Improving Deep Neural Networks

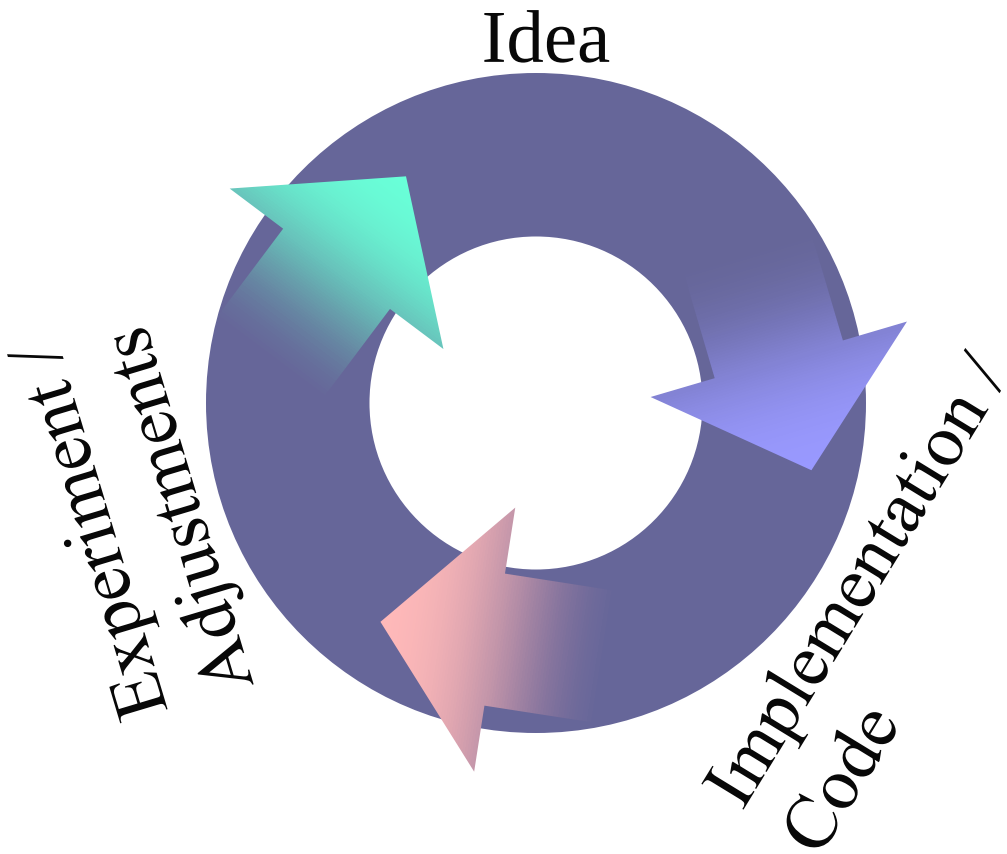
- Data set split
- Regularization
- Hyperparameter tuning
- Optimization

[DeepLearning.AI, Improving Deep Neural Networks: Hyperparameter tuning, Regularization and Optimization, https://www.coursera.org/learn/deep-neural-network/home/welcome]

[SHUBHAM JAIN, An Overview of Regularization Techniques in Deep Learning (with Python code), APRIL 19, 2018, https://www.analyticsvidhya.com/blog/2018/04/fundamentals-deep-learning-regularization-techniques/]

Machine learning – intensive iterative process

Layers
Hidden units
Learning rates
Activation function
Epochs
Batch
…



How efficiently can you go round this cycle?

Train / Val /Test split

Train set: used to learn the parameters of the model

Val set (validation set): supervises the learning generality (identify overfitting);
Used to rank different models in terms of their accuracy (decide which models to proceed further with); parameter choice and model choice

Test set: used as a proxy for unseen data and evaluate our model on test-set (brand-new data set)

Size of training/val/test split

Small / moderate data set:

- **70% / 20% /10%**

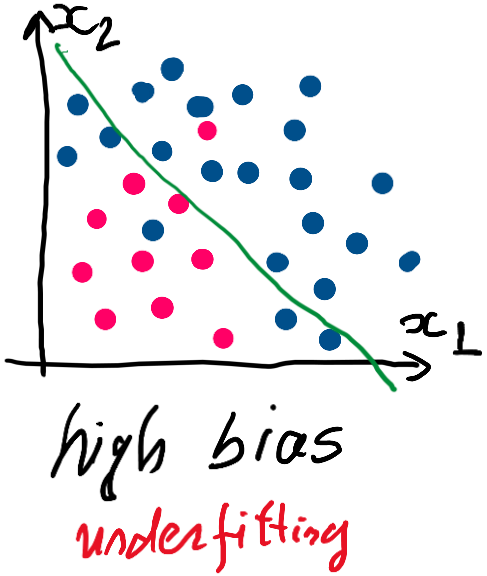
Big data set:

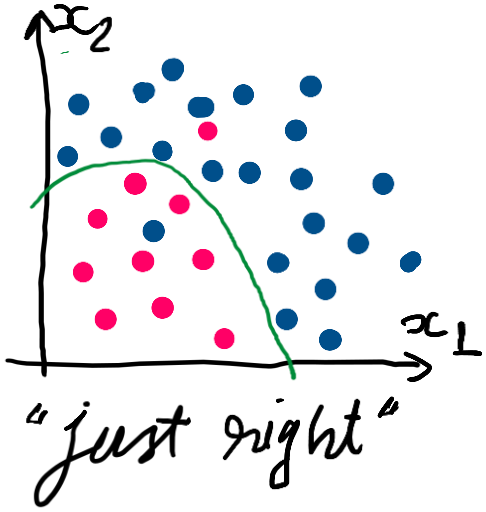
Val set ~ 1000 – 10000 example; Test set ~ 100 – 1000 example

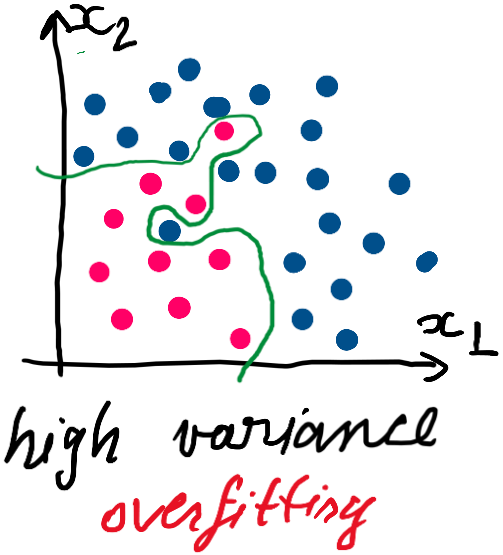
https://snji-khjuria.medium.com/everything-you-need-to-know-about-train-dev-test-split-what-how-and-why-6ca17ea6f35

Bias / Variance

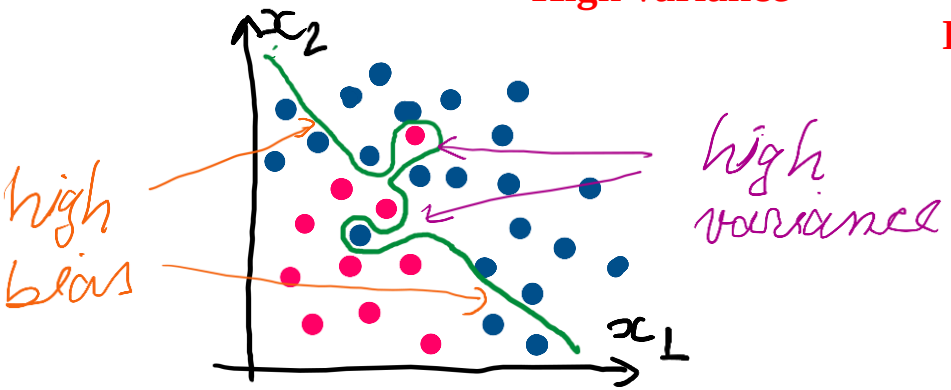
2D data; binary classifier





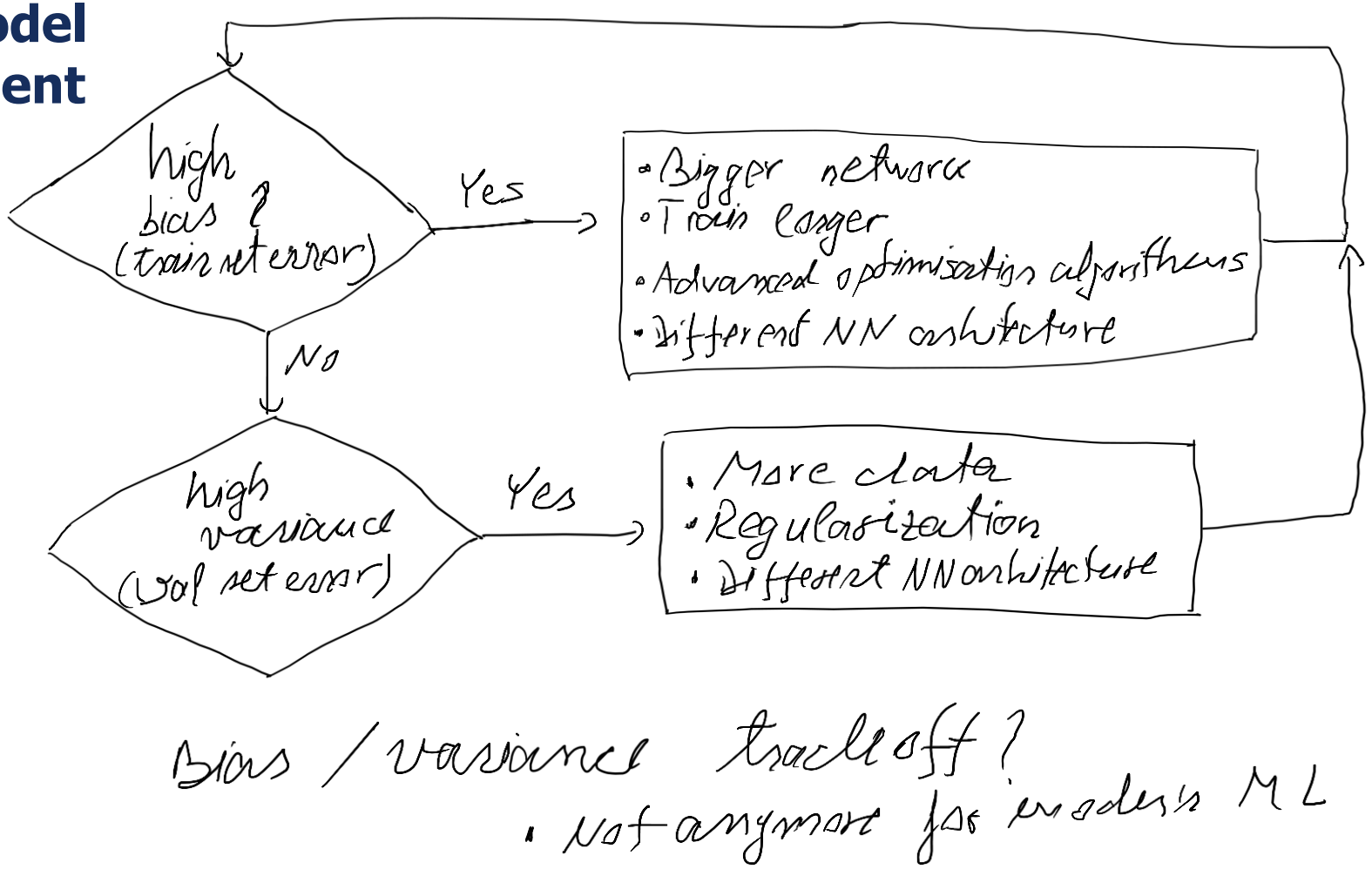


Train set error:	1%	14 %	14%	0.6%
Val set error:	12%	15 %	21%	0.9%
	High variance	Low variance High bias	High variance High bias	Low variance Low bias



Same model can present high bias in one region and high variance in another region !

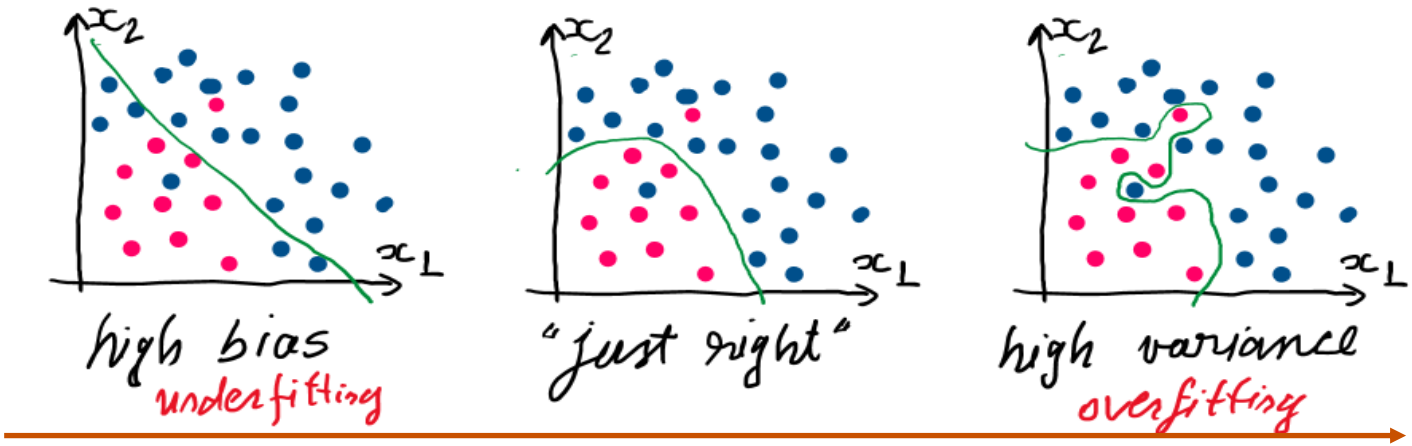
Basic recipe for ML model development



Training a bigger network almost never hurts.

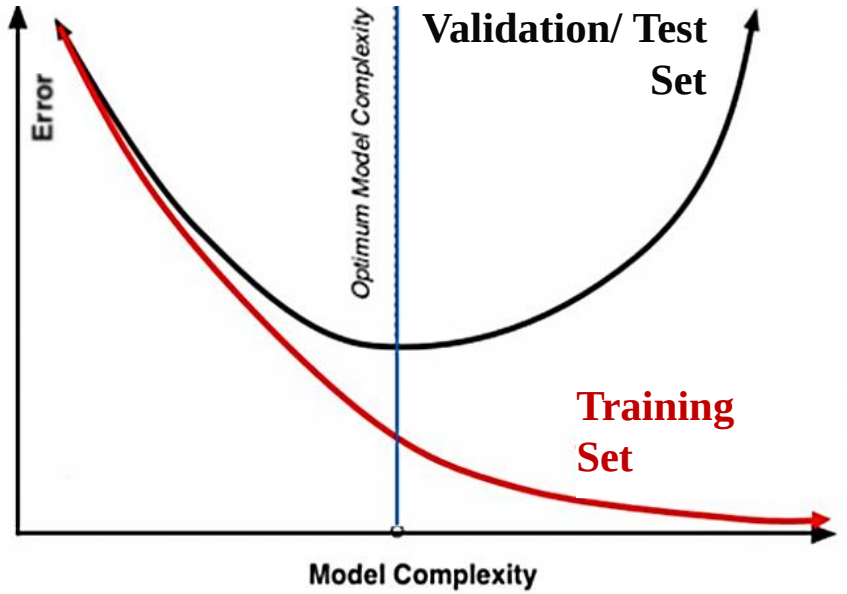
Main cost of training a neural network that's too big is just computational time, so long as you're regularizing (to avoid overfitting).

Overfitting



The model tries to learn too well the details and noise from the training data
Poor performance on the other data (validation/test data)
The complexity of the model increases
Training error decreases Validation / testing error increases

Training vs. Validation / Test Set Error



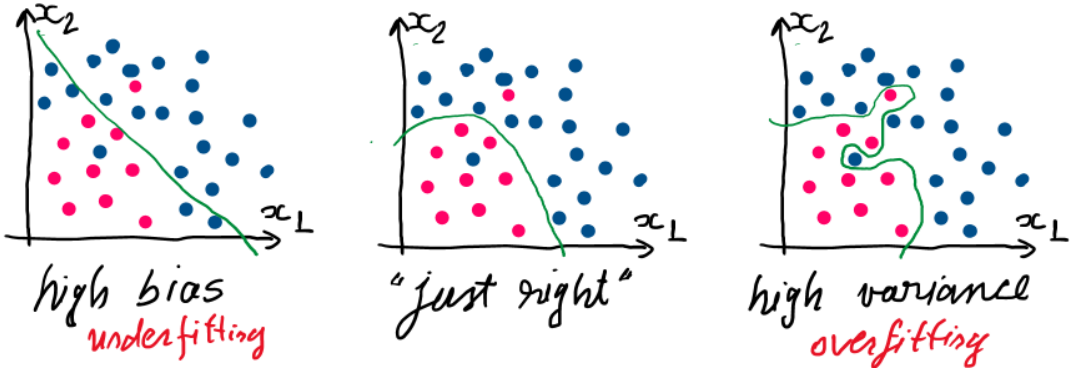
One of the most common problem data science professionals face is avoiding **overfitting**

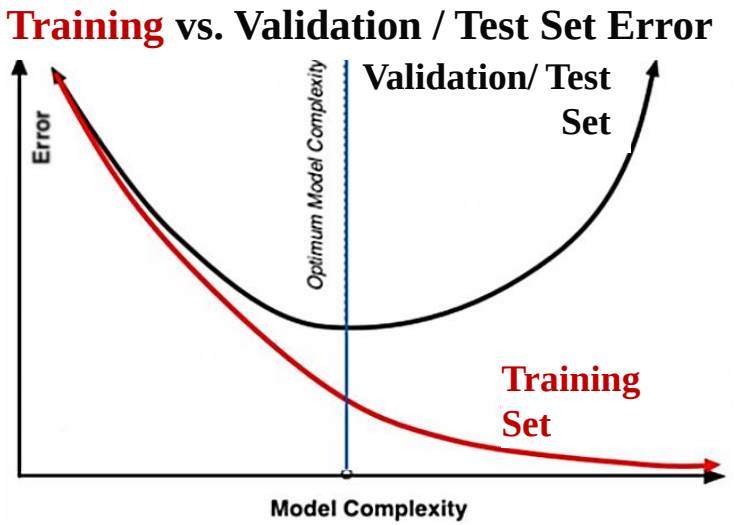
The model

- **exceptionally well on training data,**
- **quite poorly on validation data**
- **not able to make accurate predictions on test data**

[SHUBHAM JAIN, An Overview of Regularization Techniques in Deep Learning (with Python code), APRIL 19, 2018, https://www.analyticsvidhya.com/blog/2018/04/fundamentals-deep-learning-regularization-techniques/]

Regularization





- **Avoiding overfitting can single-handedly improve our model's performance**

Regularization is a technique which makes **slight modifications to the learning algorithm** such that the model **generalizes better**.

- ✓ This in turn **improves the model's performance on the new (unseen) data**

In machine learning, regularization penalizes the coefficients.

In deep learning, it actually **penalizes the weight matrices** of the nodes.

Regularization

- When you decrease the number of training parameters you usually get a lot of benefits such as smaller model making them fit into memory easier.
- However, that usually lowers the performance.
- So, the main challenge is
  - **decrease the number of parameters without lowering the performance**.

A huge regularization effect on small images would cause underfitting and a small regularization effect on large images would cause overfitting.

Mostafa Ibrahim, Google releases EfficientNetV2 — a smaller, faster, and better EfficientNet, Apr 3 2021, https://towardsdatascience.com/google-releases-efficientnetv2-a-smaller-faster-and-better-efficientnet-673a77bdd43c

L2 & L1 regularization

If neural network is overfitting the data (high variance):

- regularization
- get more training data (can't always get more training data / could be expensive to get more data

Adding regularization often help to prevent overfitting / reduce the errors in the NN

Adding L2 / L1 penalty term:

Cost function must be minimized

$$cost\_r = cost + \text{penalty term}$$

L2 regularization $$cost\_r = cost + \frac{\lambda}{2m}\sum||w||^2$$

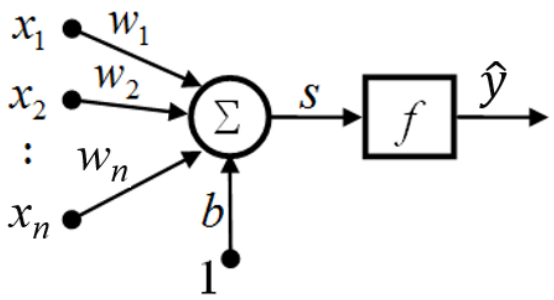
L1 regularization $$cost\_r = cost + \frac{\lambda}{2m}\sum||w||$$

λ – the regularization parameter

L2 regularization is also known as *weight decay* as it forces the weights to decay towards zero (but never zero).

For L1 regularization the weights may be reduced to zero.

Logistic regression
L2 & L1 regularization



$$s = w^T x + b \quad \hat{y} = f(s)$$

$$\hat{y} = f(w^T x + b)$$

Cost function across m examples is:

$$J(w, b) = \frac{1}{m} \sum_{i=1}^{m} \mathcal{L}(\hat{y}^{(i)}, y^{(i)})$$

minimise $J(w, b)$ over w, b

- Add regularization:

$$J(w, b) = \frac{1}{m} \sum_{i=1}^{m} \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2m} \|w\|_2^2$$

λ - regularization parameter

L_2 regularization – 2nd order

$$\|w\|_2^2 = \sum_{j=1}^{n} w_j^2 = w^T w$$ Euclidean norm

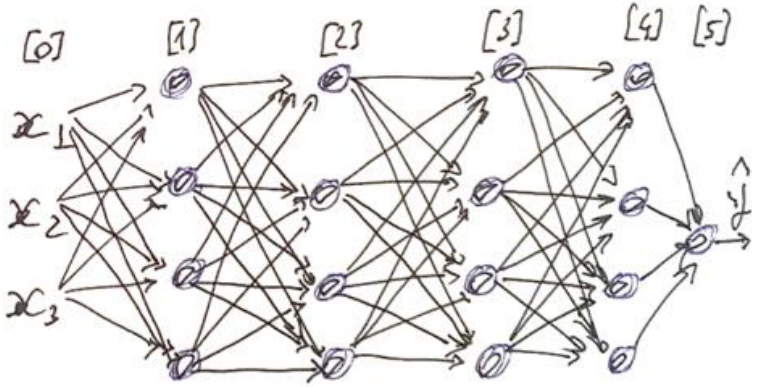
L_1 regularization – 1st order

L_1 regularization: $+\frac{\lambda}{2m} \|w\|_1$

$$\|w\|_1 = \sum_{j=1}^{n} |w_j|$$

λ is a hyperparameter to be tuned.

Neural network
L2 regularization



$$J(w^{[1]}, b^{[1]}, \dots, w^{[L]}, b^{[L]}) = \frac{1}{m} \sum_{i=1}^{m} \left(\mathcal{L}(\hat{y}^{(i)}, \hat{y}^{(i)}) \right)$$

$$\min_{w^{[\ell]}, b^{[\ell]}} J(w^{[\ell]}, b^{[\ell]}) \quad \ell = 1, \dots L$$

$$J(w^{[1]}, b^{[1]}, \dots, w^{[L]}, b^{[L]}) = \frac{1}{m} \sum_{i=1}^{m} \left(\mathcal{L}(\hat{y}^{(i)}, y^{(i)}) \right) + \frac{\lambda}{2m} \sum_{\ell=1}^{L} \| w^{[\ell]} \|_F^2$$

Cost | cross-entropy cost | regularization cost

$$\| w^{[\ell]} \|_F^2 = \sum_{i=1}^{n^{[\ell]}} \sum_{j=1}^{n^{(\ell-1)}} \left(w_{ij}^{[\ell]} \right)^2$$

$$w^{(\ell)} : \left(n^{(\ell)}, n^{(\ell-1)} \right)$$

Frobenius norm (sum of squares of elements of a matrix)

Neural network - L_2 regularization **GDA implementation**

- **Without regularization**

$$J(w^{[1]}, b^{[1]}, \dots, w^{[L]}, b^{[L]}) = \frac{1}{m} \sum_{i=1}^{m} \mathcal{L}(\hat{y}^{(i)}, y^{(i)})$$

$$w^{[l]} := w^{[l]} - \eta \, dw^{[l]} \qquad dw^{[l]} = \frac{\partial J}{\partial w^{[l]}}$$

- **With regularization**

$$J(w^{[1]}, b^{[1]}, \dots, w^{[L]}, b^{[L]}) = \frac{1}{m} \sum_{i=1}^{m} \left(\mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2m} \sum_{l=1}^{L} \| w^{[l]} \|_F^2 \right)$$

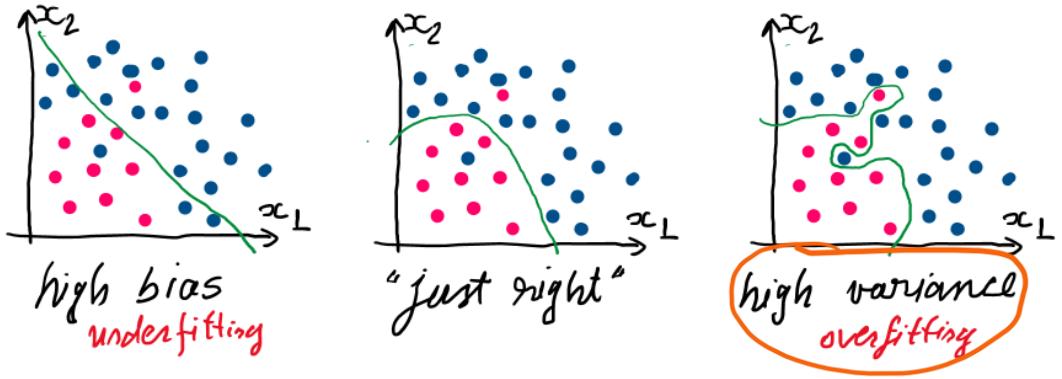
$$w^{[l]} := w^{[l]} - \eta \left(dw^{[l]} + \frac{\lambda}{m} w^{[l]} \right) = w^{[l]} - \frac{\eta\lambda}{m} w^{[l]} - \eta \, dw^{[l]}$$

$$w^{[l]} := \left(1 - \frac{\eta\lambda}{m}\right) w^{[l]} - \eta \, dw^{[l]}$$

Weight decay

- the coefficient in front of $w^{[l]} < 1$

Why L2 regularization reduces overfitting? (intuition)

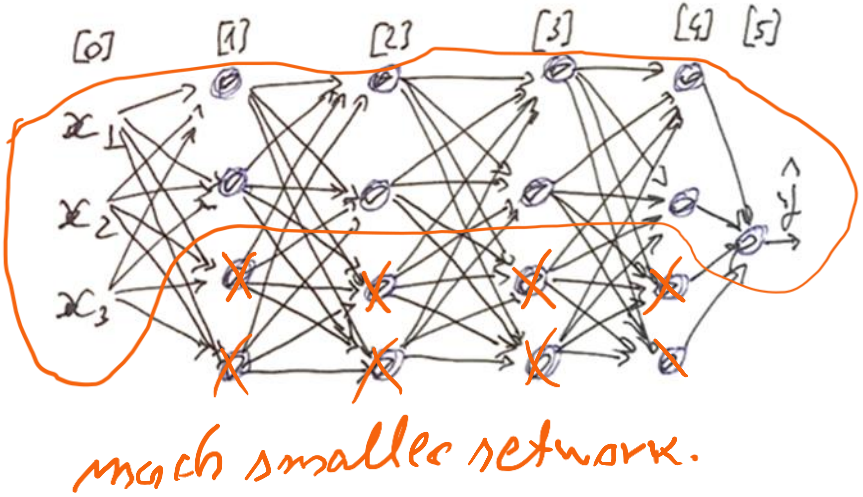


$$J(w^{[1]}, b^{[1]}, \ldots, w^{[L]}, b^{[L]}) = \frac{1}{m}\sum_{i=1}^{m} \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2m}\sum_{l=1}^{L} \|w^{[l]}\|_F^2$$

Why does this term reduce overfitting?

The *w* weights are stimulated to become very small (close to zero), to minimize *J*

$w_{ij} \sim 0$ for a lot of hidden neurons



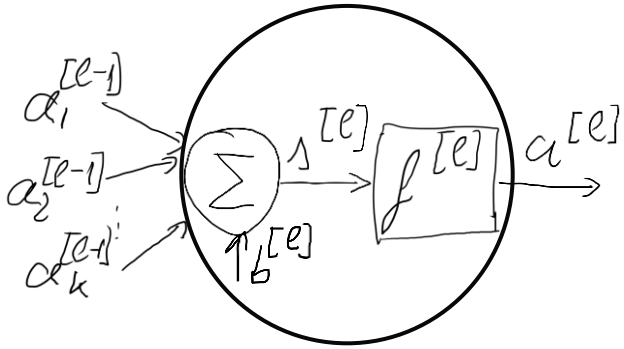
This highly simplified neural network (much smaller neural network) will take us from the overfitting case closer to the underfitting case (for large λ).

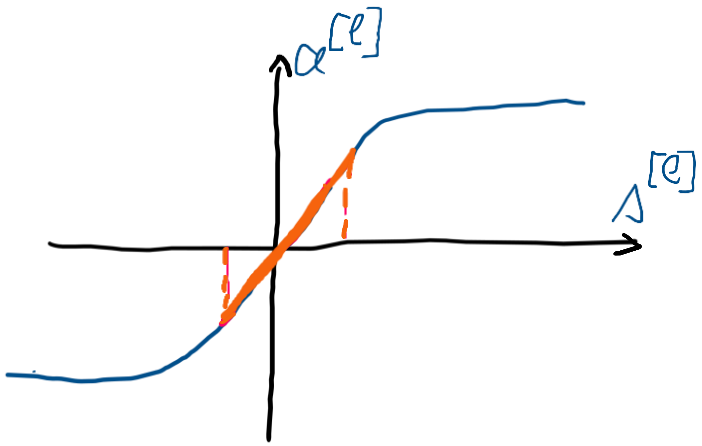
Hopefully, there will be an intermediate value of λ that leads toward just right case.

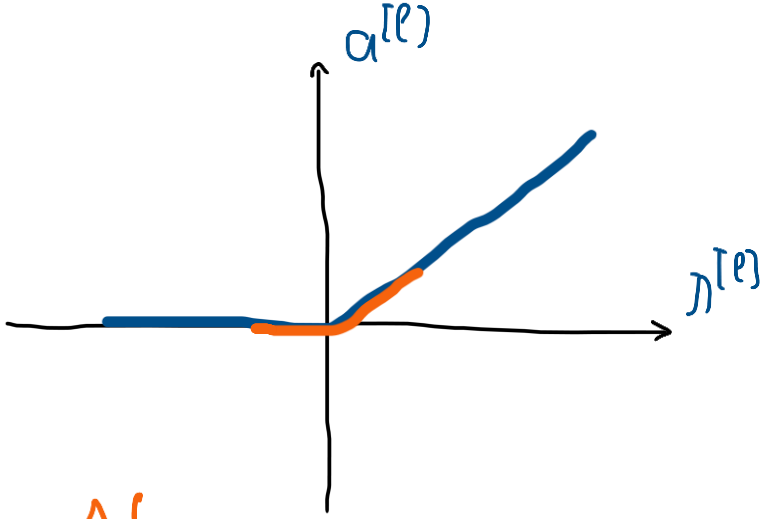
We can think of it as zeroing out or at least reducing the impact of a lot of the hidden units (especially the least significative weights).

Variance reduction

Why L2 regularization reduces overfitting? (intuition) – cont.







$\lambda \uparrow,\ w \downarrow,\ z \downarrow$

We are entering a narrow, almost linear region of the transfer function
This happens for all neurons, in all layers.

So, the NN decreases its degree of nonlinearity, approaching linearity and it cannot fit a verry complicated (highly non-linear) decision boundary

overfitting can hardly happen

Observations:

• The value of λ **is a hyperparameter that you can tune**.

• L2 regularization makes your decision boundary smoother. If λ is too large, it is also possible to "over-smooth", resulting in a model with high bias.

L2-regularization relies on the assumption that **a model with small weights is simpler than a model with large weights**.

Thus, by penalizing the square values of the weights in the cost function you drive all the weights to smaller values.

It becomes too costly for the cost function to have large weights!

This leads to a smoother model in which the output changes more slowly as the input changes.

In *keras (python)*, we can directly **apply regularization to any layer**

Sample code to apply **L2 regularization to a Dense layer**.

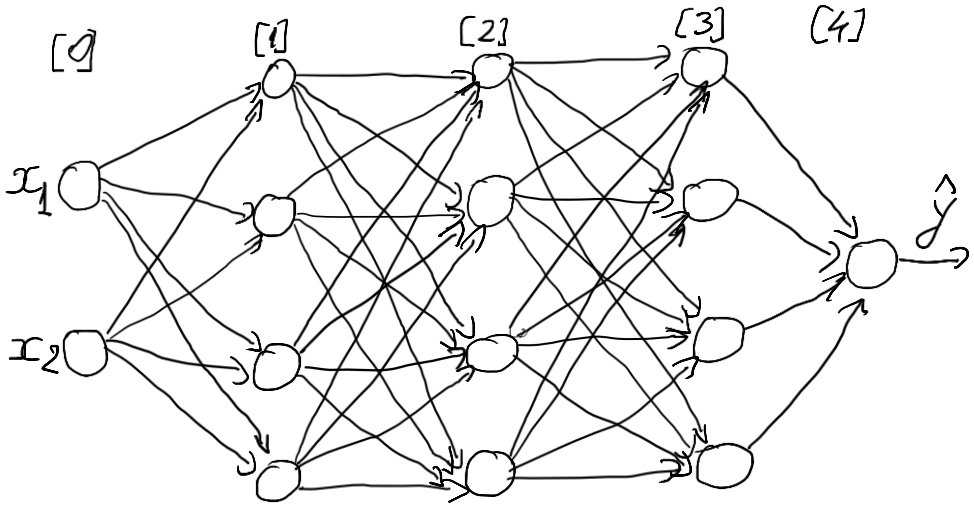
```
from keras import regularizers
model.add(Dense(64, input_dim=64,
                kernel_regularizer=regularizers.l2(l2 = 0.01)
```

0.01 is the value of regularization parameter, i.e., lambda.

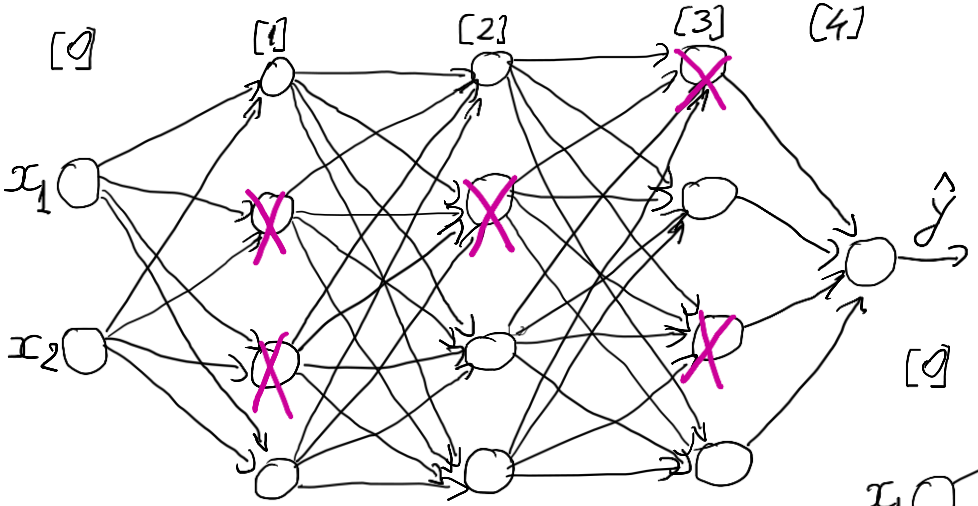
Sample code to apply **L1 regularization to a Dense layer**.

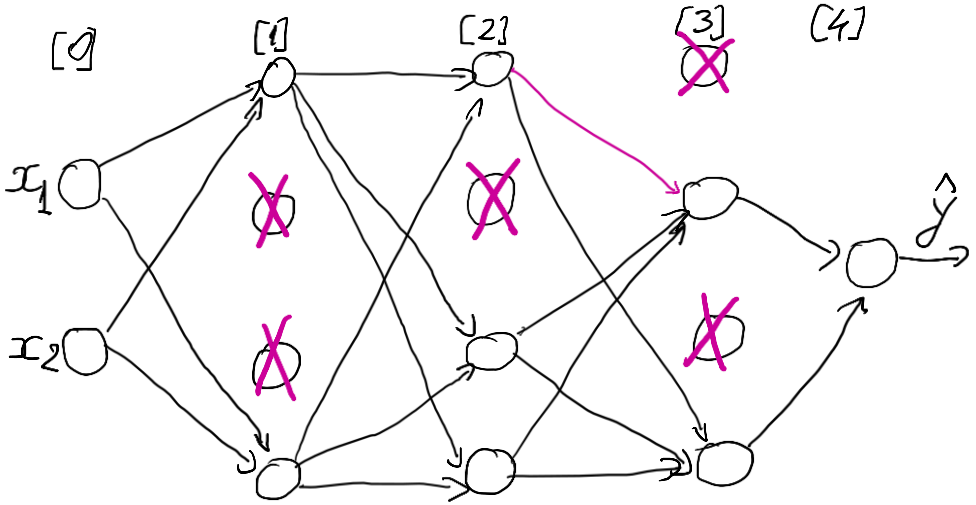
```
from keras import regularizers
model.add(Dense(64, input_dim=64,
                kernel_regularizer=regularizers.l1(l1 = 0.01)
```

Dropout regularization



At every iteration, dropout regularization **randomly** selects some nodes and removes them along with all their incoming and outgoing weights.





You end up with a much smaller, much diminished network.

Then you do back propagation training on this much diminished network.

Dropout regularization

Each training epoch has a different set of nodes and this results in a different set of outputs.
It can also be thought of as an ensemble technique in machine learning.

Ensemble models usually perform better than a single model as they capture more randomness.
Similarly, dropout also performs better than a normal neural network model.

At each epoch, you shut down (= set to zero) each neuron of a layer with a certain probability (*keep_prob*)

The dropped neurons don't contribute to the training in both the forward and backward propagations of the current training epoch.

In each training epoch, only a part of the network weights are updated (those not connected to shut-down neurons), so that the possibility of overfitting (learning by heart the training data set) is considerably diminished.

The **probability** of choosing how many nodes should be dropped is the **hyperparameter of the dropout function**.

Dropout can be applied to both the hidden layers as well as the input layers.

Dropout is usually preferred when we have a large neural network structure in order to introduce more randomness.

When you shut some neurons down, you actually modify your model.

The idea behind dropout is that at each iteration, you train a different model that uses only a subset of your neurons.

With dropout, your neurons thus become less sensitive to the activation of another specific neuron, because that other neuron might be shut down at any time.

Keras - Dropout layer

Dropout class

tf.keras.layers.Dropout(**rate**, noise_shape=None, seed=None, **kwargs)

hyperparameter

The Dropout layer randomly **sets units to 0** with a frequency of **rate** at each step during training time, which helps prevent overfitting.

Inputs not set to 0 are scaled up by 1/(1 - rate) such that the sum over all inputs is unchanged (inverted dropout).

Note that the Dropout layer only applies when training is set to True such that no values are dropped during inference.

Dropout is inactive at inference time.

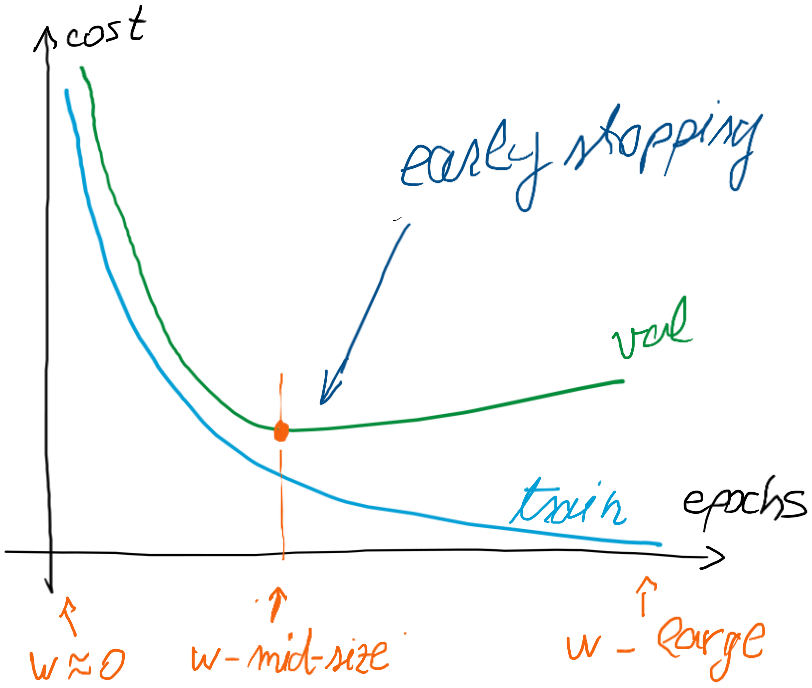
The trained network contains all neurons

[https://keras.io/api/layers/regularization_layers/dropout/]

Other regularization techniques

Early stopping

The advantage of early stopping is that running the gradient descent process just once, you get to try out values of small *w*, mid-size *w*, and large *w*, without needing to try a lot of values of the L2 regularization hyperparameter lambda.



Rather than using early stopping, one alternative is just use L2 regularization, then you can just train the neural network as long as possible.

The downside of this: you might have to try a lot of values of the regularization parameter lambda. This makes searching over many values of lambda more computationally expensive.

Other regularization techniques - Early stopping

Keras - EarlyStopping

https://keras.io/api/callbacks/early_stopping/

EarlyStopping class

```
tf.keras.callbacks.EarlyStopping(
    monitor="val_loss",
    min_delta=0,
    patience=0,
    verbose=0,
    mode="auto",
    baseline=None,
    restore_best_weights=False,
)
```

Stop training when a monitored metric has stopped improving.

Assuming the goal of a training is to minimize the loss. With this, the metric to be monitored would be 'loss', and mode would be 'min'.

A model.fit() training loop will check at end of every epoch whether the loss is no longer decreasing, considering the min_delta and patience if applicable.

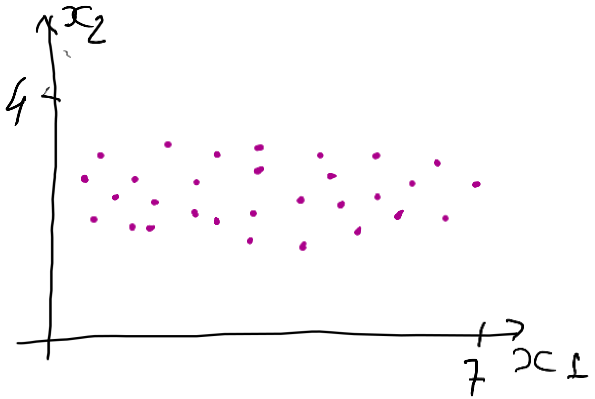
Once it's found no longer decreasing, model.stop_training is marked True and the training terminates.

```
>>> callback = tf.keras.callbacks.EarlyStopping(monitor='loss', patience=3)
>>> # This callback will stop the training when there is no improvement in
>>> # the loss for three consecutive epochs.
>>> model = tf.keras.models.Sequential([tf.keras.layers.Dense(10)])
>>> model.compile(tf.keras.optimizers.SGD(), loss='mse')
>>> history = model.fit(np.arange(100).reshape(5, 20), np.zeros(5),
...                     epochs=10, batch_size=1, callbacks=[callback],
...                     verbose=0)
>>> len(history.history['loss'])  # Only 4 epochs are run.
4
```

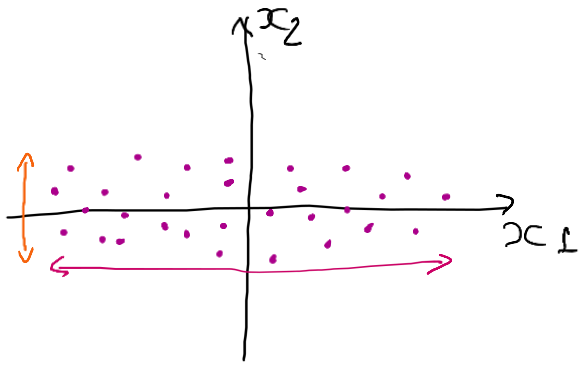
Setting up the optimization problem

- Data normalization
- Network (weights) initialization

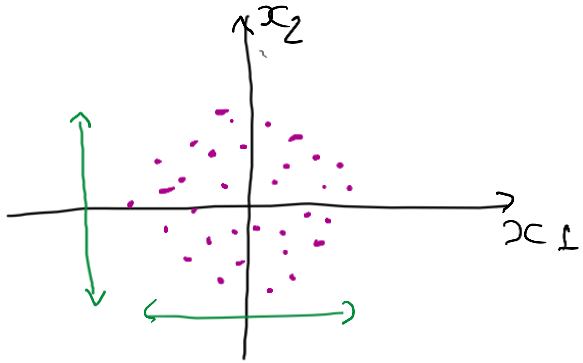
Normalizing inputs



Initial dataset



Subtract mean (zero out the mean)



Normalize the variance

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$\mu = \frac{1}{m} \sum_{i=1}^{m} x^{(i)} \; ; \; \mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}$$

$$x := x - \mu$$

μ – mean

$$\sigma^2 = \frac{1}{m} \sum_{i=1}^{m} \left(x^{(i)}\right)^2$$

σ^2 – variance

$$x := \frac{x}{\sigma}$$

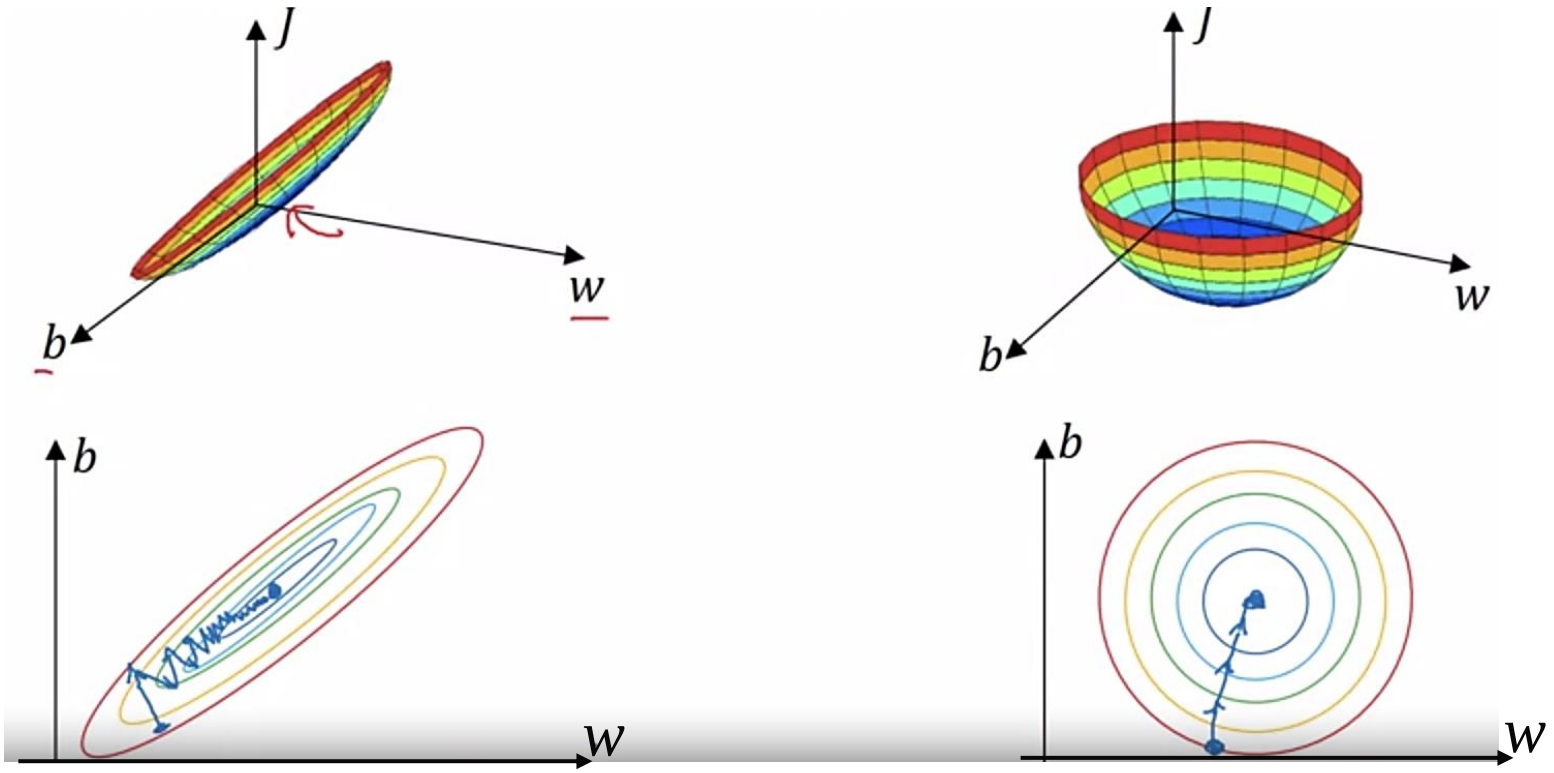
σ – standard deviation $\quad \sigma = \begin{bmatrix} \sigma_1 \\ \sigma_2 \end{bmatrix}$

Use the same μ, σ to normalize all data sets

- ✓ **Training**
- ✓ **Validation**
- ✓ **Test**

Why normalization?

$$J(w,b) = \frac{1}{m}\sum_{i=1}^{m} \mathcal{L}\left(\hat{y}^{(i)}, y^{(i)}\right)$$



Unnormalized

Very low learning rate, a lot of steps

Normalized

Go straight to the minima

J is easier and faster to optimize

[DeepLearning.AI, Improving Deep Neural Networks: Hyperparameter tuning, Regularization and Optimization, https://www.coursera.org/learn/deep-neural-network/home/welcome]

Vanishing / exploding gradients – network initialization

(Very) Deep neural network have a **major setback**

- **vanishing gradient**
- **exploding gradient**

Exploding gradient

In deep networks, **error gradients can accumulate** during an update and result in very large gradients. The explosion occurs through exponential growth by repeatedly multiplying gradients through the network layers that have values larger than 1.0.

These in turn result in large updates to the network weights, and in turn, an unstable network. At an extreme, the values of weights can become so large as to overflow and result in NaN values.

Vanishing gradient

When *n* hidden layers use an activation that give small gradients (below unity, like the sigmoid function), *n* small derivatives are multiplied together. Thus, the **error gradient decreases exponentially** as we propagate down to the initial layers.

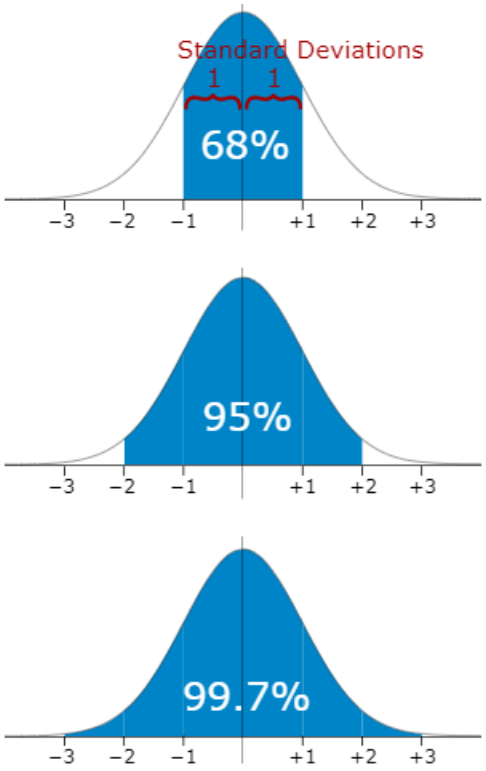
A small gradient means that the weights and biases of the initial layers will not be updated effectively with each training session. Since these initial layers are often crucial to recognizing the core elements of the input data, it can lead to overall inaccuracy of the whole network.

Vanishing / exploding gradients – network initialization

Partial solution – careful choice of the **random initialization of the network** (initial weights)

$$W^{[l]} = \text{np.random.randn}(n^{[l]}, n^{[l-1]}) * \text{np.sqrt}\left(\frac{cst}{n^{[l-1]}}\right)$$

standard normal distribution
(mean = 0, standard deviation = 1)



Introduces a variance that depends on the number of input features for the layer

Can be seen as a hyperparameter to be tuned

$cst = 2$ for *ReLU* activation function
$cst = 1$ for *tanh* activation function

Hopefully, that makes the weights not explode too quickly and not decay to zero too quickly, so you can train a reasonably deep network without the weights or the gradients exploding or vanishing too much.

Overfitting and regularization - recommended reading

http://neuralnetworksanddeeplearning.com/chap3.html#overfitting_and_regularization

Setting a DNN –recommended exercise

http://playground.tensorflow.org/#activation=relu&regularization=L2&batchSize=5&dataset=xor&regDataset=reg-gauss&learningRate=0.03&regularizationRate=0.001&noise=20&networkShape=2&seed=0.93433&showTestData=false&discretize=true&percTrainData=70&x=true&y=true&xTimesY=false&xSquared=false&ySquared=false&cosX=false&sinX=false&cosY=false&sinY=false&collectStats=false&problem=classification&initZero=false&hideText=false

Augmentation, L2 regularization, dropout implementation – recommended programimg exercise

https://colab.research.google.com/drive/1moK2cq2SSgJLB68uNyvjyrGQKjwh8hKU?usp=sharing

To download the dataset:

https://drive.google.com/drive/folders/10HMkJbgl0XVtxGngP7NS1uWM9LbgrGez?usp=sharing

Tuning process

The processes that drive performance and generate good results systematically

Hyperparameters:

- Learning rate – most important
- Learning rate decay
- Mini-batch size
- Momentum term; hyperparameters of the optimization algorithms
- Number of layers
- Number of hidden units

Set regularization method and params