Advanced Section #1: Moving averages, optimization algorithms, understanding dropout and batch normalization

AC 209B: Data Science 2

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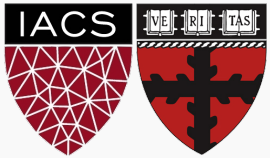


Lecture Outline

Moving averages

Optimization algorithms

Tuning the learning rate

Gradient checking

How to address overfitting

Dropout

Batch normalization

Moving averages

Moving averages

- Given a stationary process $x[n]$ and a sequence of observations $x_1, x_2, \ldots, x_n, \ldots$, we want to estimate the average of all values ***dynamically***.
- We can use a ***moving average*** for instant n:

$$\overline{x}_{n+1} = \frac{1}{n}(x_1 + x_2 + \ldots + x_n)$$

- **To save computations and memory**:

$$\begin{aligned}\overline{x}_{n+1} &= \frac{1}{n}\sum_{i=1}^{n} x_i = \frac{1}{n}\left(x_n + \sum_{i=1}^{n-1} x_i\right) = \frac{1}{n}\left(x_n + (n-1)\frac{1}{n-1}\sum_{i=1}^{n-1} x_i\right) \\ &= \frac{1}{n}\left(x_n + (n-1)\overline{x}_n\right) = \overline{x}_n + \frac{1}{n}\left(x_n - \overline{x}_n\right)\end{aligned}$$

- Essentially, for $\alpha_n = 1/n$,

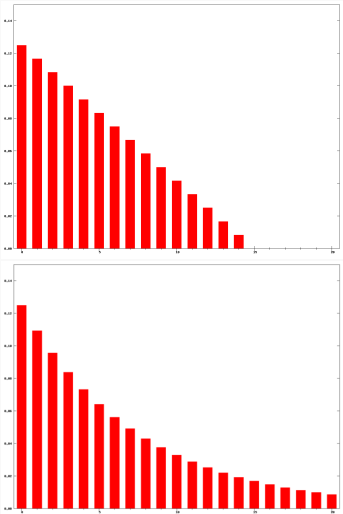
$$\boxed{\overline{x}_{n+1} = \overline{x}_n + \alpha_n\left(x_n - \overline{x}_n\right)}$$

Weighted moving averages

- Previous step size $\alpha_n = 1/n$ is dynamic.
- From **stochastic approximation theory**, the estimate converges to the true value with probability 1, if

$$\sum_{i=1}^{\infty} \alpha_i = \infty \qquad \text{and} \qquad \sum_{i=1}^{\infty} \alpha_i^2 < \infty$$

- $\alpha_n = \frac{1}{n}$ satisfies the previous conditions.
- Constant α does not satisfy the second!!
- This can be useful to track ***non-stationary*** processes.



Exponentially weighted moving average

- Update rule for constant step size is

$$\begin{aligned}
\overline{x}_{n+1} &= \overline{x}_n + \alpha\,(x_n - \overline{x}_n) \\
&= \alpha x_n + (1-\alpha)\overline{x}_n \\
&= \alpha x_n + (1-\alpha)[\alpha x_{n-1} + (1-\alpha)\overline{x}_{n-1}] \\
&= \alpha x_n + (1-\alpha)\alpha x_{n-1} + (1-\alpha)^2\overline{x}_{n-1}] \\
&= \alpha x_n + (1-\alpha)\alpha x_{n-1} + (1-\alpha)^2\alpha x_{n-2} + \ldots + (1-\alpha)^{n-1}\alpha x_1 + (1-\alpha)^n\overline{x}_1 \\
&= \boxed{(1-\alpha)^n\overline{x}_1 + \sum_{i=1}^{n}\alpha(1-\alpha)^{n-i}x_i}
\end{aligned}$$

- Note that $(1-\alpha)^n + \sum_{i=1}^{n}\alpha(1-\alpha)^{n-i} = 1$.
- With infinite terms we get

$$\lim_{n\to\infty}\overline{x}_n = \lim_{n\to\infty}\frac{x_n + (1-\alpha)x_{n-1} + (1-\alpha)^2x_{n-2} + (1-\alpha)^3x_{n-3} + \ldots}{1 + (1-\alpha) + (1-\alpha)^2 + (1-\alpha)^3 + \ldots}$$

Exponentially weighted moving average

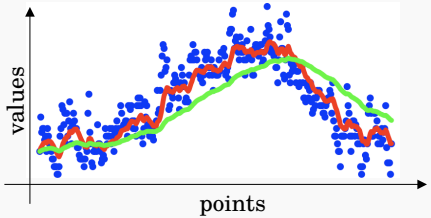
- Recap update rule, but change $1 - \alpha = \beta$

$$\overline{x}_{n-1} = \beta \overline{x}_{n-1} + (1 - \beta) x_n,$$

- β controls the amount of points to consider (variance):
- **Rule of thumb:**

$$N = \frac{1+\beta}{1-\beta} \text{ amounts to 86\% of influence.}$$

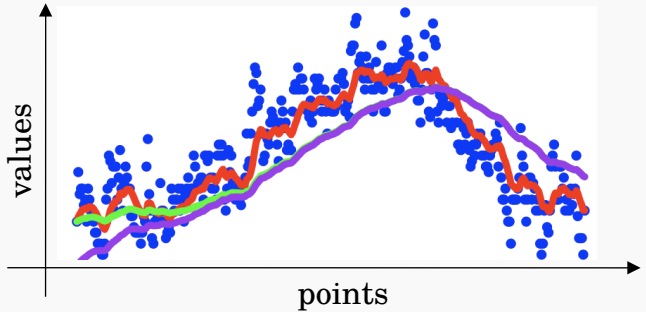
  - $\beta = 0.9$ corresponds to 19 points.
  - $\beta = .98$ corresponds to 99 points (wide window).
  - $\beta = 0.5$ corresponds to 3 points (susceptible to outliers).



Bias correction

- The rule of thumb works for sufficiently large N.
- Otherwise, the first values are biased.
- We can correct the variance with:

$$\overline{x}_n^{\text{corrected}} = \frac{\overline{x}_n}{1-\beta^t}.$$



Bias correction II

- The bias correction can in practice be ignored (Keras does not implement it).
- Origin of bias comes from zero initialization:

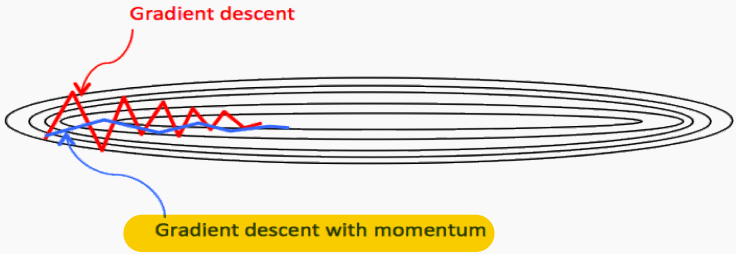
$$\overline{x}_{n+1} = \beta^n \underbrace{\overline{x}_1}_{0} + (1-\beta)\sum_{i=1}^{n} \beta^{n-i} x_i$$

- Derivation:

$$\begin{aligned}
\mathbb{E}[\overline{x}_{n+1}] &= \mathbb{E}\left[(1-\beta)\sum_{i=1}^{n} \beta^{n-i} x_i\right] \\
&= \mathbb{E}[x_n](1-\beta)\sum_{i=1}^{n} \beta^{n-i} + \zeta \\
&= \mathbb{E}[x_n](1-\beta^n) + \zeta
\end{aligned}$$

Optimization algorithms

Gradient descent



- Gradient descent will have high variance if the problem is ill-conditioned.
- Aim to estimate directions of high variance and reduce their influence.
- Descent with momentum, RMSprop or Adam, help reduce the variance and speed up convergence.

Gradient descent with momentum

- The algorithm:

  On iteration t for W update:

  Compute dW on current mini-batch.

  $v_{dW} = \beta v_{dW} + (1 - \beta) dW$.

  $W = W - \alpha v_{dW}$.

- Gradient with momentum performs an exponential moving average over the gradients.
- This will reduce the variance and give more stable descent directions.
- Bias correction is usually not applied.

RMSprop

- The algorithm:

  1: On iteration t for W update:

  2: Compute dW on current mini-batch.

  3: $s_{dW} = \beta_2 s_{dW} + (1 - \beta_2) dW^2$.

  4: $W = W - \alpha \frac{dW}{\sqrt{s_{dW}} + \epsilon}$.

- $\epsilon = 10^{-8}$ controls numerical stability.
- High variance gradients will have larger values $\rightarrow$ the squared averages will be large $\rightarrow$ reduces the step size.
- Allows a higher learning rate $\rightarrow$ faster convergence.

Adaptive moment estimation (Adam)

- The algorithm:

1: On iteration t for W update:

2: Compute dW on current mini-batch.

3: $v_{dW} = \beta_1 v_{dW} + (1 - \beta_1) dW.$

4: $s_{dW} = \beta_2 s_{dW} + (1 - \beta_2) dW^2.$

5: $v^{\text{corrected}} = \frac{v_{dW}}{1 - \beta_1^t}$

6: $s^{\text{corrected}} = \frac{s_{dW}}{1 - \beta_2^t}$

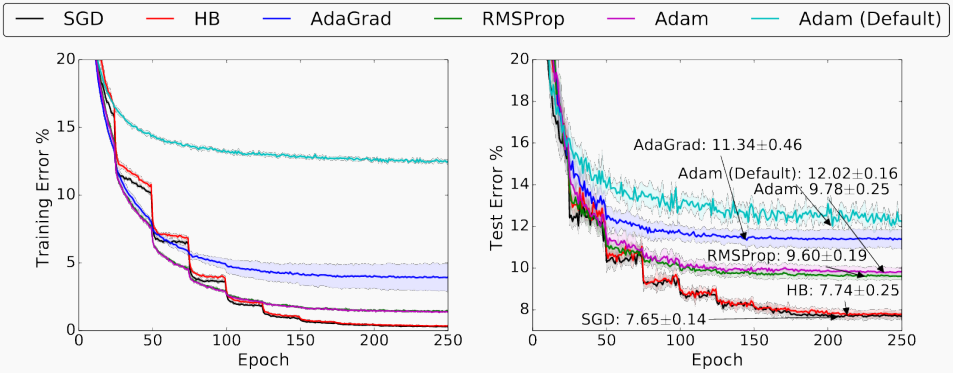
7: $W = W - \alpha \frac{v^{\text{corrected}}}{\sqrt{s_{dW}} + \epsilon}.$

AMSGrad

- Adam/RMSprop fail to converge on certain convex problems.
- Reason is that some important descent directions are weakened by high second order estimations.
- AMSGrad proposes a conservative fix where second order moment estimator can only increase.
- The algorithm:

1: On iteration t for W update:
2: Compute dW on current mini-batch.
3: $v_{dW}^{n+1} = \beta_1 v_{dW}^{n} + (1-\beta_1)dW$.
4: $s_{dW}^{n+1} = \beta_2 s_{dW}^{n} + (1-\beta_2)dW^2$.
5: $\hat{s}_{dW}^{n+1} = \max(\hat{s}_{dW}^{n}, s_{dW}^{n+1})$
6: $W = W - \alpha \frac{v^{\text{corrected}}}{\sqrt{\hat{s}_{dW}^{n+1}+\epsilon}}$.

Marginal value of adaptive gradient methods



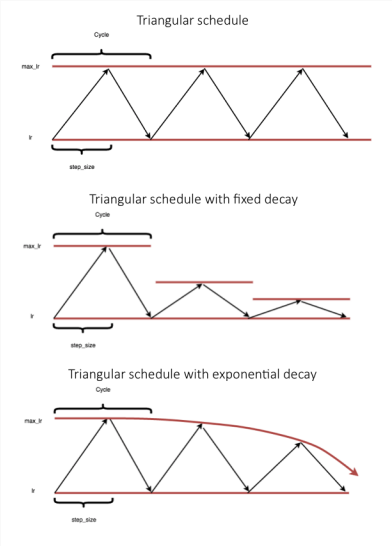
(a) CIFAR-10 (Train)

(b) CIFAR-10 (Test)

Tuning the learning rate

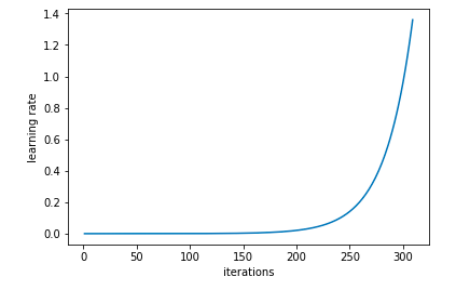
Cyclical Learning Rates for Neural Networks

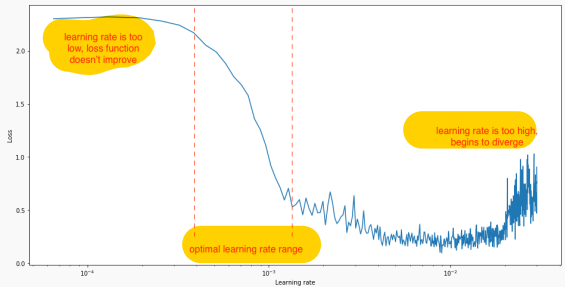
- Use cyclical learning rates to escape local extreme points.
- Saddle points are abundant in high dimensions, and convergence becomes very slow. Furthermore, they can help escape sharp local minima (overfitting).
- Cyclic learning rates raise the learning rate periodically: **short term negative effect and yet achieve a longer term beneficial effect.**
- Decreasing learning rates may still help reduce error towards the end.



Estimating the learning rate

- How can we get a good LR estimate?
- Start with a small LR and increase it on every batch exponentially.
- Simultaneously, compute loss function on validation set.
- This also works for finding bounds for cyclic LRs.



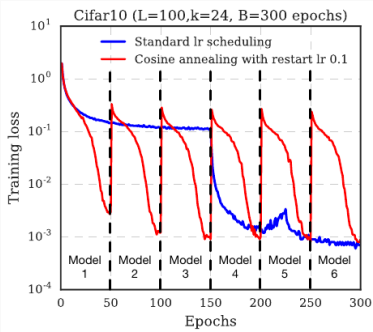


SGD with Warm Restarts

- Key idea: restart every T_i epochs. **Record best estimates before restart**.
- Restarts are not from scratch, but from last estimate, and learning rate is increased.

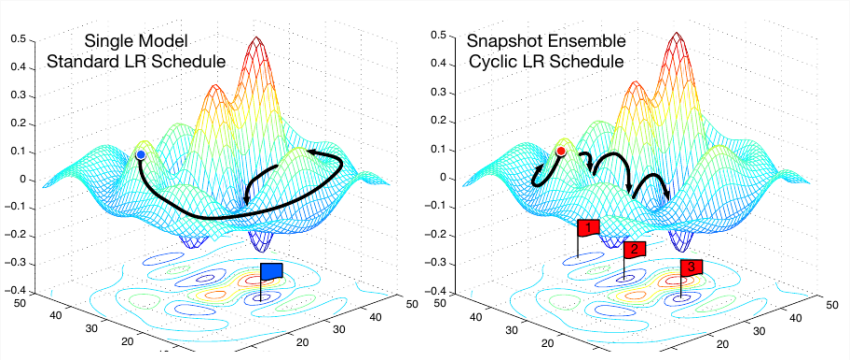
$$\alpha_t = \alpha^i_{\min} + \frac{1}{2}(\alpha^i_{\max} - \alpha^i_{\min})(1 + \cos(\frac{T_c ur}{T_i}\pi))$$

- The cycle can be lengthened with time.
- $\alpha^i_{\min}$ and $\alpha^i_{\max}$ can be decayed after a cycle.



Snapshot ensembles: Train 1, get M for free

- Ensemble networks are much more robust and accurate than individual networks.
- They constitute another type of regularization technique.
- The novelty is to train a single neural network, but obtain M different models.
- The idea is to converge to M different local optima, and save network parameters.



Snapshot ensembles II

- Different initialization points, or hyperarameter choices may converge to different local minima.
- Although these local minima may perform similarly in terms of averaged errors, they may not make the same mistakes.
- Ensemble methods train many NN, and then optimize through majority vote, or averaging of the prediction outputs.
- The proposal uses a cycling step size procedure (cosine), in which the learning rate is abruptly raised and wait for new convergence.
- The final ensemble consists of snapshots of the optimization path.

Snapshot ensembles III

	Method	C10	C100	SVHN	Tiny ImageNet
ResNet-110	Single model	5.52	28.02	1.96	46.50
	NoCycle Snapshot Ensemble	5.49	26.97	1.78	43.69
	SingleCycle Ensembles	6.66	24.54	1.74	42.60
	Snapshot Ensemble ($\alpha_0 = 0.1$)	5.73	25.55	**1.63**	40.54
	Snapshot Ensemble ($\alpha_0 = 0.2$)	**5.32**	**24.19**	1.66	**39.40**
Wide-ResNet-32	Single model	5.43	23.55	1.90	39.63
	Dropout	4.68	22.82	1.81	36.58
	NoCycle Snapshot Ensemble	5.18	22.81	1.81	38.64
	SingleCycle Ensembles	5.95	21.38	1.65	35.53
	Snapshot Ensemble ($\alpha_0 = 0.1$)	**4.41**	**21.26**	1.64	35.45
	Snapshot Ensemble ($\alpha_0 = 0.2$)	4.73	21.56	**1.51**	**32.90**
DenseNet-40	Single model	5.24*	24.42*	1.77	39.09
	Dropout	6.08	25.79	1.79*	39.68
	NoCycle Snapshot Ensemble	5.20	24.63	1.80	38.51
	SingleCycle Ensembles	5.43	22.51	1.87	38.00
	Snapshot Ensemble ($\alpha_0 = 0.1$)	4.99	23.34	**1.64**	37.25
	Snapshot Ensemble ($\alpha_0 = 0.2$)	**4.84**	**21.93**	1.73	**36.61**
DenseNet-100	Single model	3.74*	19.25*	-	-
	Dropout	3.65	18.77	-	-
	NoCycle Snapshot Ensemble	3.80	19.30	-	-
	SingleCycle Ensembles	4.52	18.38		
	Snapshot Ensemble ($\alpha_0 = 0.1$)	3.57	18.12	-	-
	Snapshot Ensemble ($\alpha_0 = 0.2$)	**3.44**	**17.41**	-	-

Gradient checking

Gradient checking

- Useful technique to debug code of manual implementations of neural networks.
- Not intended for training of networks, but it can help to identify errors in a backpropagation implementation.
- Derivative of a function:

$$f'(x) = \lim_{\epsilon \to 0} \frac{f(x+\epsilon) - f(x-\epsilon)}{2\epsilon} \approx \frac{f(x+\epsilon) - f(x-\epsilon)}{2\epsilon}.$$

- The approximation error is in the order $O(\epsilon^2)$.
- In the multivariate case, the ϵ term affects a single component:

$$\frac{df(\theta)}{d\theta_r} \approx \frac{f(\theta_r^+) - f(\theta_r^-)}{2\epsilon}$$

where $\theta_r^+ = (\theta_1, \ldots, \theta_r + \epsilon, \ldots, \theta_n)$, $\theta_r^- = (\theta_1, \ldots, \theta_r - \epsilon, \ldots, \theta_n)$.

Algorithm for gradient checking

1: Reshape input vector in a column vector θ.
2: **for** each r component **do**
3: $\quad \theta_{\text{old}} \leftarrow \theta_r$
4: $\quad$ Calculate $f(\theta_r^+)$ and $f(\theta_r^-)$.
5: $\quad$ Compute approx. $\frac{df(\theta)}{d\theta_r}$.
6: $\quad$ Restore $\theta_r \leftarrow \theta_{\text{old}}$
7: **end for**
8: Verify relative error is below some threshold:

$$\xi = \frac{\|d\theta^{\text{approx}} - d\theta\|}{\|d\theta^{\text{approx}}\| + \|d\theta\|}$$

How to address overfitting

Estimators

- Point estimation is the attempt to provide the single "best" prediction of some quantity of interest:

$$\hat{\boldsymbol{\theta}}_m = g(\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)}).$$

  - $\boldsymbol{\theta}$: true value.
  - $\hat{\boldsymbol{\theta}}_m$: estimator for m samples.
- Frequentist perspective: $\boldsymbol{\theta}$ fixed but unkwown.
- Data is random $\implies$ $\hat{\boldsymbol{\theta}}_m$ is a r.v.

Bias and Variance

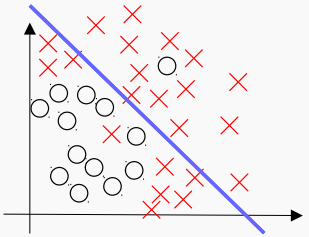
- Bias: expected deviation from the true value.
- Variance: deviation from the expected estimator.

  Examples:
  - Sample mean: $\hat{\mu}_m = \frac{1}{m}\sum_i \mathbf{x}^{(i)}$
  - Sample variance $\hat{\sigma}_m^2 = \frac{1}{m}\sum_i (x^{(i)} - \hat{\mu}_m)^2$:

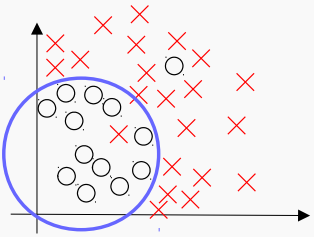
$$\mathbb{E}[\hat{\sigma}_m^2] = \frac{m-1}{m}\sigma^2$$

  - Unbiased sample variance: $\tilde{\sigma}_m^2 = \frac{1}{m-1}\sum_i (x^{(i)} - \hat{\mu}_m)^2$
- How to choose estimators with different statistics?
  - Mean square error (MSE).
  - Cross-validation: **empirical**.

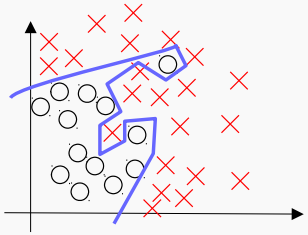
Bias-Variance Example



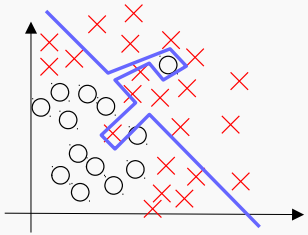
high bias &
underfitting



appropriate



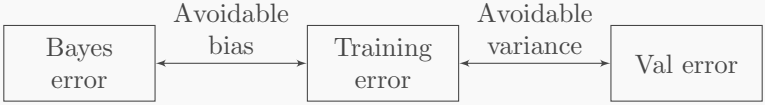
high variance &
overfitting



high bias & variance

Diagnose bias-variance

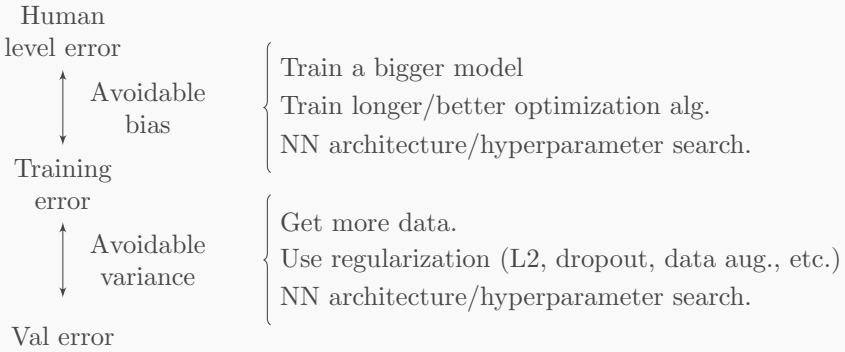
- In high dimensions we cannot draw decision curves to inspect bias-variance.
- We calculate error values to infer the source of errors on the training set, as well as on the val set.
- To determine bias, we need a base line, such as human level performance.



- Example:

Human level error	$\approx 0\%$			
Training error	0.5%	15%	1%	12%
Val error	1%	16%	11%	20%
	low bias low variance	high bias	high variance	high bias high variance

Orthogonalization

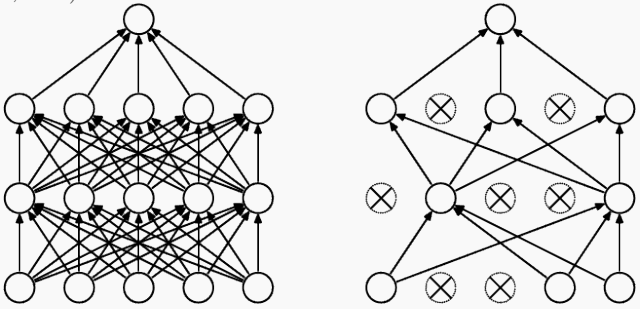


- Orthogonalization aims to decompose the process to adjust NN performance.
- It assumes the errors come from different sources and uses a systematic approach to minimize them.
- Early stopping is a popular regularization mechanism, but couples the bias and variance errors.

Dropout

Dropout

- Regularization technique for deep NN.
- Employed at training time.
- Eliminates the output of some units randomly.
- Can be used in combination with other regularization techniques (such as L2, batch normalization, etc.).

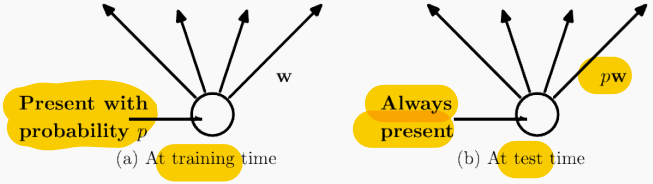


(a) Standard Neural Net

(b) After applying dropout.

Motivation and direct implementation

- **Purpose**: prevent the co-adaptation of feature detectors for a set of neurons, and avoid overfitting.
  - It enforces the neurons to develop an individual role on their own given an overall population behavior.
  - Training weights are encouraged to be spread along the NN, because no neuron is permanent.
- **Interpretation**: training examples provide gradients from different, randomly sampled architectures.
- **Direct implementation**:
  - At training time: eliminate the output of some units randomly.
  - At test time: all units are present.



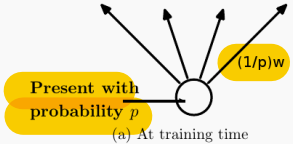
Inverted dropout

- Current implementations use ***inverted dropout***
  - Weighting is performed during training.
  - Does not require re-weighting at test time.
- In particular, for layer l,

$$z^{[l]} = \frac{1}{p_l} W^{[l]} D^{[l]} a^{[l-1]} + b^{[l]}$$
$$a^{[l]} = g(z^{[l]}),$$

- Notation:

p_l : Retention probability.
$D^{[l]}$: Dropout activations.
$a^{[l-1]}$: Output from previous layer.
$W^{[l]}$: Layer weights.
$b^{[l]}$: Offset weights.
$z^{[l]}$: Linear output.
$g(\cdot)$: Nonlinear activation function.



(a) At training time

(b) At test time

Understanding dropout

We aim to understand dropout as a regularization technique on simplified neural architectures such as:

- ***Linear networks***.
- ***Logistic regression***.
- ***Deep networks***.

These results are are based on the following reference:

Pierre Baldi and Peter J Sadowski, "Understanding dropout,"
in *Advances in Neural Information Processing Systems*, 2013, pp. 2814–2822.

Dropout in linear networks

- **Linear network**: all activations units correspond to the identity function.
- For a single training example we get

$$z^{[l]} = W^{[l]} D^{[l]} z^{[l-1]}.$$

- The expectation over all possible network realizations:

$$\mathbb{E}\{z^{[l]}\} = p_l W^{[l]} z^{[l-1]},$$

- p_l corresponds to the probability of keeping a unit on layer l.

Dynamics of a single linear unit

- Consider the error terms for the averaged ensemble network, and dropout:

$$E^{\text{ens}} = (y^{(i)} - p_l W^{[l]} x^{(i)})^2$$
$$E^{\text{d}} = (y^{(i)} - W^{[l]} D^{[l]} x^{(i)})^2.$$

- We want to minimize these cost functions.

1. Compute the gradients.
2. Take expectation over dropout realizations.
3. Obtain:

$$\mathbb{E}\{E^{\text{d}}\} = E^{\text{ens}} + \sum_{r=1}^{n_1} \frac{1}{2} \text{var}(D^{[l]})(x_r^{(i)})^2 w_r^2$$

- Dropout corresponds to a regularized cost function of the ensemble network.

Dropout in logistic regression

- Single logistic unit with n inputs:

$$\sigma(z) = a^{[1]} = \frac{1}{1+e^{-z}} \text{ and } z = w^T x.$$

- The ***normalized weighted geometric mean*** over al possible network configurations corresponds to a feedforward pass of the averaged weights.

$$\text{NWGM} = \frac{G}{G+G'} = \frac{1}{1+e^{-\sum_j pw_j x_j}} = \sigma(pz).$$

- Definitions:
  - Total number of network configurations: $m = 2^n$.
  - $a_1^{[1]}, \ldots, a_m^{[1]}$ possible outcomes.
  - Weighted geometric mean: $G = \prod_i (a_i^{[1]})^{P_i}$.
  - Weighted geometric mean of the complements $G' = \prod_i (1 - a_i^{[1]})^{P_i}$.

Dynamics of a single logistic unit

- The result from a single linear unit generalizes to a sigmoidal unit as well.
- The expected gradient of the dropout network:

$$\mathbb{E}\left\{\frac{\partial E^{\mathrm{d}}}{\partial w_i}\right\} \approx \frac{\partial E^{\mathrm{ens}}}{\partial w_i} + \lambda \sigma'(pz) x_i^2 \operatorname{var}(p) w_i.$$

- The expectation of the dropout gradient corresponds approximately to the gradient of the ensemble network plus a ridge regularization term.

Dropout in Deep Neural Networks

- Network of sigmoidal units.
- Output of unit i in layer l: $a_i^{[l]} = \sigma\Big(\sum_j W_{ij}^{[l]} a^{[l-1]}\Big)$
- ***Normalized weighted geometric mean***:

$$\mathrm{NWGM}(a_i^{[l]}) = \frac{\Pi_N (a_i^{[l]})^{P(N)}}{\Pi_N (1 - a_i^{[l]})^{P(N)} + \Pi_N (a_i^{[l]})^{P(N)}}$$

  where N ranges over all possible configuration networks.
- Averaging properties of dropout:

$$\mathbb{E}\{a_i^{[l]}\} = \sigma\Big(\mathbb{E}\Big\{\sum_j W_{ij}^{[l]} a_i^{[l-1]}\Big\}\Big)$$

- **Take-home message:** the expected dropout gradient corresponds to an approximated ensemble network, regularized by an adaptive weight decay with a propensity for self-consistent variance minimization.
- **Convergence** can be understood via analysis of stochastic gradient descent.

Batch normalization

Problems of deep networks

- Adaptive reparametrization, motivated by the difficulty of training very deep models.
- Parameters from all layers are updated at the same time.
  - composition of many functions can have unexpected results because all functions have been changed simultaneously.
  - learning rate becomes difficult to tune.
- Consider a linear network with a single neuron per layer and single input.
- We update $w \leftarrow w - \epsilon g$, where $g = \nabla_w J$:

$$\hat{y} \leftarrow (w^{[1]} - \epsilon g^{[1]})(w^{[2]} - \epsilon g^{[2]}) \dots (w^{[L]} - \epsilon g^{[L]})x.$$

- Previous update has many high order components, that can influence greatly the value of $\hat{y}$.

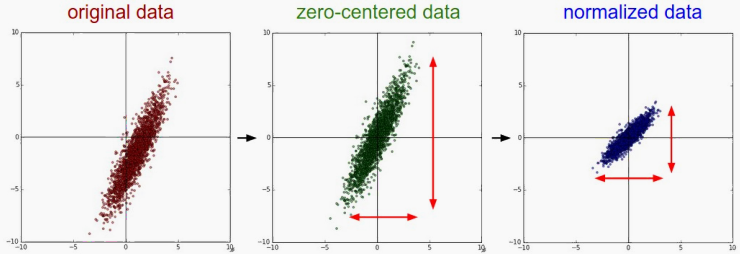
Input normalization

- The method is inspired by the normalization step normally applied to an input:

$$\widetilde{X}^{\{i\}} = \frac{X^{\{i\}} - \mu}{\sigma + \epsilon}$$

where $\epsilon = 10^{-8}$ is frequently used,

$$\mu = \frac{1}{m}\sum_r x^{\{i\}(r)}, \text{ and } \sigma^2 = \frac{1}{m}\sum_r (x^{\{i\}(r)} - \mu)^2.$$



Batch normalization

- Batch normalization extends the concept to other hidden layers.

$$Z^{\{i\}[l]}_{\text{norm}} = \frac{Z^{\{i\}[l]} - \mu^{\{i\}[l]}}{\sigma^{\{i\}[l]} + \epsilon}$$

where

$$\mu^{\{i\}[l]} = \frac{1}{m}\sum_r z^{\{i\}[l](r)}, \text{ and } (\sigma^{\{i\}[l]})^2 = \frac{1}{m}\sum_r (z^{\{i\}[l](r)} - \mu^{\{i\}[l]})^2.$$

- i refers to the mini-batch index; m to the number of elements.
  - the normalization depends on the minibatch.
- The outcome is rescaled with new parameters:

$$\widetilde{Z}^{\{i\}[l]} = \gamma^{\{i\}[l]} Z^{\{i\}[l]}_{\text{norm}} + \beta^{\{i\}[l]},$$

where $\gamma^{\{i\}[l]}$ and $\beta^{\{i\}[l]}$ are incorporated in the learning process.

Batch normalization

- The scheme has the same expressive capabilities
  - setting $\beta^{\{i\}[l]} = \mu^{\{i\}[l]}$ and $\gamma^{\{i\}[l]} = \sigma^{\{i\}[l]}$.
- The weights from one layer do not affect the statistics (first and second order) of the next layer.
- The offsets $b^{[l]}$ become obsolete.
- **Testing:** a weighted average on all parameters:

$$\gamma_t = \beta\gamma_t + (1-\beta)\gamma^{\{i\}[l]}$$
$$\beta_t = \beta\beta_t + (1-\beta)\beta^{\{i\}[l]}$$
$$\mu_t = \beta\mu_t + (1-\beta)\mu^{\{i\}[l]}$$
$$\sigma_t = \beta\sigma_t + (1-\beta)\sigma^{\{i\}[l]}$$