (no dropout).
- Surely we must compensate?

At test time

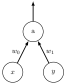


Consider this simple partial network

- During testing if we do not compensate:

$$a_{\text{test}} = w_0 x + w_1 y$$

At test time



Consider this simple partial network

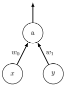
- During dropout training:
  1. Each input activation x and y is switched off with probability $1 - p$.
  2. The possible input activations are

inputs	probability
$(0,0)$	$(1-p)^2$
$(x,0)$	$p(1-p)$
$(0,y)$	$(1-p)p$
(x,y)	p^2

  3.

$$\begin{aligned} \mathsf{E}[a_{\text{training}}] &= (1-p)^2(w_0 0 + w_1 0) + p(1-p)(w_0 x + w_1 0) \\ &\quad + p(1-p)(w_0 0 + w_1 y) + p^2(w_0 x + w_1 y) \\ &= p\,(w_0 x + w_1 y) \end{aligned}$$

At test time



Consider this simple partial network

- During **testing** if we do not compensate:

$$a_{\text{test}} = w_0 x + w_1 y$$

- During **dropout training**:

$$\mathsf{E}[a_{\text{training}}] = p\,(w_0 x + w_1 y) = p\, a_{\text{test}}$$

$\Longrightarrow$ have to compensate at test time by scaling the activations by p.

Must compensate at test time

- Must scale the activations so for each neuron:
  output at test time = expected output at training time

- Don't drop activations but have to compensate

$$\begin{aligned}
\mathbf{x}^{(1)} &= \max(0, W_1 \mathbf{x}^{(0)} + \mathbf{b}_1) * p \\
\mathbf{x}^{(2)} &= \max(0, W_2 \mathbf{x}^{(1)} + \mathbf{b}_2) * p \\
\mathbf{x}^{(3)} &= \text{SoftMax}(W_3 \mathbf{x}^{(2)} + \mathbf{b}_3)
\end{aligned}$$

More common: Inverted Dropout

- During **training**:

$$\begin{aligned}
\mathbf{x}^{(1)} &= \max(0, W_1 \mathbf{x}^{(0)} + \mathbf{b}_1) \\
\mathbf{u}_2 &= (\text{rand}(\text{size}(\mathbf{x}^{(1)})) < p)/p \quad \longleftarrow \text{Note } /p \\
\mathbf{x}^{(1)} &= \mathbf{x}^{(1)} .* \mathbf{u}_2 \\
\mathbf{x}^{(2)} &= \max(0, W_2 \mathbf{x}^{(1)} + \mathbf{b}_2) \\
\mathbf{u}_2 &= (\text{rand}(\text{size}(\mathbf{x}^{(2)})) < p)/p \quad \longleftarrow \text{Note } /p \\
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\mathbf{x}^{(3)} &= \text{SoftMax}(W_3 \mathbf{x}^{(2)} + \mathbf{b}_3)
\end{aligned}$$

- $\Longrightarrow$ At **test time** no scaling necessary:

$$\begin{aligned}
\mathbf{x}^{(1)} &= \max(0, W_1 \mathbf{x}^{(0)} + \mathbf{b}_1) \\
\mathbf{x}^{(2)} &= \max(0, W_2 \mathbf{x}^{(1)} + \mathbf{b}_2) \\
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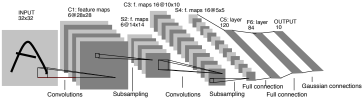
\end{aligned}$$

Convolutional Neural Networks (ConvNets)

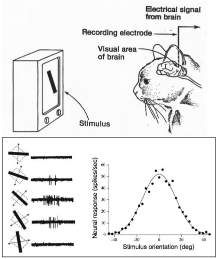
Convolutional Neural Networks



LeNet-5 (LeCun '98)

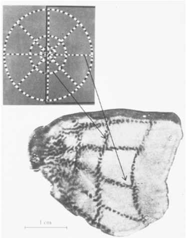
ConvNets: Some history

Hubel & Wiesel cat experiments 1968



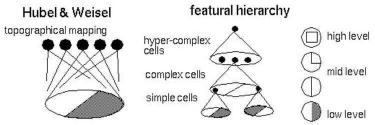
- Discovered *visual cortex* consists of a hierarchy of simple, complex, and hyper-complex cells. (Experiments in 50's & 60's)
- Hubel & Wiesel won the Nobel prize (1981).

Hubel & Wiesel



Topographical mapping in the cortex: nearby cells in cortex represented nearby regions in the visual field.

Hierarchical organization



Neurocognitron

Neocognitron: A Self-organizing Neural Network Model for a Mechanism of Pattern Recognition Unaffected by Shift in Position by Kunihiko Fukushima, 1980.

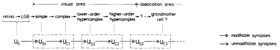
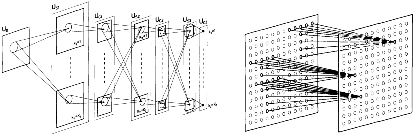


Fig. 1. Correspondence between the hierarchy model by Hubel and Wiesel, and the neural network of the neocognitron

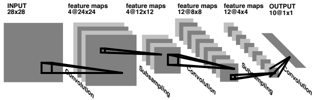
Inspired by Hubel & Wiesel model



sandwich architecture (SCSCSC...)

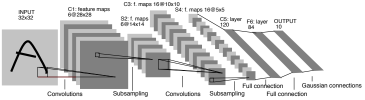
simple cells: modifiable parameters, **complex cells**: perform pooling

LeCun's *LeNet* ConvNets



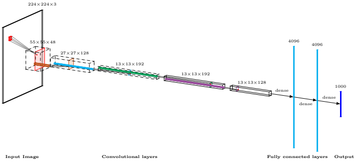
LeNet 1 '90

$\downarrow$



LeNet 5 '95

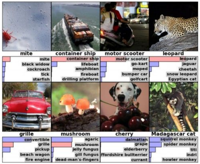
AlexNet



ImageNet Classification with Deep Convolutional Neural Networks by Krizhevsky, Sutskever, Hinton, 2012

Fast-forward to today: ConvNets are everywhere

Classification

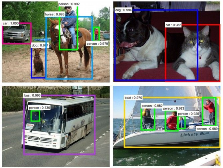


Retrieval

[Krizhevsky 2012]

Fast-forward to today: ConvNets are everywhere

Detection



Segmentation

[Faster R-CNN: Ren, He, Girshick, Sun 2015]

[Farabet et al., 2012]

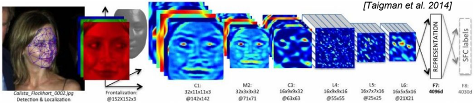
Fast-forward to today: ConvNets are everywhere

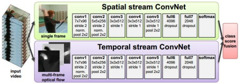
self-driving cars

NVIDIA Tegra X1

Fast-forward to today: ConvNets are everywhere

[Taigman et al. 2014]





[Simonyan et al. 2014]

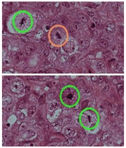
[Goodfellow 2014]

Fast-forward to today: ConvNets are everywhere

[Toshev, Szegedy 2014]

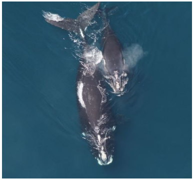
[Mnih 2013]

Fast-forward to today: ConvNets are everywhere



[Ciresan et al. 2013]

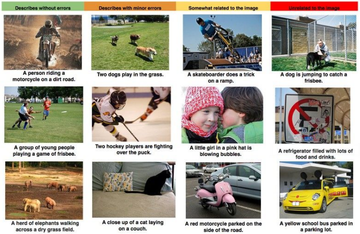
[Sermanet et al. 2011]
[Ciresan et al.]



Whale recognition, Kaggle Challenge

Mnih and Hinton, 2010

Image Captioning



[Vinyals et al., 2015]