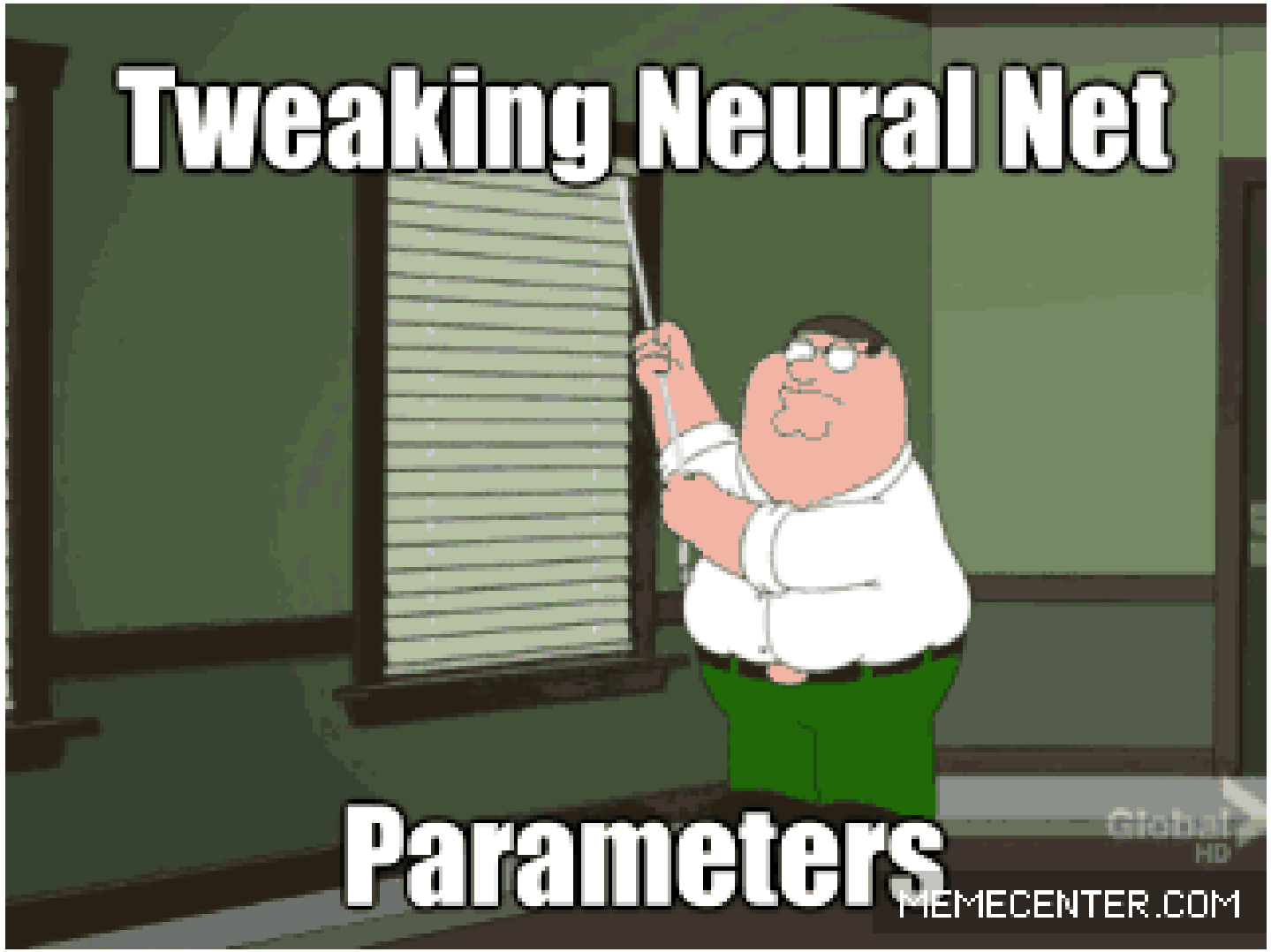
How to Train ~~Your Dragon~~ ConvNets

Stephen Baek

Factors Affecting Your Training Result:

- Network architecture
  - How many layers? How many neurons? Kernel size?
  - Skip connection? Inception (network-in-network)?
- Choice of activation functions
  - Sigmoid? Tanh? ReLU? LeakyReLU? PReLU? Others?
- Data preprocessing and sampling (Data distribution)
  - Data mean and standard deviation, minimum, maximum, noise
  - Train-val-test split, batching
  - Data augmentation, synthetic data, etc.
- ConvNet initialization
  - Initial solution for gradient descent (initial neuron weights and biases)
  - Transfer learning
- Network regularization
  - Dropouts, L1/L2 regularizers, early stopping, multi-task learning, ensemble, etc.
- Loss functions
  - MAE? MSE? LogCosh? Huber? Cross-entropy? Kullback-Leibler? Others?
- Optimization methods
  - Gradient descent? Momentum? Nesterov correction? Adaptive gradient? Adam? Nadam?
- So many other parameters to consider

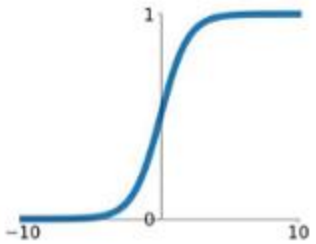

Tweaking Neural Net
Parameters
MEMECENTER.COM

Activation Functions

Recap: Activation Functions

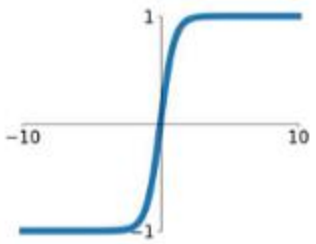
Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



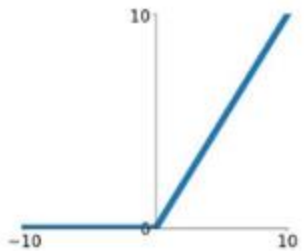
tanh

$$\tanh(x)$$



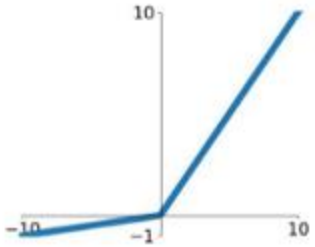
ReLU

$$\max(0, x)$$



Leaky ReLU

$$\max(0.1x, x)$$

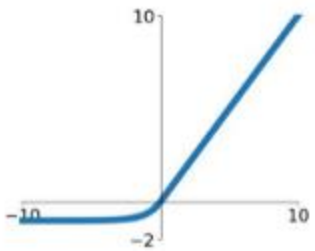


Maxout

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



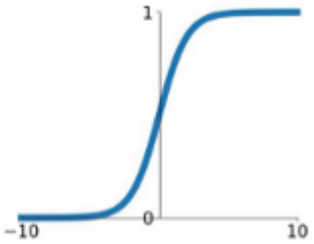
https://medium.com/@shrutijadon10104776/survey-on-activation-functions-for-deep-learning-9689331ba092

Historically the most popular choice: Sigmoid

- Brain analogy: saturating “firing rate” of a neuron
- Crushes input values to [0, 1].
  - Problems:
    1. Kills off gradients when saturated.
    2. Outputs are always non-negative (not zero-centered).
    3. Exponential! (computationally expensive)

Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



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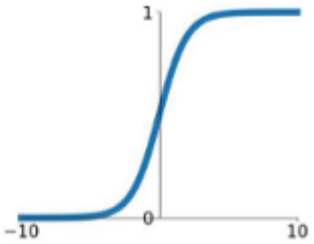
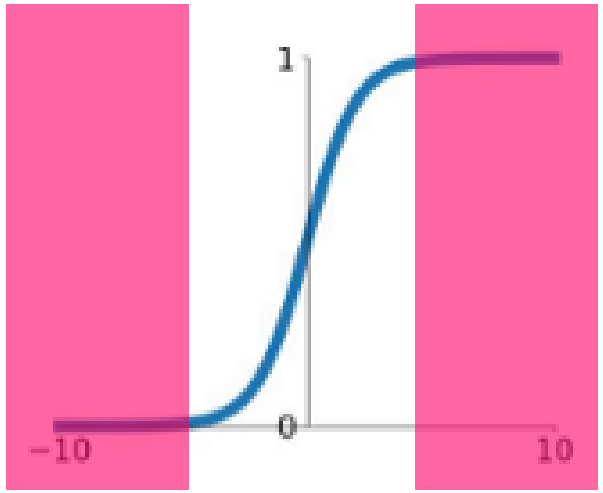
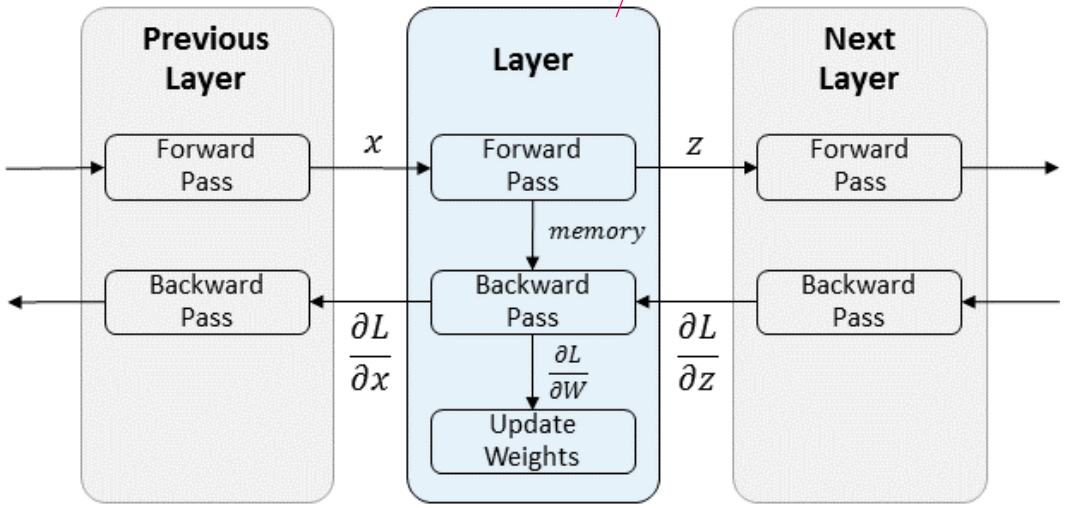


$$\frac{\partial \mathcal{L}}{\partial x} = \frac{\partial \mathcal{L}}{\partial \sigma}\frac{\partial \sigma}{\partial x}$$

$\frac{\partial \sigma}{\partial x}$ → 0



$$\frac{\partial \sigma}{\partial x} = 0$$



https://www.mathworks.com/help/nnet/ug/define-custom-deep-learning-layers.html

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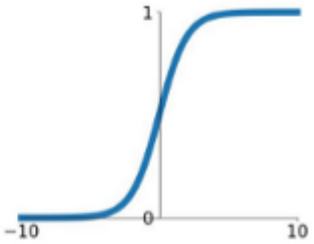

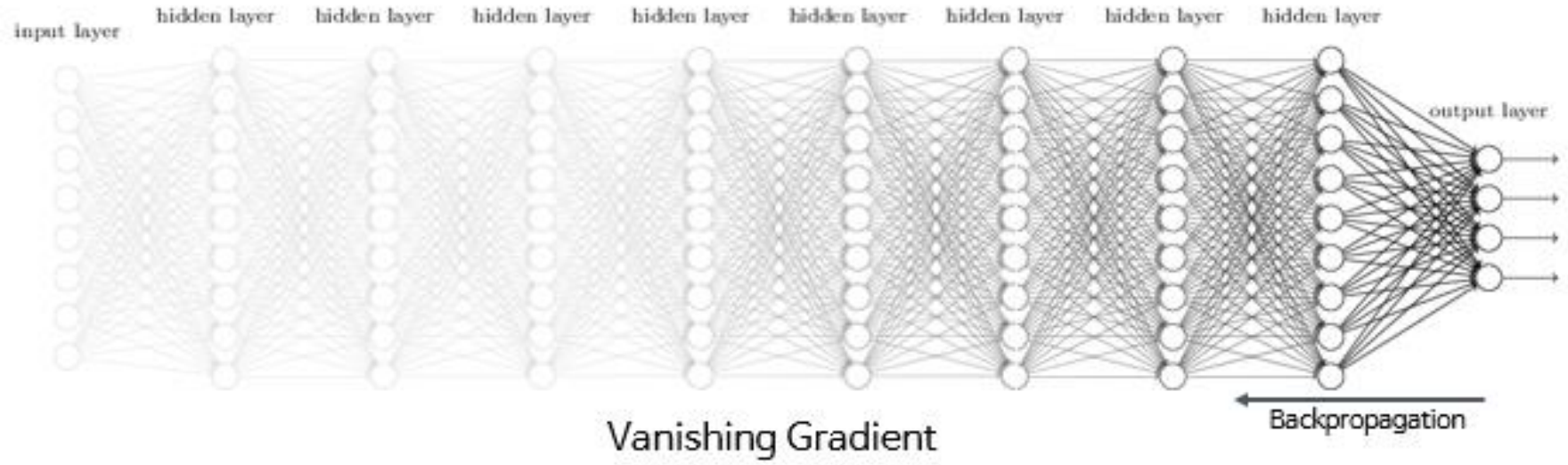

Vanishing Gradient

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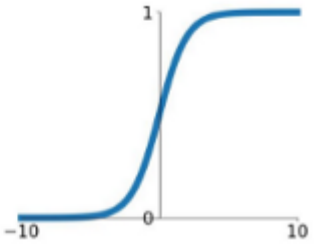
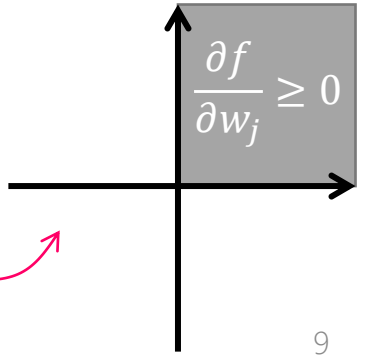


Q. What happens to the gradient if all the input to a neuron is always non-negative? i.e., $x_j \geq 0, \ \forall x_j$

$$f(x \mid \mathbf{w}, b) = \sum_j w_j x_j + b$$

$$\frac{\partial f}{\partial w_j} = x_j \geq 0 \ \ \forall j \quad \Rightarrow \quad \mathbf{w} \leftarrow \mathbf{w} - \alpha \frac{\partial \mathcal{L}}{\partial f} \frac{\partial f}{\partial \mathbf{w}}$$

scalar vector (gradient)



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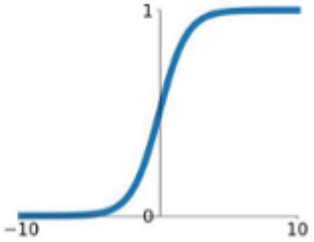

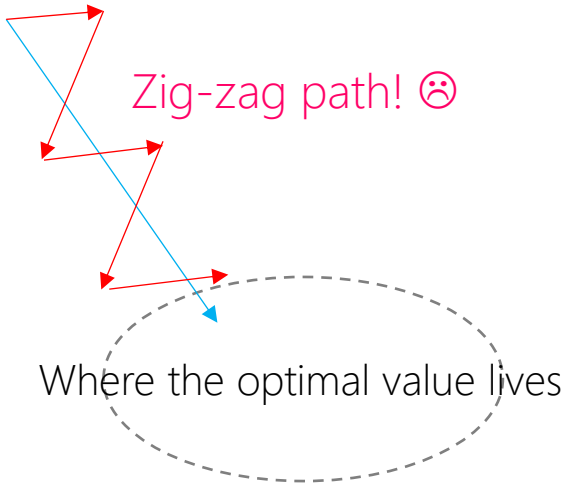

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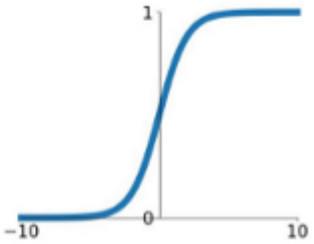


Operation	Input	Output	Algorithm	Complexity
Addition	Two n-digit numbers N, N	One n+1-digit number	Schoolbook addition with carry	$\Theta(n)$, $\Theta(\log(N))$
Subtraction	Two n-digit numbers N, N	One n+1-digit number	Schoolbook subtraction with borrow	$\Theta(n)$, $\Theta(\log(N))$
Multiplication	Two n-digit numbers	One 2n-digit number	Schoolbook long multiplication	$O(n^2)$
			Karatsuba algorithm	$O(n^{1.585})$
			3-way Toom–Cook multiplication	$O(n^{1.465})$
			k-way Toom–Cook multiplication	$O(n^{\log(2k-1)/\log k})$
			Mixed-level Toom–Cook (Knuth 4.3.3-T)[2]	$O(n\, 2^{\sqrt{2\log n}} \log n)$
			Schönhage–Strassen algorithm	$O(n \log n \log\log n)$
			Fürer's algorithm[3]	$O(n \log n\, 2^{O(\log^* n)})$
Division	Two n-digit numbers	One n-digit number	Schoolbook long division	$O(n^2)$
			Newton–Raphson division	$O(M(n))$
Square root	One n-digit number	One n-digit number	Newton's method	$O(M(n))$
Modular exponentiation	Two n-digit numbers and a k-bit exponent	One n-digit number	Repeated multiplication and reduction	$O(M(n)\, 2^k)$
			Exponentiation by squaring	$O(M(n)\, k)$
			Exponentiation with Montgomery reduction	$O(M(n)\, k)$

https://en.wikipedia.org/wiki/Computational_complexity_of_mathematical_operations

Hyperbolic Tangent (LeCun et al. 1991)

- "Rescaled sigmoid"

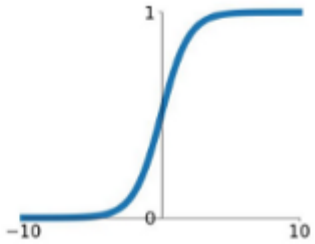
$$2\frac{1}{1+e^{-x}} - \frac{(1+e^{-x})}{1+e^{-x}} = \frac{1-e^{-x}}{1+e^{-x}}$$

$$\tanh(x) = \frac{e^{x}-e^{-x}}{e^{x}+e^{-x}} = \frac{1-e^{-2x}}{1+e^{-2x}}$$

- Now it's zero-centered ☺
  - but still…
    - Kills off gradients when saturated.
    - Exponential! (computationally expensive)

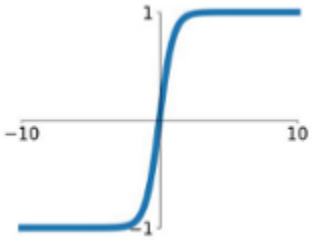
Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



tanh

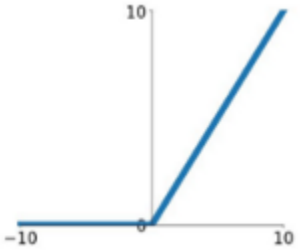
$$\tanh(x)$$



Rectified Linear Unit (Krizhevsky et al., 2012)

ReLU

$$\max(0, x)$$



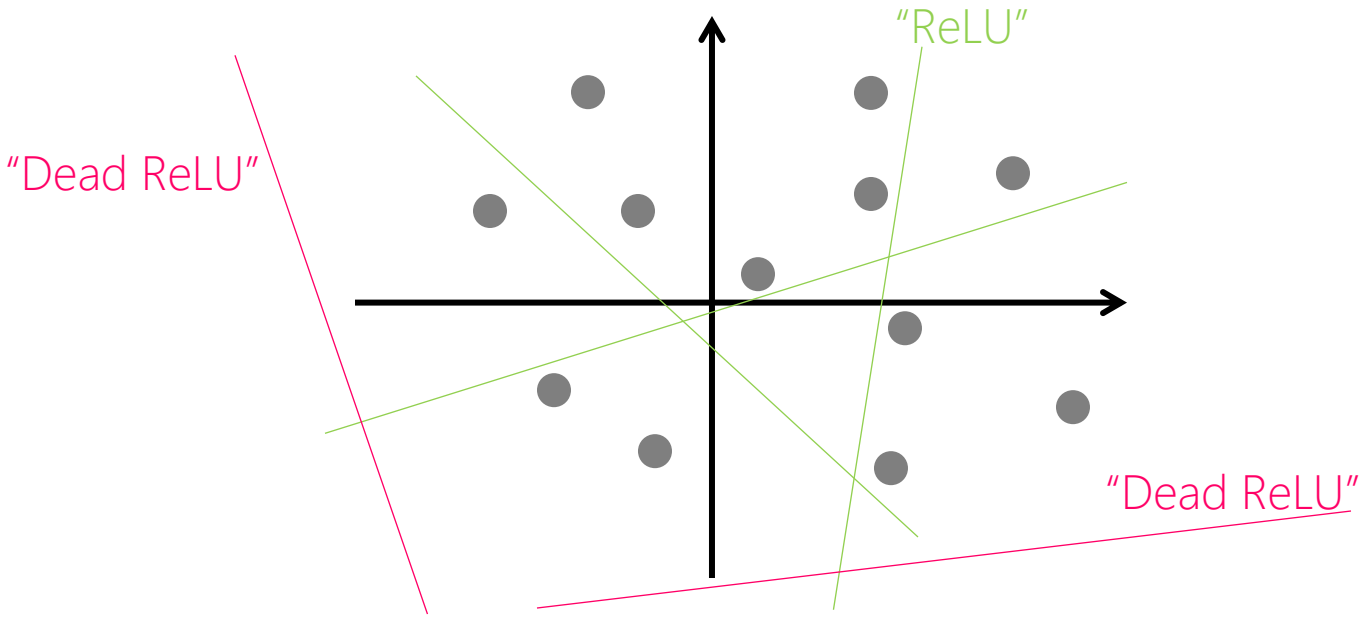
- No saturation when $x > 0$ ☺
- Computationally super efficient. ☺
- Actually, biologically more plausible (modern neuroscience) ☺

- In practice, converges much faster than sigmoid or tanh. ☺

- Not zero-centered though… ☹
- Zero gradient when $x < 0$ → "Dead ReLU" neurons ☹

Rectified Linear Unit (Krizhevsky et al., 2012)

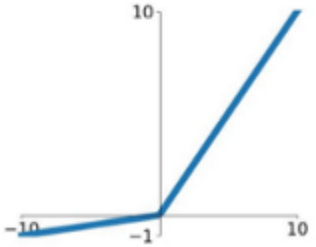
- Dead ReLU
  - A "dead" ReLU always outputs zero for any input.
  - This happens when a large negative bias term is developed.
  - In turn, the dead ReLU neuron will not take any role in the network.
  - “Decision plane” outside the data space.



“Leaky” ReLU (Mass et al., 2013)

- No saturation
- No dead ReLU situation

Leaky ReLU
$\max(0.1x, x)$



- Leaky ReLU

$$f(x) = \max(\alpha x, x)$$

  - α is set by the user

- Parametric Leaky ReLU (PReLU) (He et al., 2015)

$$f(x) = \max(\alpha x, x)$$

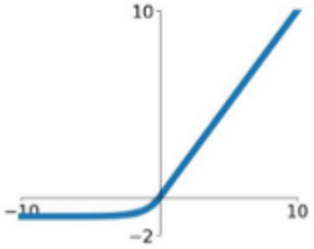
  - α is learned from data (backprop)

Exponential Linear Units (Clevert et al., 2015)

- All the benefits of ReLU, plus…
  - Close to zero-mean output
  - Negative saturation → robustness to noise than Leaky ReLUs

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



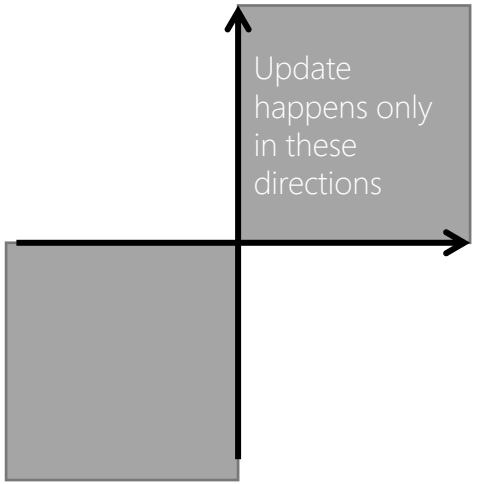
- … but at expenses of computing exponential… ☹

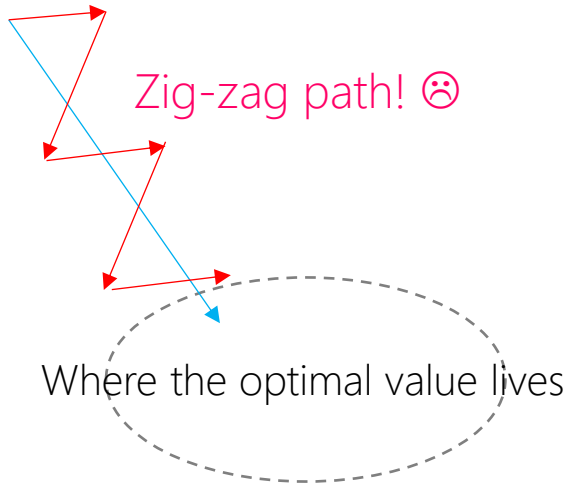
TL;DR

- “Never” use sigmoid
- tanh is good for some cases.
- ReLU is always the good starting point.
- Try out Leaky ReLU, PReLU, ELU, etc. See if they give any better result.

Data Normalization & Whitening

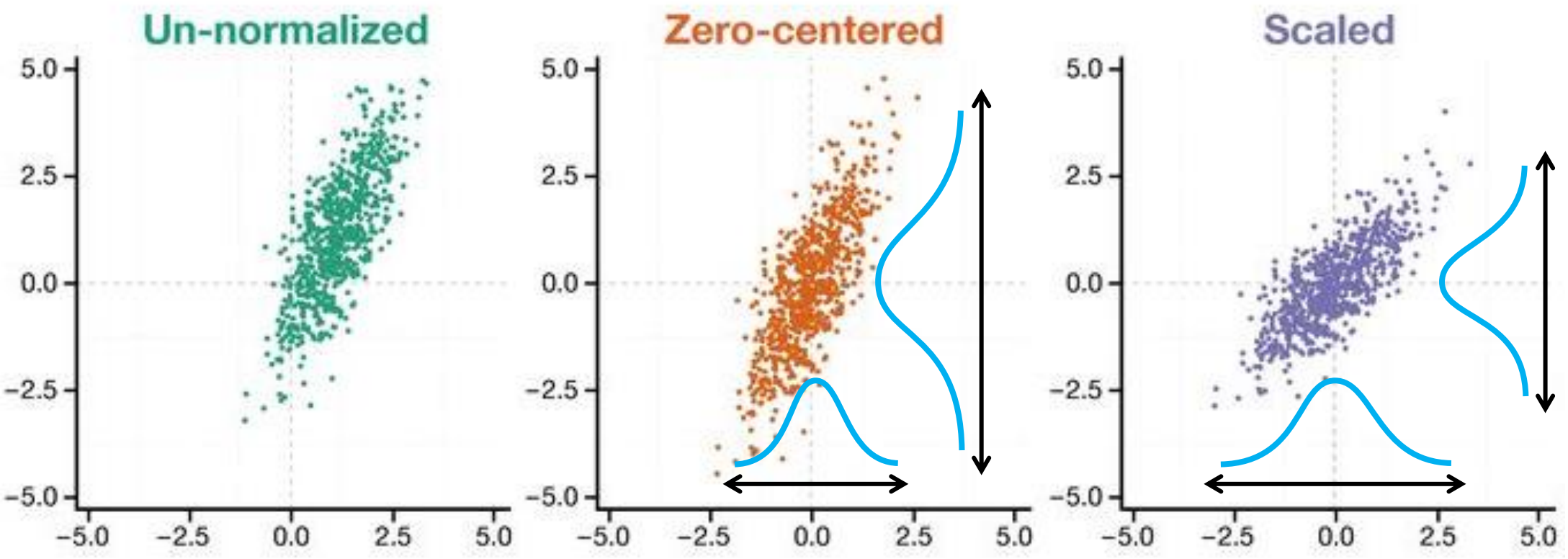
Recall: when inputs to a neuron ≥ 0





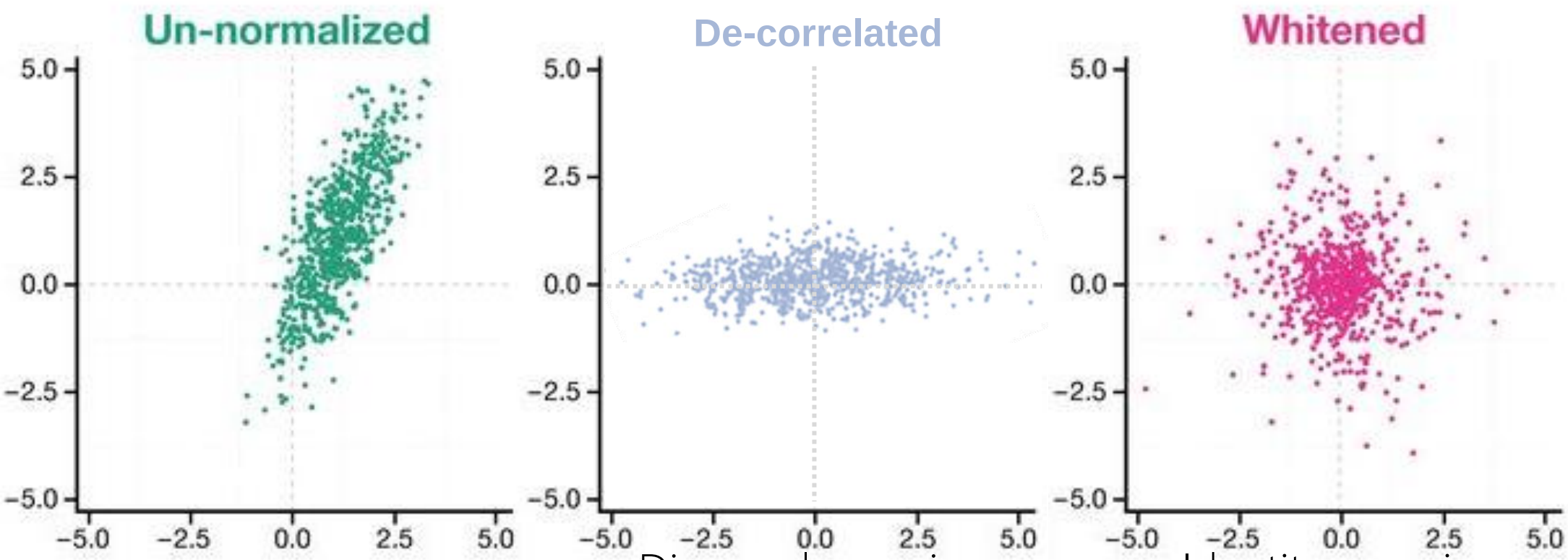
- This also means you need zero-centered data!

Standard Normalization



Angermueller et al. (2016). Deep learning for computational biology. Molecular Systems Biology 12:878

PCA Whitening



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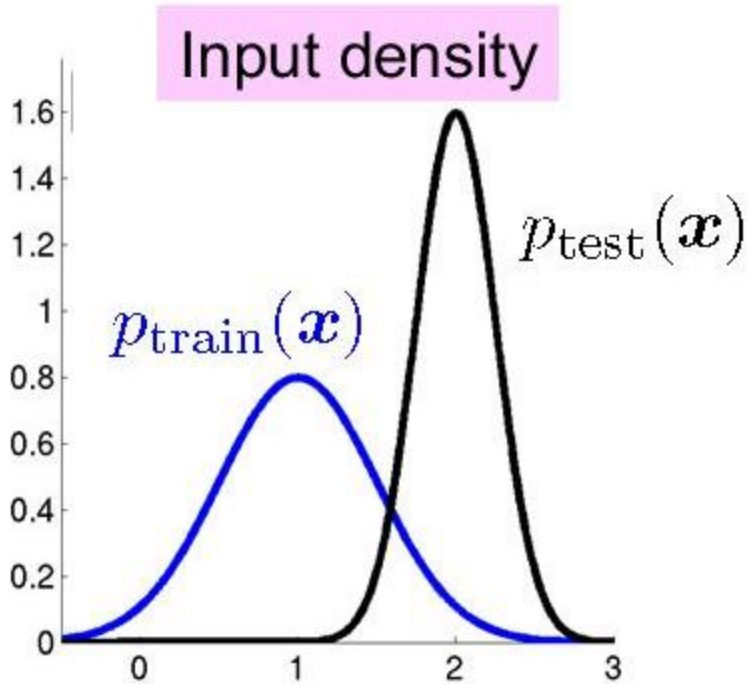
Batch Normalization

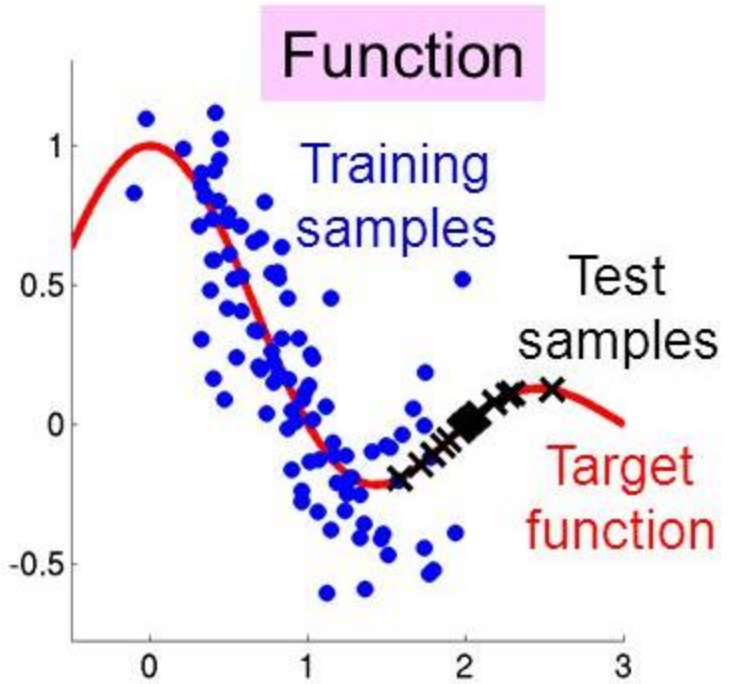
- So, we just learned that the input layer can benefit from normalization.
- Why not do the same thing also for the hidden layers?

- Ioffe and Szegedy. (2015) https://arxiv.org/pdf/1502.03167.pdf

Covariate Shift

- Test samples have different distribution than training.
- Bit of "extrapolation" is required.





Batch Normalization

- Idea: Improve training by mitigating internal covariate shift.

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: γ, β
Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma^2_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma^2_{\mathcal{B}} + \epsilon}} \qquad \text{// normalize}$$

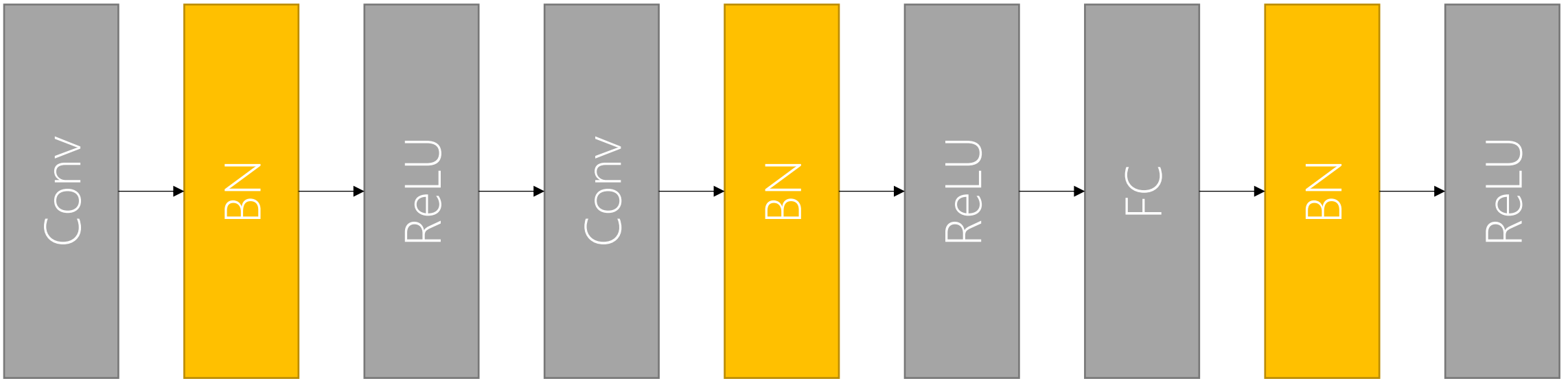
$$y_i \leftarrow \gamma\widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

Algorithm 1: Batch Normalizing Transform, applied to activation x over a mini-batch.

Ioffe and Szegedy (2015).

Batch Normalization

- Batch normalization layers are added typically after FC/Conv and before nonlinearity (activation).



Batch Normalization (Advantages)

- Allows each layer of a network to learn by itself a little bit more independently of other layers.
- Allows higher learning rates because BN makes sure that there's no neuron that goes extremely high or extremely low (i.e. no gradient explosion).
- Enables stable training at larger batch sizes (Bjorck et al., 2018; De & Smith, 2020)
- Noise statistics among batch → Slight regularization effect (Hoffer et al., 2017; Luo et al., 2019).
- Smoothens the loss landscape (Santurkar et al., 2018).
- Becomes less dependent to initialization

Reading (Optional):
- Bjorck et al. 2018: https://arxiv.org/pdf/1806.02375.pdf
- De & Smith 2020: https://arxiv.org/pdf/2002.10444.pdf
- Hoffer et al. 2017: https://arxiv.org/pdf/1705.08741.pdf
- Luo et al. 2019: https://arxiv.org/pdf/1809.00846.pdf
- Santurkar et al. 2018: https://proceedings.neurips.cc/paper/2018/file/905056c1ac1dad141560467e0a99e1cf-Paper.pdf

Batch Normalization (Disadvantages)

- Surprisingly expensive computationally. Incurs memory overhead (Rota Bulo et al., 2018)
- Significantly increases the time required to evaluate the gradient in some networks (Gitman & Ginsburg, 2017)
- Introduces a discrepancy between the behavior of the model during training and at inference time (Summers & Dinneen, 2019; Singh & Shrivastava, 2019)

Reading (Optional):

- Rota Bulo et al. 2018: https://openaccess.thecvf.com/content_cvpr_2018/papers/Bulo_In-Place_Activated_BatchNorm_CVPR_2018_paper.pdf
- Gitman & Ginsburg 2017: https://arxiv.org/pdf/1709.08145.pdf
- Summers & Dinneen 2019: https://arxiv.org/pdf/1906.03548.pdf
- Sing & Shrivastava 2019: https://arxiv.org/pdf/1904.06031.pdf

Initializing Weights

Weight Initialization

- Simplest way: W = 0 (or some constant)
  - What happens in this case? (hint: local gradient direction)

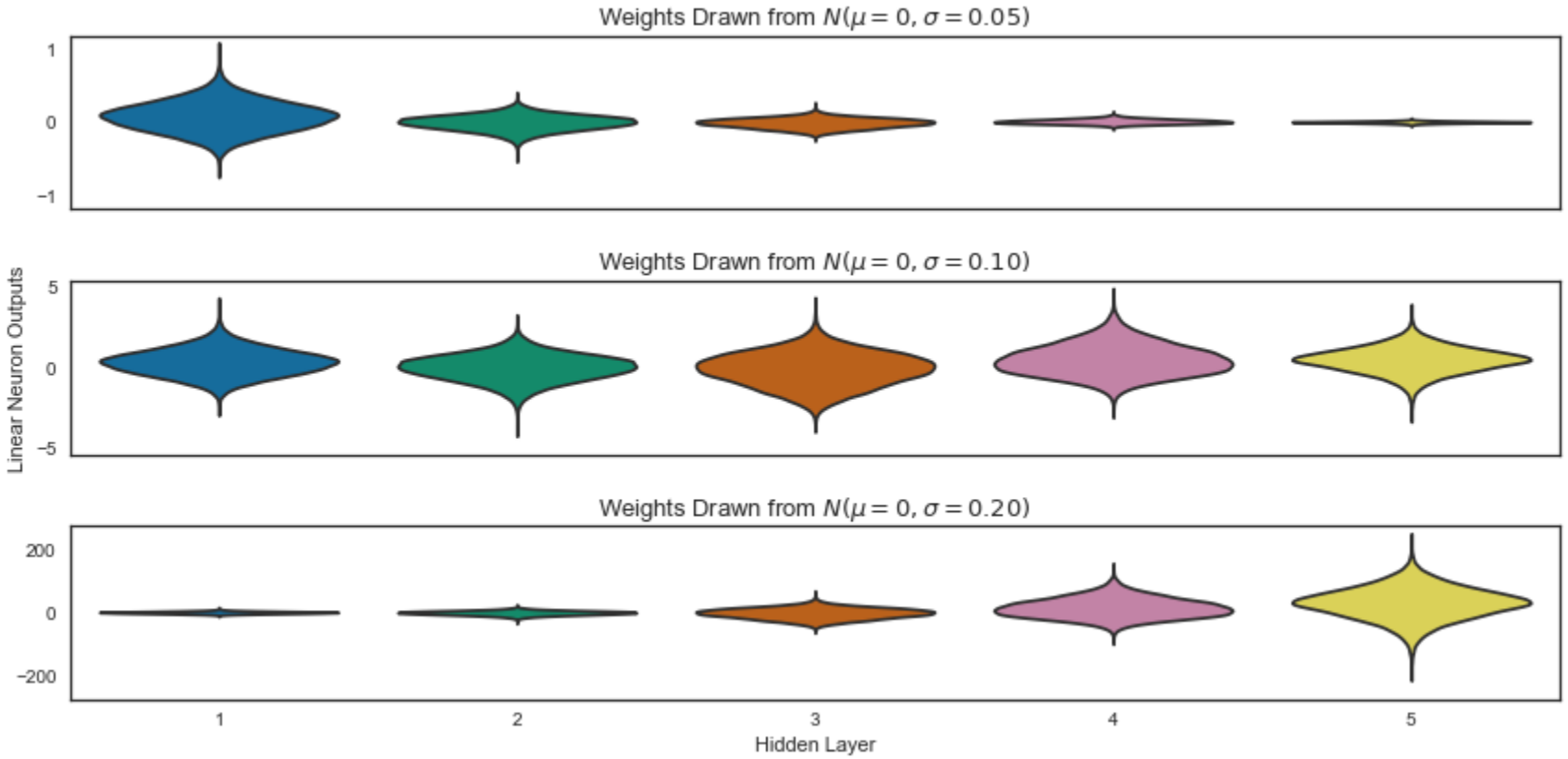
- Weight values move in the same direction!
- Never do this!

Random Initialization of Weights

- In practice, neural weights are initialized with some random number.
- Magnitude of the random number matters.
  - Too small → weights dwindle to zero
  - Too big → weights explode
- You need to find an “appropriate” sized random numbers.

Random Initialization of Weights

- Activations of each hidden layer after one forward pass through the network.



https://intoli.com/blog/neural-network-initialization/

How to find the appropriate range?

- Xavier Initialization (Glorot and Bengio 2010): $\mathrm{std}(W_i) = 1/\sqrt{n}$
  - Suppose input X with n components and a linear neuron with random weights W:
$$Y = W_1X_1 + W_2X_2 + \cdots + W_nX_n$$
  - Then, assuming W_iX_i are uncorrelated (Bienayme formula),
$$\mathrm{Var}(Y) = \mathrm{Var}\left(\sum_i W_iX_i\right) = \sum_i \mathrm{Var}(W_iX_i) = n\mathrm{Var}(W_iX_i)$$
  - Meanwhile,
$$\mathrm{Var}(W_iX_i) = E(X_i)^2\mathrm{Var}(W_i) + E(W_i)^2\mathrm{Var}(X_i) + \mathrm{Var}(W_i)\mathrm{Var}(X_i) = \mathrm{Var}(W_i)\mathrm{Var}(X_i)$$
  - which gives…
$$\mathrm{Var}(Y) = \mathrm{nVar}(W_i)\mathrm{Var}(X_i)$$
  - Therefore, to constrain $\mathrm{Var}(Y) = \mathrm{Var}(X_i)$, we need $\mathrm{nVar}(W_i) = 1$

$$\begin{aligned}
Var(XY) &= E[(XY)^2] - \{E[XY]\}^2 && (\because Var(A) = E[A^2] - \{E[A]\}^2)\\
&= E[X^2Y^2] - \{E[X]E[Y]\}^2 && (\because \text{X and Y are independent})\\
&= E[X^2]E[Y^2] - E[X]^2E[Y]^2\\
&= (\sigma_x^2 + \mu_x^2)(\sigma_y^2 + \mu_y^2) - \mu_x^2\mu_y^2 && (\because E[A^2] = Var(A) + \{E[A]\}^2)\\
&= \sigma_x^2\sigma_y^2 + \sigma_x^2\mu_y^2 + \sigma_y^2\mu_x^2 + \mu_x^2\mu_y^2 - \mu_x^2\mu_y^2\\
&= \sigma_x^2\sigma_y^2 + \sigma_x^2\mu_y^2 + \sigma_y^2\mu_x^2
\end{aligned}$$

How to find the appropriate range?

- In case of ReLU, Xavier initialization doesn't hold.
  - Derivation of Xavier initialization: assumes a linear neuron.
  - Works alright for Sigmoid and tanh, but not for "rectifiers"

- To over-simplify, half of the outputs (the negative part) dies out under ReLU

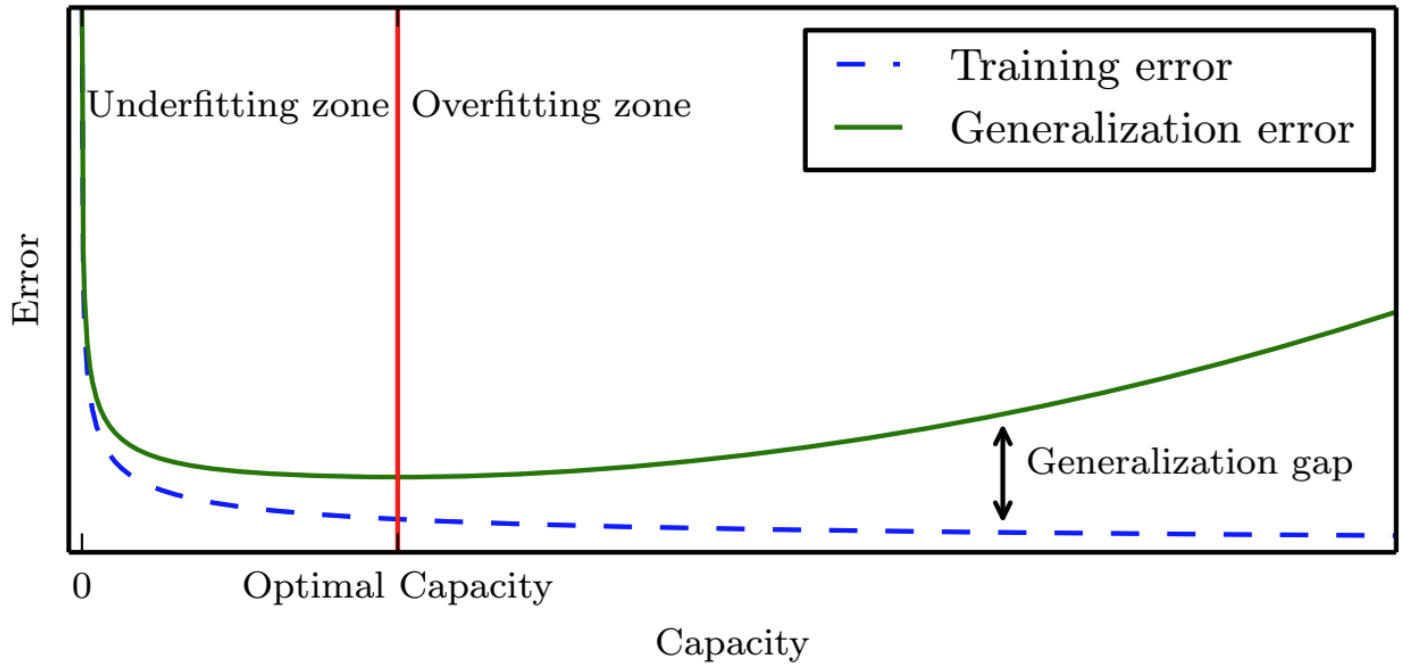
- He et al. (2015): $\mathbf{std}(W_i) = 2/\sqrt{n}$

Dropout


THE BEST WAY TO
EXPLAIN OVERFITTING

Basic Concepts

- The ability to perform well on *unobserved inputs* is called generalization.
- Underfitting: when the model is not able to obtain sufficient training error.
- Overfitting: when the gap between training and generalization error too large.



Dropout

- More abstract-level view of overfitting

What network has seen from the training set

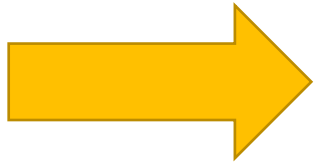
"Too fluffy, it's not a cat"

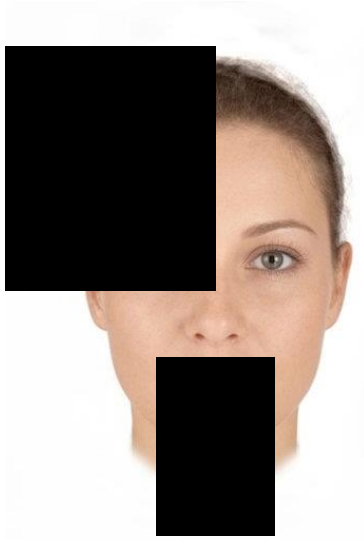
"Too fat. Not a cat"

...

Dropout

- An idea: “let’s hide some information while training”
  - Missing information → incentivize generalization of observation





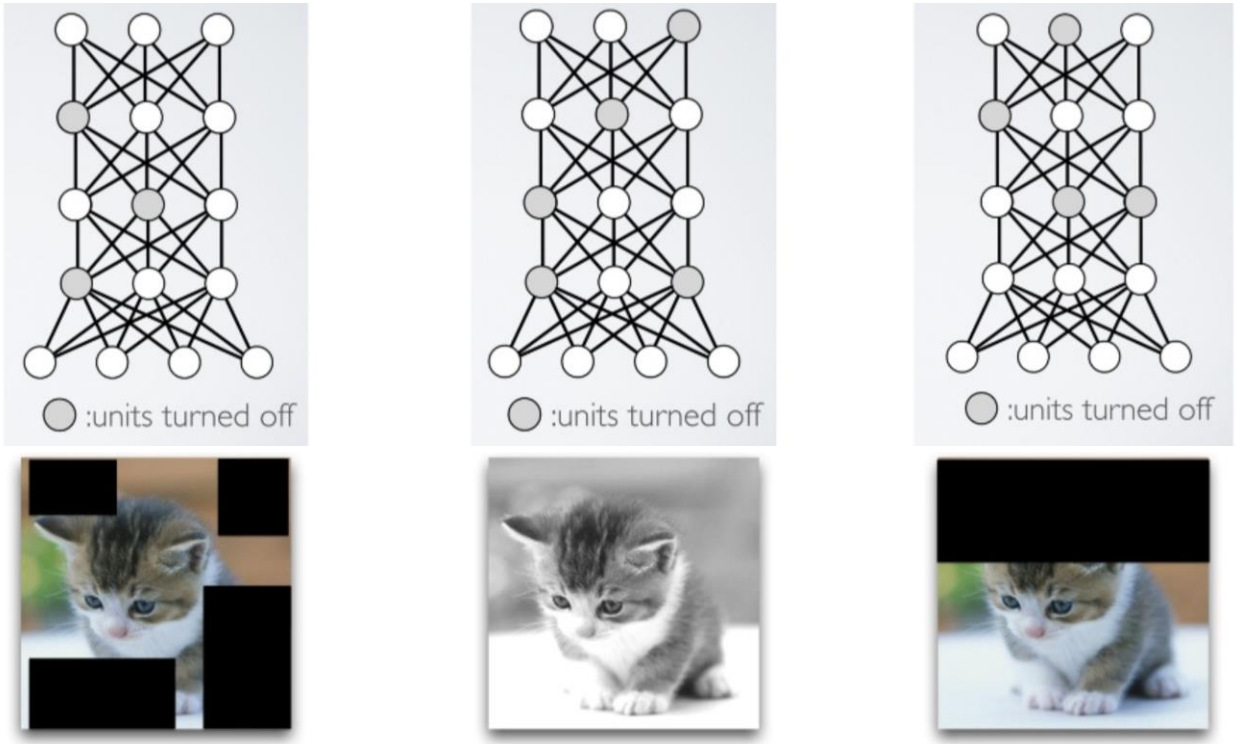
Human face:
“has to have two eyes, two eyebrows,
one nose with two nostrils, upper and lower lips,
two ears, …”

“an eye and a nose
→ face”

“chin, lips, and nose
→ face”

Dropout

- But how?
  - Randomly turn off neurons (set inputs to zero) while training



Dropout

- A bonus: increase of training data in a funny way!
  - How many?
    - Example: a FC layer with 4096 units
      - Possible combinations of turning on/off: $\mathbf{2^{4096}} \approx \mathbf{10^{1233}}$ cases
      - cf) the total number of atoms in the universe: $\mathbf{10^{82}}$ approx.

Dropout

- Dropout happens only at training time. No dropout during test time.
- Dropout layers can be added to any location in the computational graph.
  - Typically before Conv or FC layers.
- Dropout rate can be controlled independently per each dropout layer.

Data Augmentation

Is this a cat?

How about this?

How about now?

How about now?

How about now?

How about now?

How about now?

How about now?

How about now?

Data Augmentation

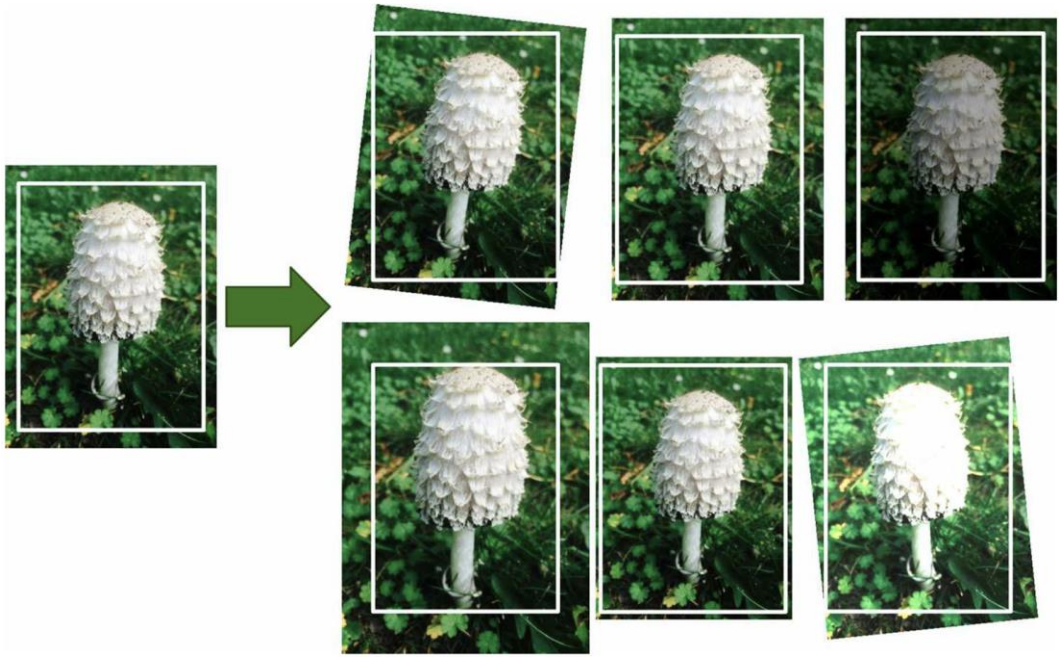
- Random rotation, scale, crop, color change in training set

- Even some crazy ideas… because why not?:
  - Stretch
  - Shear
  - Lens distortion

- Point: Stochasticity!

Data Augmentation

- Make the model generalize better by training it on more data
- If the amount of data available is limited, get around by creating “fake” data and augment them into the training set. How?
- Augmentation has been particularly effective for object recognition. Image transformations (ie. translating, rotating, cropping, brightness correcting, ect) often greatly improve generalization.



Injecting noise and label smoothing

- Injecting (random) noise in the inputs can be a form of data augmentation.
- Injecting noise to output labels? It can be harmful to maximize log p(y|x) when y is a mistake.
- Prevent this by explicitly model the noise on the label: y is correct with probability 1 - $\boldsymbol{\varepsilon}$ (epsilon) with small constant $\boldsymbol{\varepsilon}$

$$\frac{\epsilon}{k-1} \text{ and } 1-\epsilon$$

- Label smoothing regularizes a model on a softmax with k output values by replacing hard label 0 and 1 with

Regularization

Preventing weights going crazy…

- Too flexible weights → Too flexible models → Overfit!

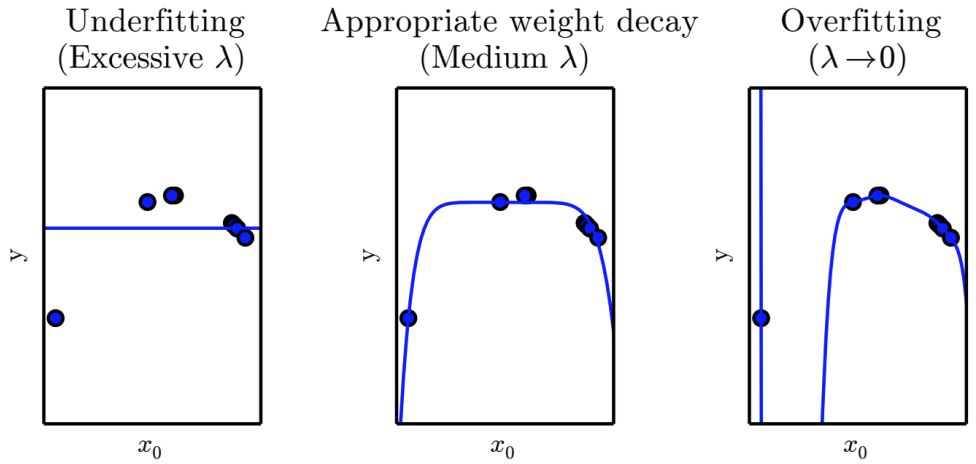
- You can *regularize* (meaning, prevent the size of weights going too big) by adding a regularization term in the loss function.

$$L(W,b) = \frac{1}{N}\sum_{i=1}^{N}\left\|y^{(i)} - f\left(x^{(i)} \mid W,b\right)\right\|^2 + \lambda R(W,b)$$

Regularization

- Regularization is the modification made to a learning algorithm that is intended to reduce its generalization error but not its training error.
- For example, we can modify the loss function for linear regression to include a preference for the weights to have smaller L2 norm as a regularizer:

$$J(\mathbf{w}) = \mathcal{L}_{\text{mse}}(\mathbf{X}_{\text{train}}, \mathbf{y}_{\text{train}}) + \lambda \mathbf{w}^\top \mathbf{w}$$



Parameter Norm Penalties

- Many regularization approaches are based on limiting the model capacity by adding a parameter norm penalty to the objective (loss) function:

$$J(\mathbf{w}; \mathbf{X}, \mathbf{y}) = \mathcal{L}(\hat{\mathbf{y}}, \mathbf{y}) + \lambda \Omega(\mathbf{w})$$

Data Loss Norm Penalty

where $\boldsymbol{\lambda}$ is a hyperparameter that controls the relative contribution of the norm penalty term, $\boldsymbol{\Omega}$, relative to the standard data loss function L

- Larger value of $\boldsymbol{\lambda}$ correspond to more regularization
- Setting $\boldsymbol{\lambda}$ to 0 results in no regularization
- Norm penalty $\boldsymbol{\Omega}$ penalizes only the weights of the affine transformation
- Different choice of $\boldsymbol{\Omega}$ can result in different solutions being preferred.

L2 Parameter Regularization

- L2 regularization is aka Ridge Regression or Tikhonov regularization
- The L2 norm penalty commonly known as weight decay

$$J(\mathbf{w}; \mathbf{X}, \mathbf{y}) = \mathcal{L}(\hat{\mathbf{y}}, \mathbf{y}) + \frac{\lambda}{2}||\mathbf{w}||^2$$

$$\nabla_{\mathbf{w}} J(\mathbf{w}; \mathbf{X}, \mathbf{y}) = \nabla_{\mathbf{w}} \mathcal{L}(\hat{\mathbf{y}}, \mathbf{y}) + \lambda \mathbf{w}$$

To take a single **Gradient Descent** step to update the weights:

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \nabla_{\mathbf{w}} J(\mathbf{w}; \mathbf{X}, \mathbf{y})$$

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha(\nabla_{\mathbf{w}} \mathcal{L}(\hat{\mathbf{y}}, \mathbf{y}) + \lambda \mathbf{w})$$

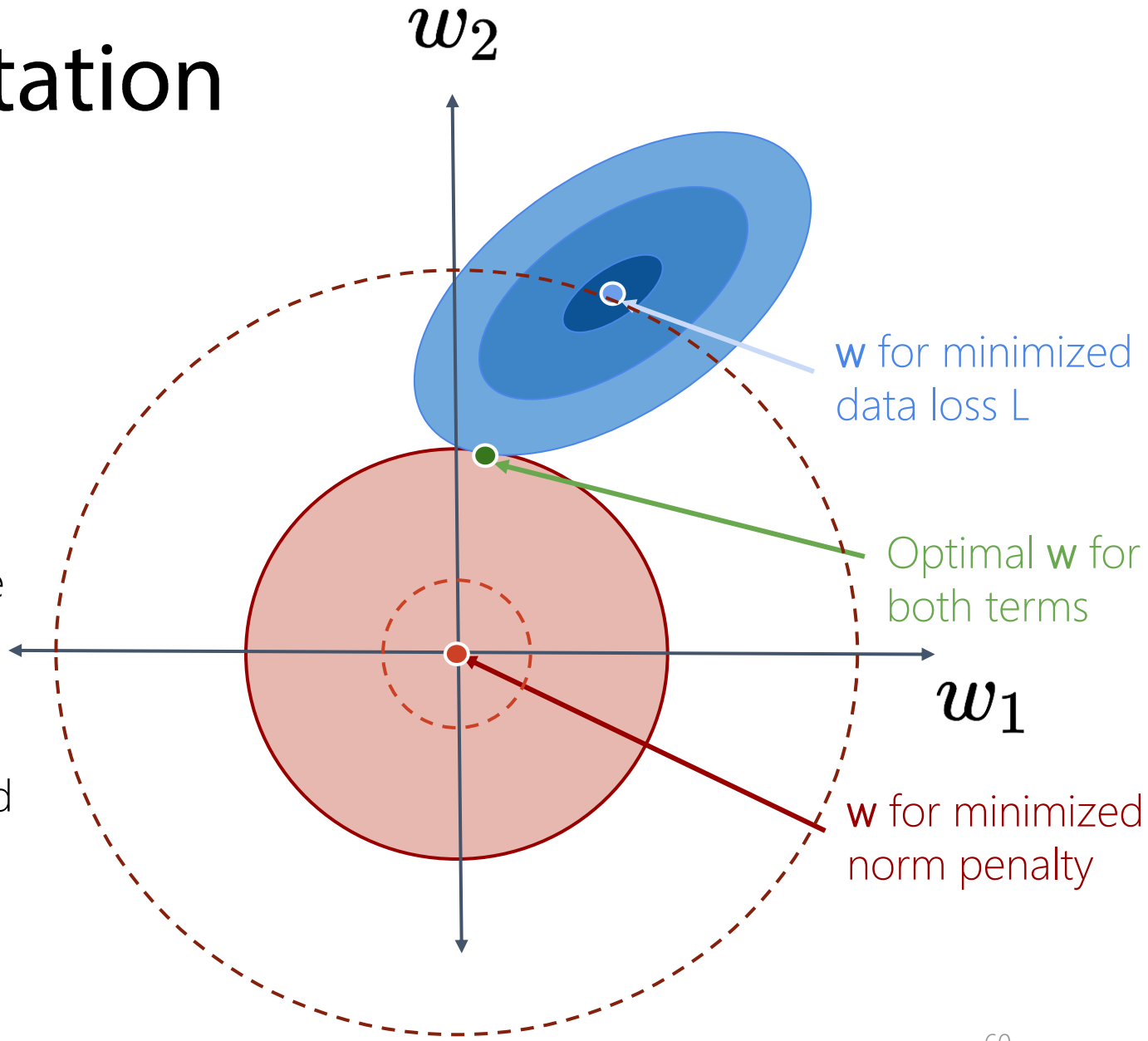
$$\mathbf{w} \leftarrow (1 - \alpha\lambda)\mathbf{w} - \alpha \nabla_{\mathbf{w}} \mathcal{L}(\hat{\mathbf{y}}, \mathbf{y})$$

< 1

Shrink the weight vector before gradient update

Geometric Interpretation

- L2 regularizations $||w||^2$ can be geometrically represented as concentric (red) circles.
- When circle is too small, the params are not useful to the model.
- When the circle region (in red) grows, due to its shape the region intersects the data contour closer to the origin, L2 makes both parameters shrink and w1 near zero.
- When the circle grows too large, you end up with a similar params as data loss.



L1 Parameter Regularization

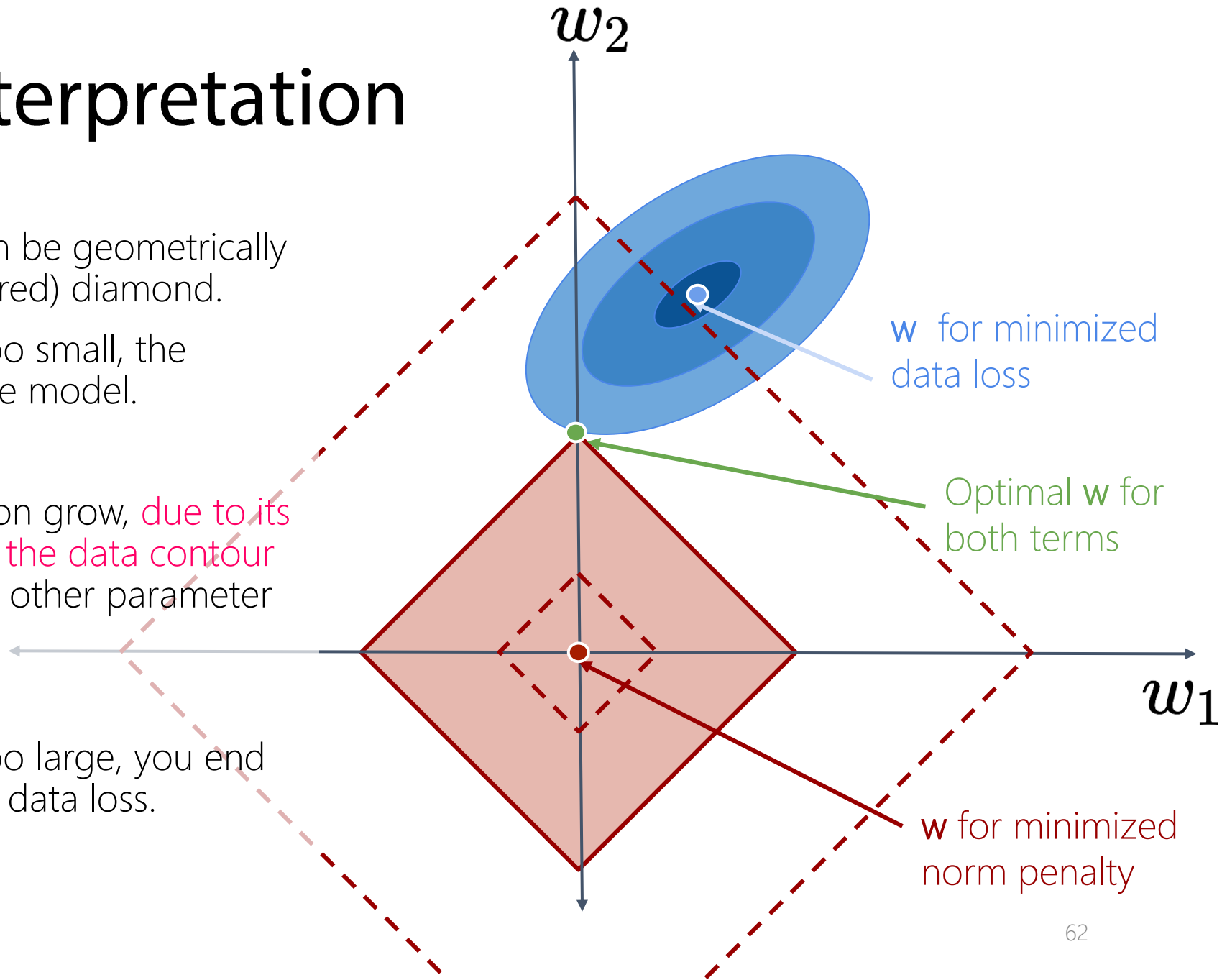
- L1 regularization is aka LASSO (least absolute shrinkage and selection operator)
- L1 norm commonly is known as the Manhattan Distance.

$$J(\mathbf{w}; \mathbf{X}, \mathbf{y}) = \mathcal{L}(\hat{\mathbf{y}}, \mathbf{y}) + \lambda ||\mathbf{w}||_1$$
$$\nabla_{\mathbf{w}} J(\mathbf{w}; \mathbf{X}, \mathbf{y}) = \nabla_{\mathbf{w}} \mathcal{L}(\hat{\mathbf{y}}, \mathbf{y}) + \lambda \mathbf{sign}(\mathbf{w})$$

- The regularization to the gradient no longer scale linearly with each $\mathbf{w}$, instead it is a constant factor with a sign equal to $\mathbf{sign}(\mathbf{w})$. Thus, there is no clean algebraic solution to approximates J as we have just seen in L2 regularization
- L1 norm makes the parameters to become sparse (contains lots of zeros)
- L1 norm tends to cause a subset of the network weights to become zero, suggesting that the corresponding signal may safely be discarded (dead neuron).

Geometric Interpretation

- L1 regularizations $||w||^1$ can be geometrically represented as concentric (red) diamond.
- When diamond region is too small, the params are not useful to the model.
- When as the diamond region grow, due to its shape the region intersects the data contour on one of the axis, thus the other parameter is zero out.
- When diamond region is too large, you end up with a similar params as data loss.



Elastic Net

- Is a middle ground between Ridge (L2) and Lasso (L1) with a ratio r.

$$J(\mathbf{w};\mathbf{X},\mathbf{y}) = \mathcal{L}(\hat{\mathbf{y}},\mathbf{y}) + r\lambda||\mathbf{w}||_1 + (1-r)\lambda||\mathbf{w}||_2^2$$

LASSO

RIDGE

Geometric Interpretation

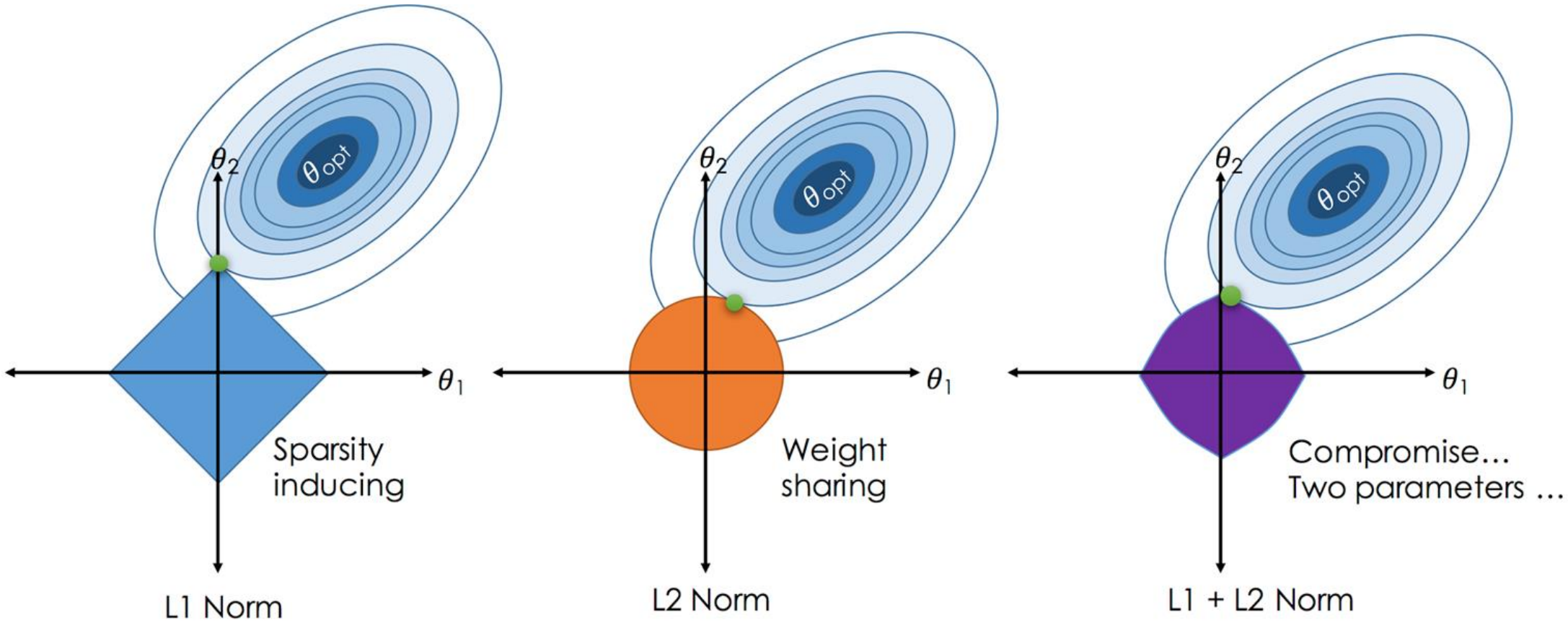
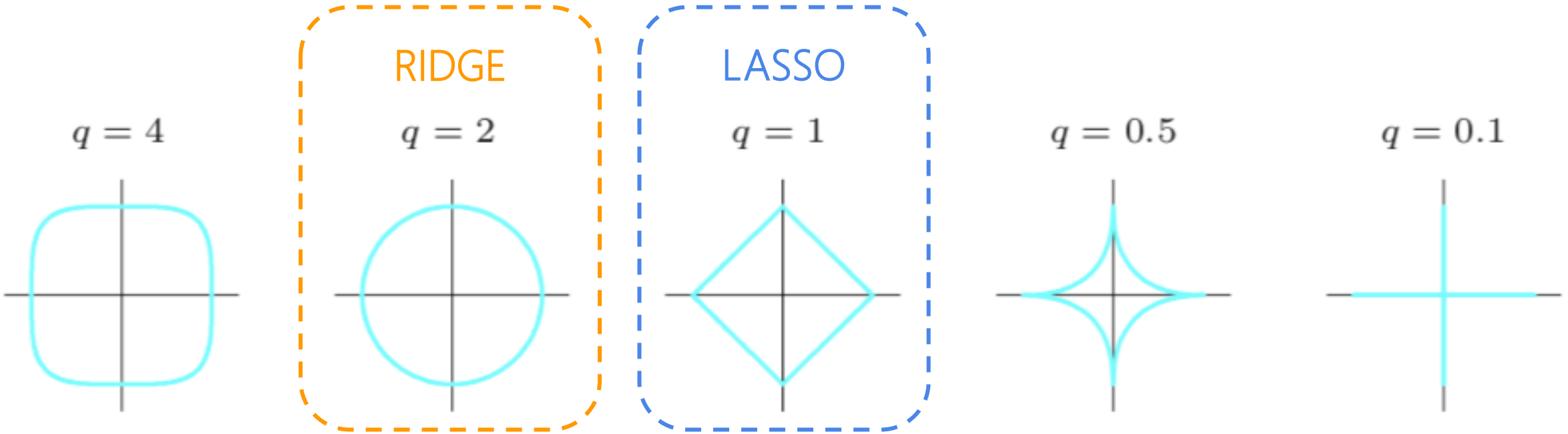


*Figure from Yin Hu, Medium

Family of Parameter Norm Models

$$J(\mathbf{w}; \mathbf{X}, \mathbf{y}) = \mathcal{L}(\hat{\mathbf{y}}, \mathbf{y}) + \lambda ||\mathbf{w}||_q$$



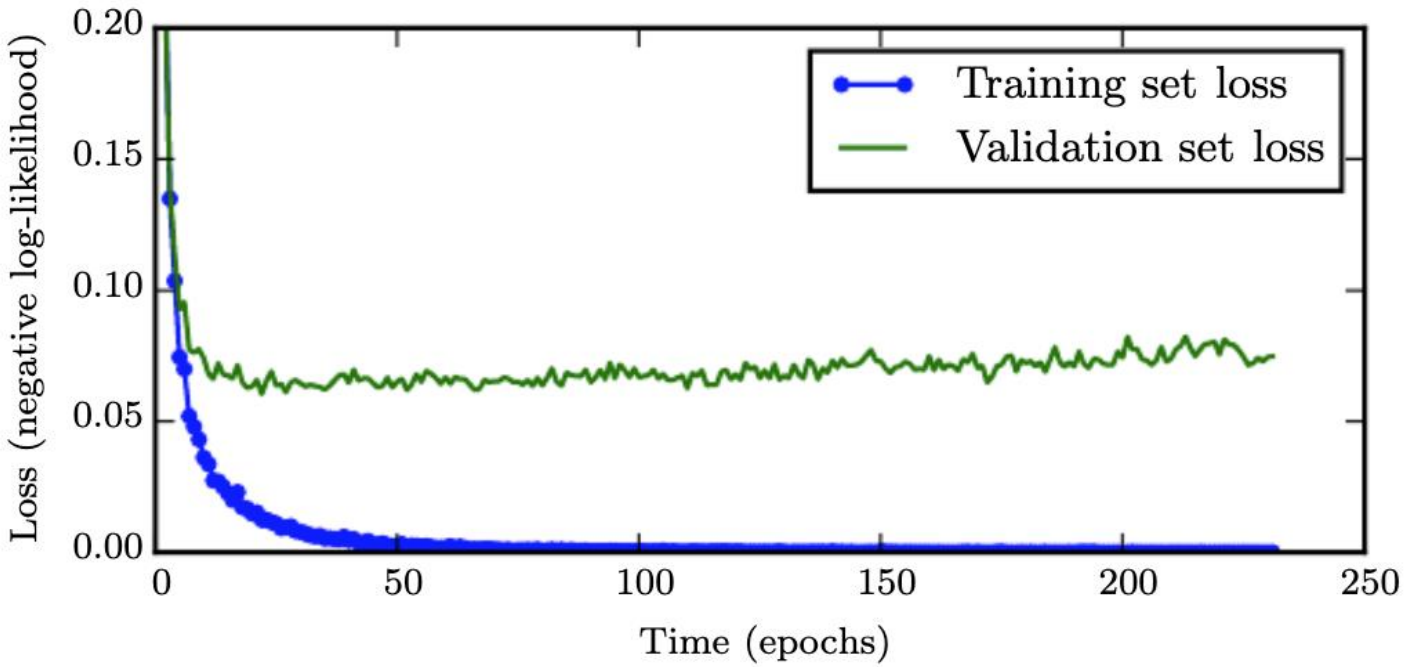
TL;DR

- It is preferable to have at least a little bit of regularization. Ridge (L2) is a good default.
- If you suspect that only a few features are actually useful, use Lasso (L1)
- Lasso may behave erratically when # features > # examples → use Elastic Net

Early Stopping

Early Stopping

- When training large models with sufficient capacity to overfit the task, we often observe reliably that training error decreases steadily over time, but validation error begins to rise again → we can stop at the lowest validation error!
- The most commonly used form of regularization in deep learning: simple yet effective!



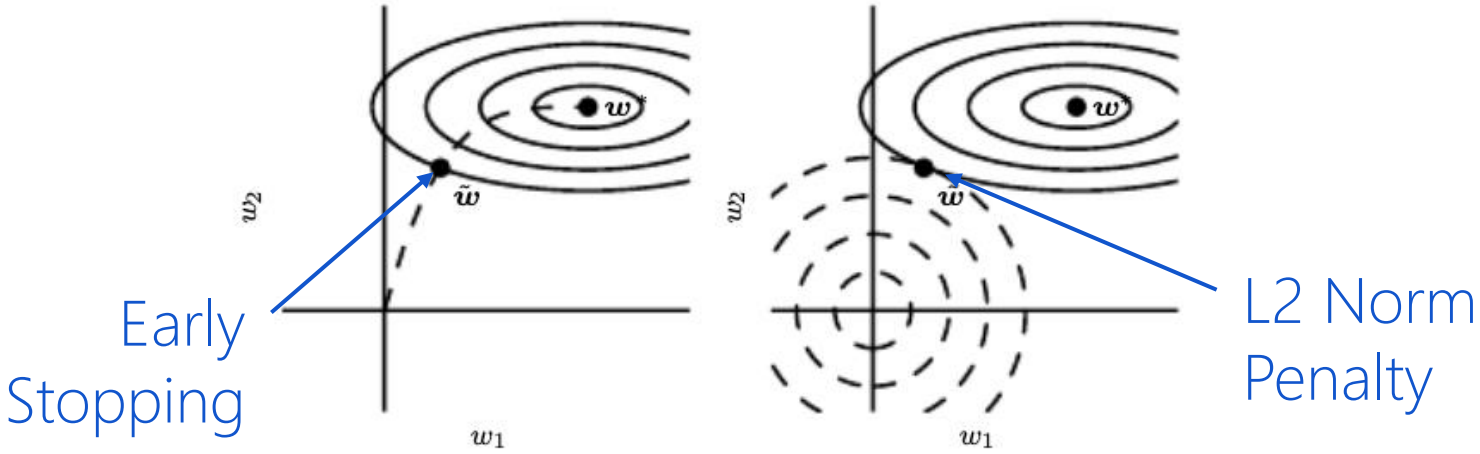
Early Stopping: Algorithm

Algorithm 7.1 The early stopping meta-algorithm for determining the best amount of time to train. This meta-algorithm is a general strategy that works well with a variety of training algorithms and ways of quantifying error on the validation set.

Let n be the number of steps between evaluations.
Let p be the "patience," the number of times to observe worsening validation set error before giving up.
Let $\boldsymbol{\theta}_o$ be the initial parameters.
$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}_o$
$i \leftarrow 0$
$j \leftarrow 0$
$v \leftarrow \infty$
$\boldsymbol{\theta}^* \leftarrow \boldsymbol{\theta}$
$i^* \leftarrow i$
while $j < p$ **do**
  Update $\boldsymbol{\theta}$ by running the training algorithm for n steps.
  $i \leftarrow i + n$
  $v' \leftarrow \text{ValidationSetError}(\boldsymbol{\theta})$
  if $v' < v$ **then**
    $j \leftarrow 0$
    $\boldsymbol{\theta}^* \leftarrow \boldsymbol{\theta}$
    $i^* \leftarrow i$
    $v \leftarrow v'$
  else
    $j \leftarrow j + 1$
  end if
end while
Best parameters are $\boldsymbol{\theta}^*$, best number of training steps is i^*.

Early Stopping: Properties

- Is a very efficient hyperparameter selection method (saves the best set).
- Controls the model capacity by determining how many steps to fit the training data (and reduce the computational cost of the training procedure)
- Unobtrusive form of regularization as almost no change in training procedure
- Can be used either alone or with other regularization strategies
- Is equivalent to L2 regularization, and better because it automatically determines the correct amount of regularization while L2 requires the tuning of hyperparameter $\boldsymbol{\lambda}$



Beyond SGD:
Fancier Optimization Methods

Thought Experiment on Gradient Descent

- Q. What does it take to evaluate loss?

$$\mathcal{L}(\boldsymbol{\theta}) = \sum_{i=1}^{N} \left\| \mathbf{y}^{(i)} - f\left(\mathbf{x}^{(i)} | \boldsymbol{\theta}\right) \right\|^2$$

Thought Experiment on Gradient Descent

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- A. The function value $f\left(\mathbf{x}^{(i)} | \, \boldsymbol{\theta}\right)$ need to be evaluated for all $\mathbf{x}^{(i)}$ in the dataset.

Thought Experiment on Gradient Descent

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- Q. What about the gradient?

Thought Experiment on Gradient Descent

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- A. Same! Backpropagation needs to happen for all and each $\mathbf{x}^{(i)}$

Thought Experiment on Gradient Descent

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- Q. Then what happens to the gradient descent algorithm?

Thought Experiment on Gradient Descent

- Q. What does it take to evaluate loss?

$$\mathcal{L}(\boldsymbol{\theta}) = \sum_{i=1}^{N} \left\| \mathbf{y}^{(i)} - f\left(\mathbf{x}^{(i)} | \boldsymbol{\theta}\right) \right\|^2$$

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- Q. What about the gradient?
- A. Same! Backpropagation needs to happen for all and each $\mathbf{x}^{(i)}$

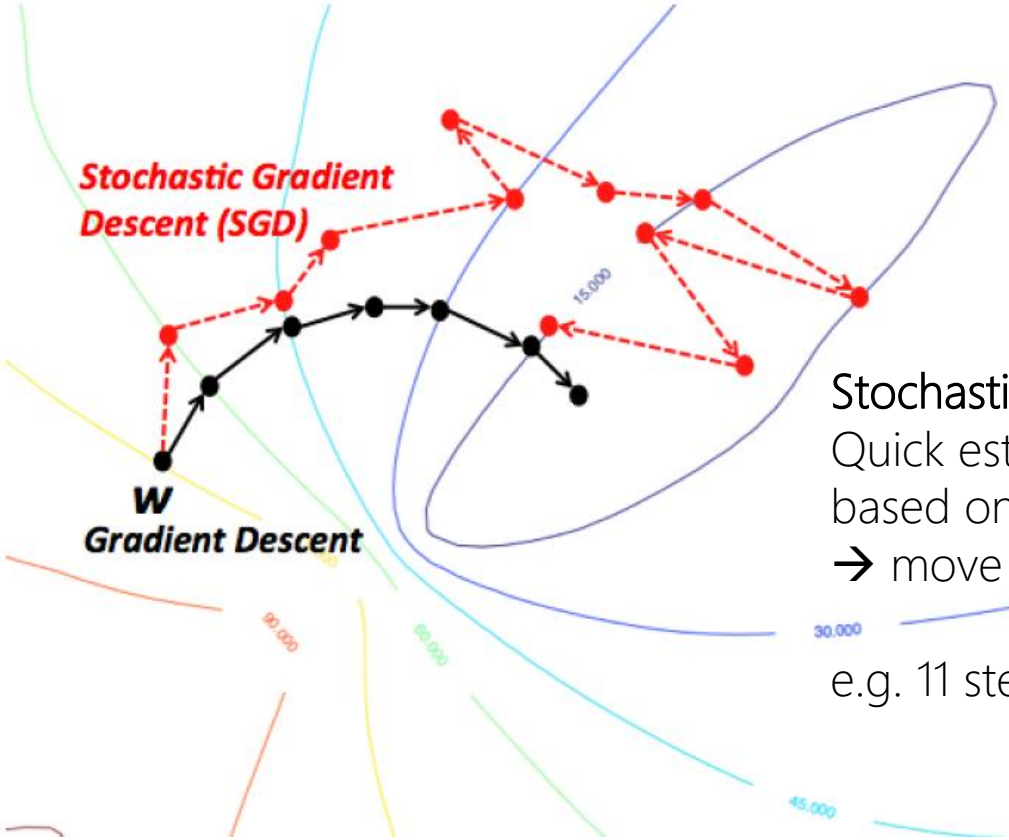
- Q. Then what happens to the gradient descent algorithm?
- A. Computational time increases exponentially as N goes up.

Stochastic Gradient Descent (SGD)

- Idea:

Gradient Descent
Compute everything
→ make the optimal one step

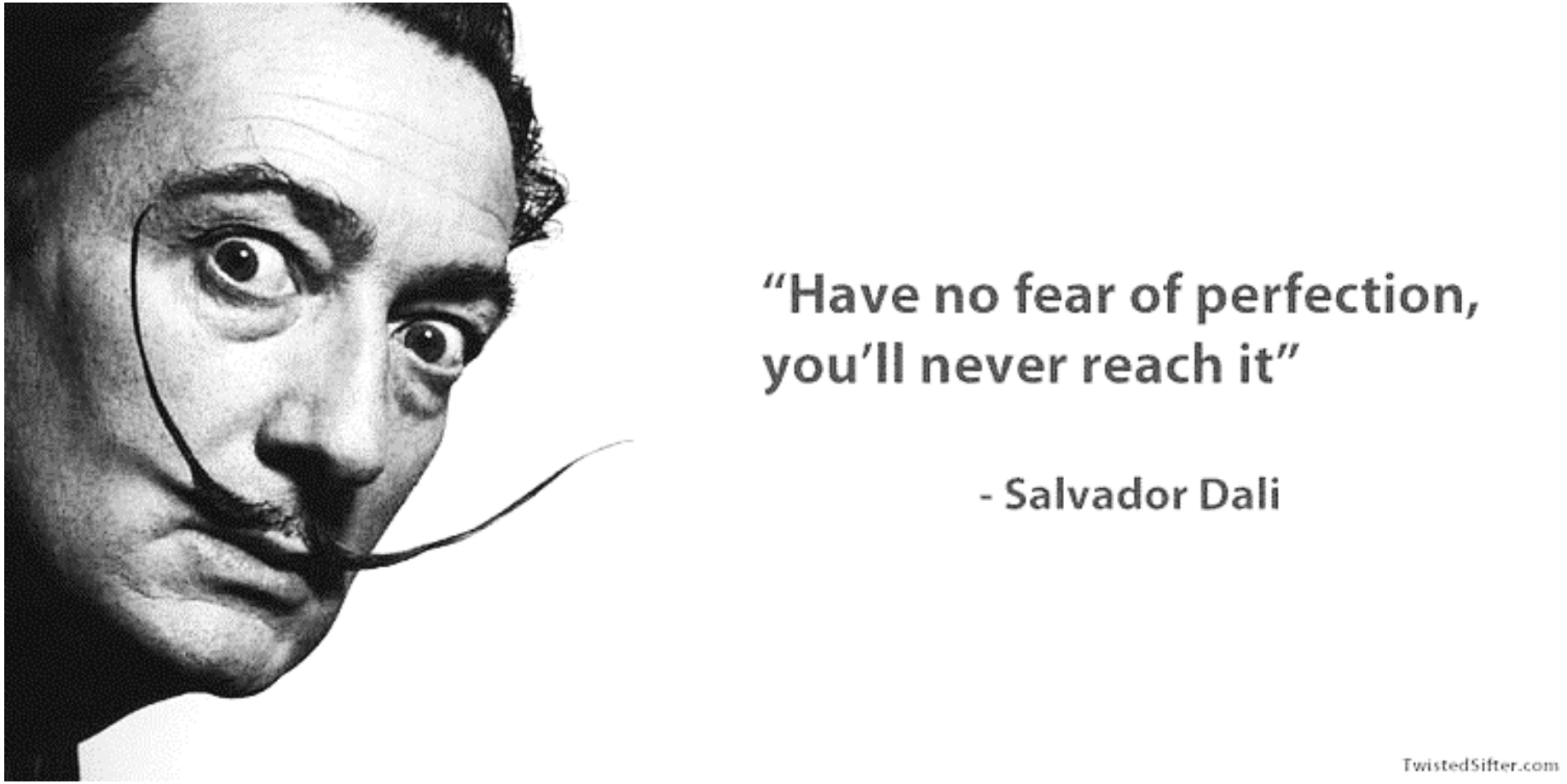
e.g. 6 steps * 1 hr/step = 6 hrs



Stochastic Gradient Descent
Quick estimation of the gradient
based on a small batch
→ move quickly even if it's not the optimal

e.g. 11 steps * 5 min/step = 55 min

Stochastic Gradient Descent (SGD)

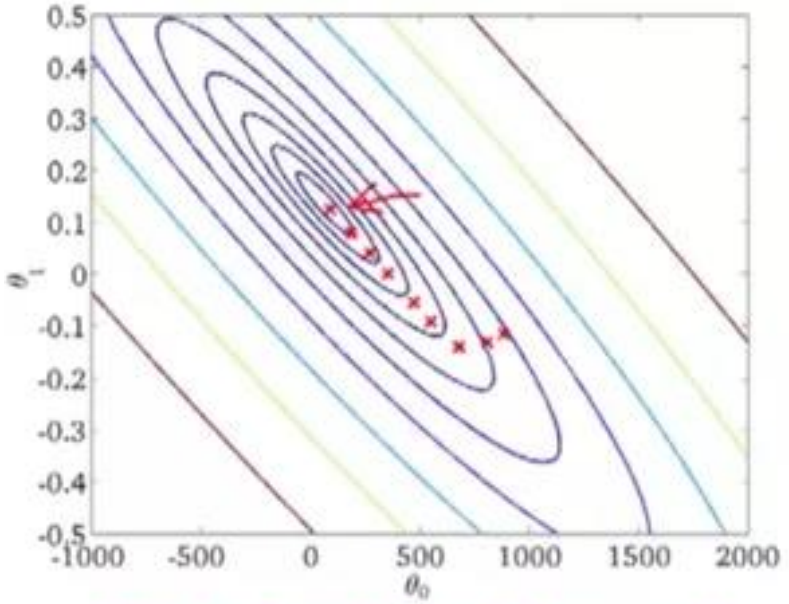


Stochastic Gradient Descent (SGD)

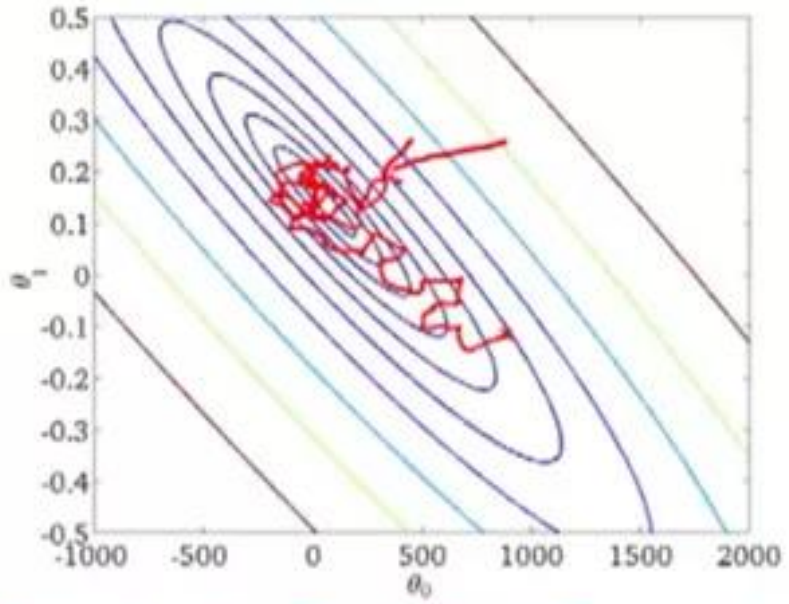
1. Randomly shuffle dataset
2. Repeat until converge {
    for a mini-batch {
        compute gradient only with the mini-batch
        update weights
    }
}

Stochastic Gradient Descent (SGD)

- Gradients come from mini-batches, so they can be noisy and inaccurate!



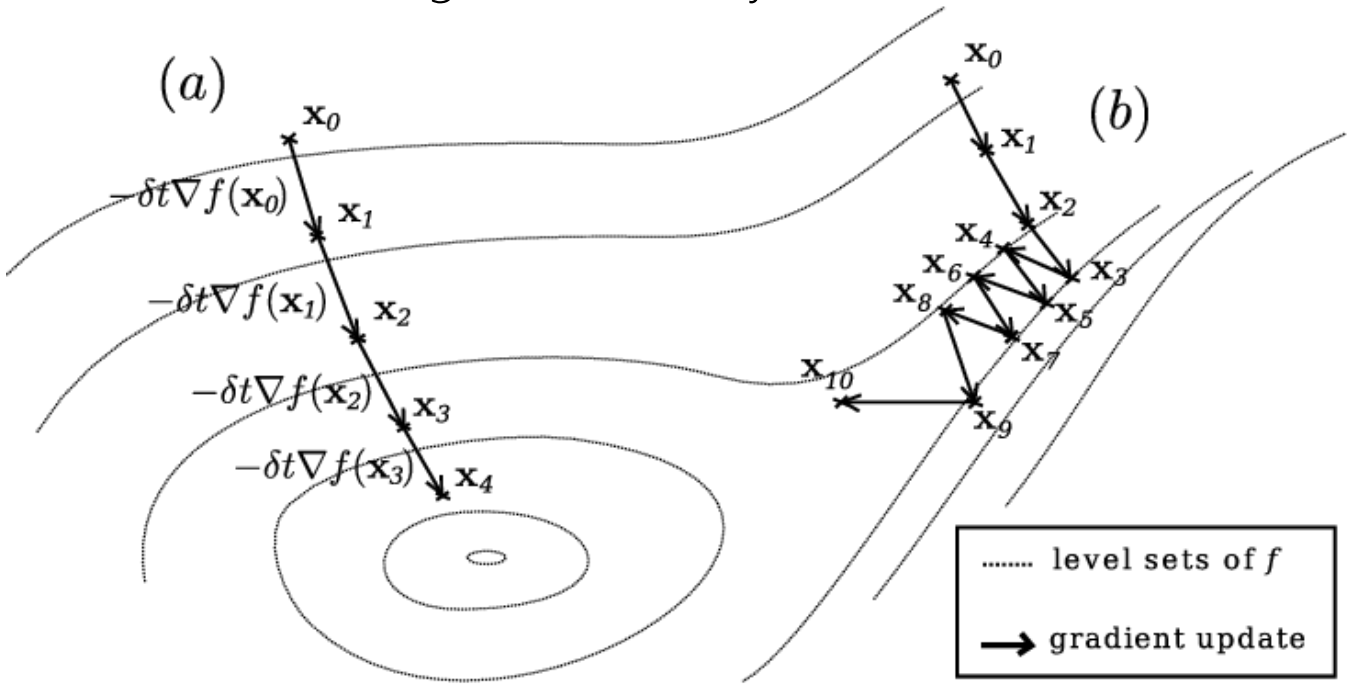
Batch Gradient Descent



Stochastic Gradient Descent

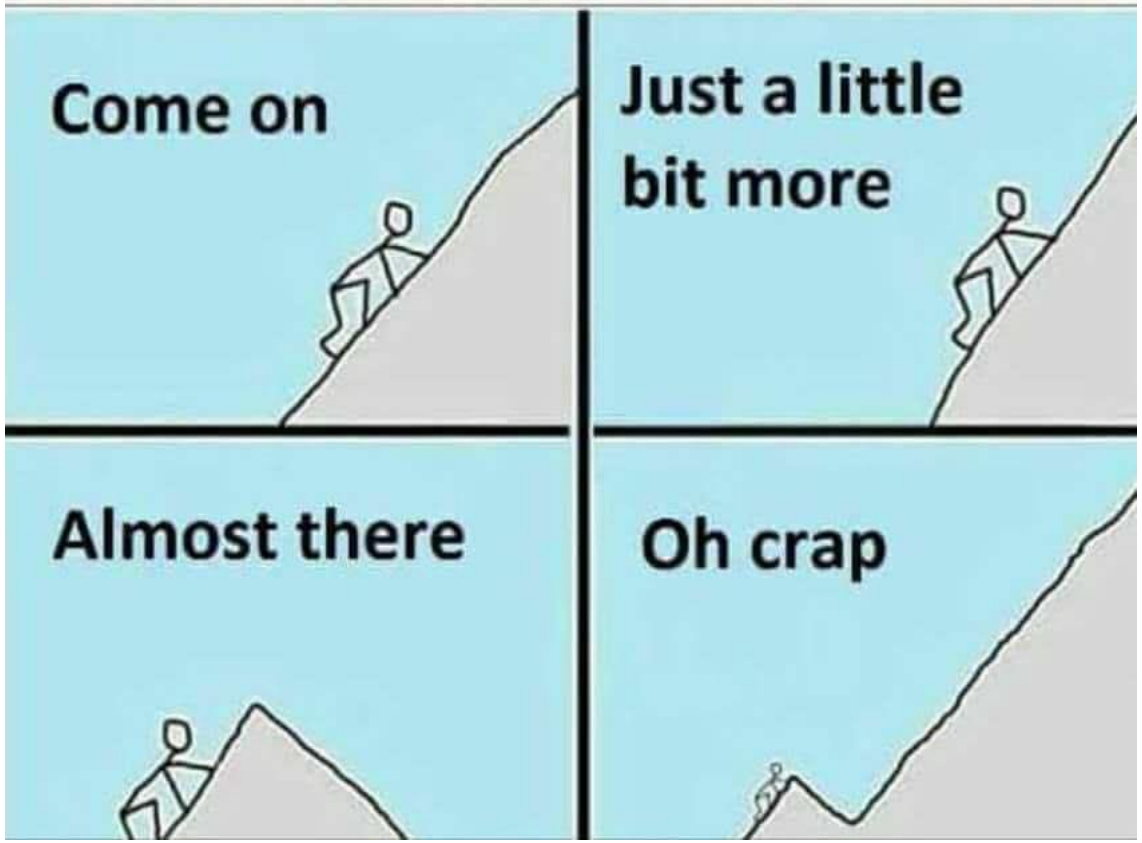
Problems of SGD

- "long-narrow valley"
  - What if your loss function happens to be steep in one direction but "flat" in another…
  - Condition number: ratio of largest to smallest singular value of the Hessian.
  - Large condition number → long-narrow valley



Problems of SGD

- Local minima or Saddle points → zero gradient! → No update (gets stuck)



Momentum

- Idea: let's build up a velocity (momentum)!

- SGD

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

- SGD + Momentum

$$v_{t+1} = \rho v_t + \nabla f(x_t)$$
$$x_{t+1} = x_t - \alpha v_{t+1}$$

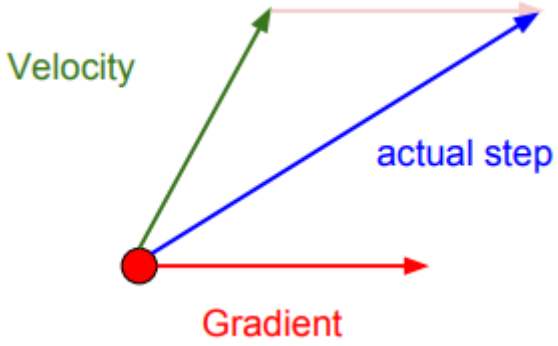
  - ρ: "friction" or "drag". Causes decrease of velocity. Typically 0.9 or 0.99

SGD + Momentum

- Discuss:
  - High condition number (long-narrow valley)
  - Local minima and saddle points
  - Noisy gradient

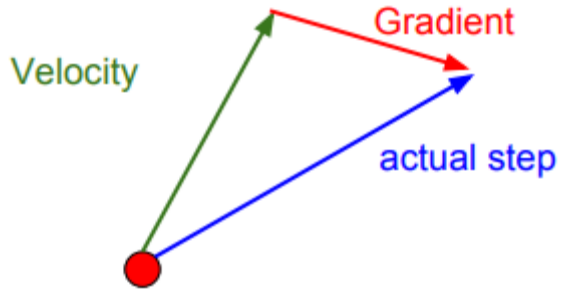
Nesterov Momentum

- Vanilla momentum method: Current gradient + Current velocity.



$$v_{t+1} = \rho v_t + \nabla f(x_t)$$
$$x_{t+1} = x_t - \alpha v_{t+1}$$

- Nesterov Version: Look ahead to the point where the current velocity would take us. Take the gradient there and perform the update.



☹

$$v_{t+1} = \rho v_t - \alpha \nabla f(x_t + \rho v_t)$$
$$x_{t+1} = x_t + v_{t+1}$$

Nesterov Momentum

- $v_{t+1} = \rho v_t - \alpha \nabla f(x_t + \rho v_t),\ x_{t+1} = x_t + v_{t+1}$

- We want to update in terms of x_t and $\nabla f(x_t)$, NOT $\nabla f(x_t + \rho v_t)$.

- Luckily, this can be rearranged by the change of variables: $\tilde{x}_t = x_t + \rho v_t$

$$
\begin{aligned}
v_{t+1} &= \rho v_t - \alpha \nabla f(\tilde{x}_t) \\
\tilde{x}_{t+1} &= \tilde{x}_t - \rho v_t + v_{t+1} + \rho v_{t+1} \\
&= \tilde{x}_t + v_{t+1} + \rho(v_{t+1} - v_t)
\end{aligned}
$$

AdaGrad

- Perform element-wise scaling of the gradient
  - Scale factors determined based on the historical sum of squares…

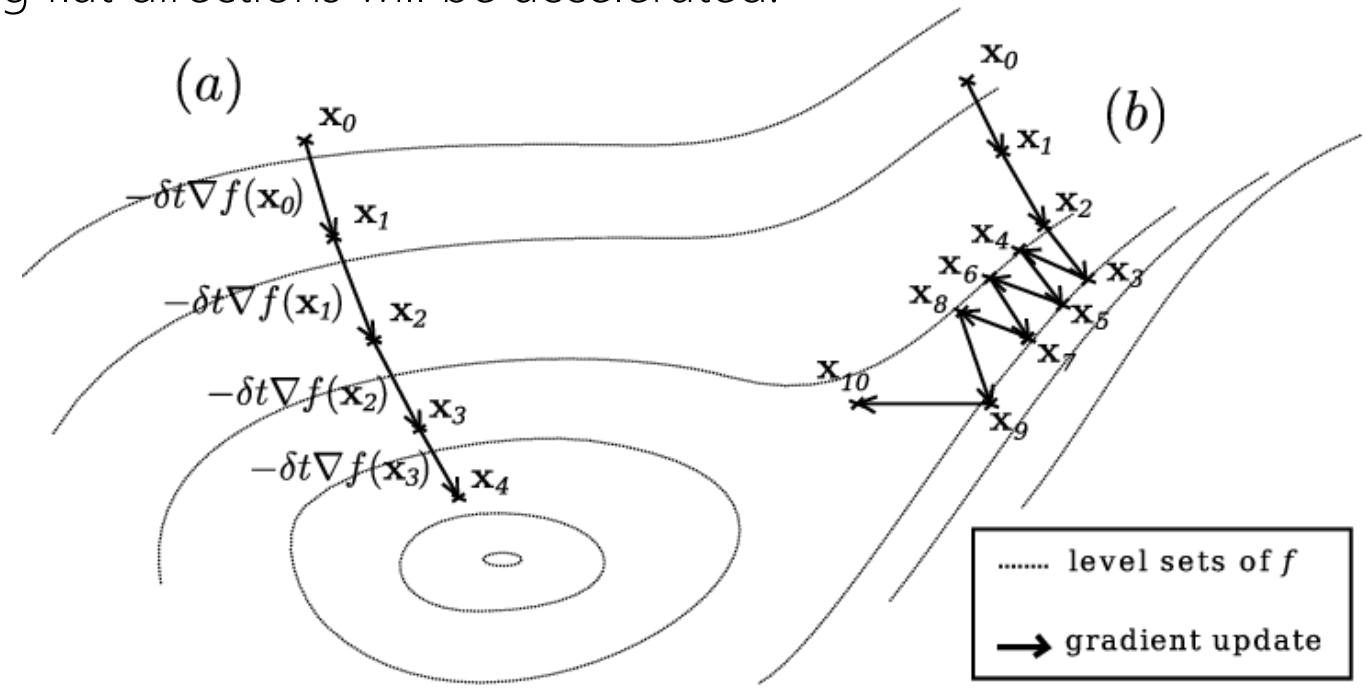
```
scale_factor = 0

for iter in range(0, MAX_ITER):
    dx = backpropagate(x)   # compute gradient
    scale_factor += dx*dx
    x -= learning_rate * dx / (np.sqrt(scale_factor) + epsilon)
```

- The element-wise scaling has an effect of "per-parameter learning rates" or "adaptive learning rates," thus, the name Adaptive Gradient.

AdaGrad

- Long narrow valley: what happens with AdaGrad?
  - Step size along steep directions will be damped.
  - Step size along flat directions will be accelerated.



AdaGrad

- Historical sum: what happens with AdaGrad after many iterations?
  - Step size decays to zero… ☹

```
scale_factor = 0

for iter in range(0, MAX_ITER):
    dx = backpropagate(x)   # compute gradient
    scale_factor += dx*dx
    x -= learning_rate * dx / (np.sqrt(scale_factor) + epsilon)
```

RMSProp

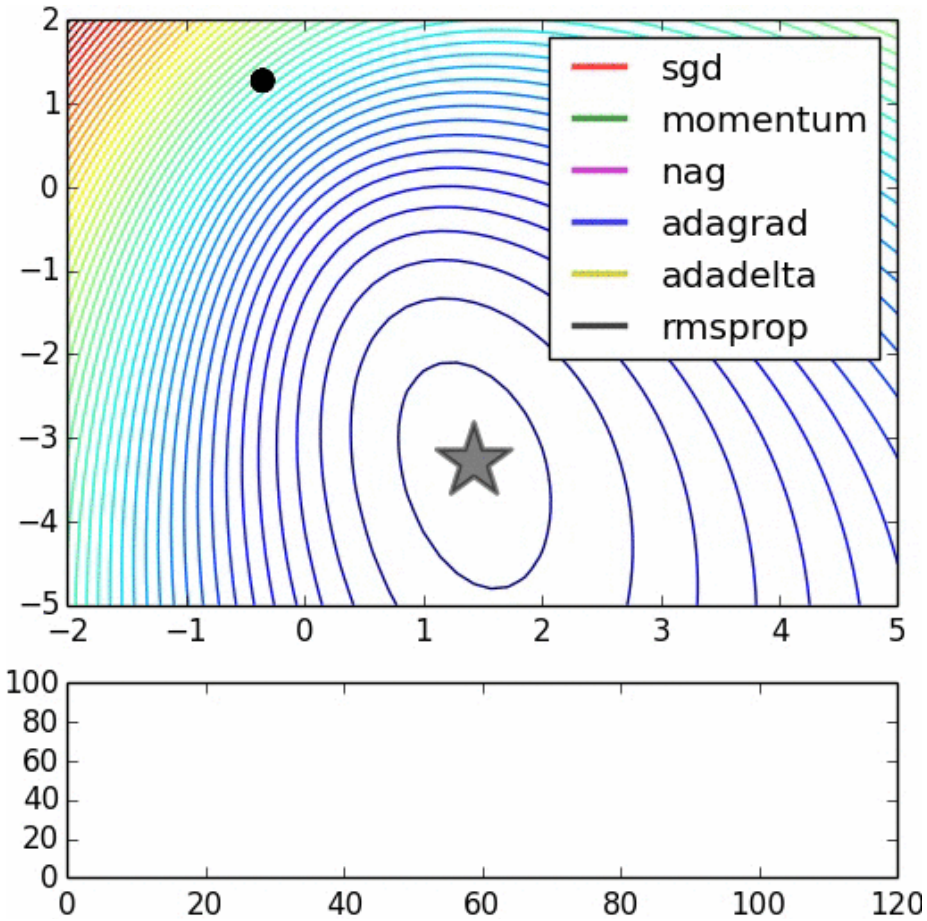
- AdaGrad (step size decays to zero):

```
scale_factor = 0
for iter in range(0, MAX_ITER):
    dx = backpropagate(x)   # compute gradient
    scale_factor += dx*dx
    x -= learning_rate * dx / (np.sqrt(scale_factor) + epsilon)
```

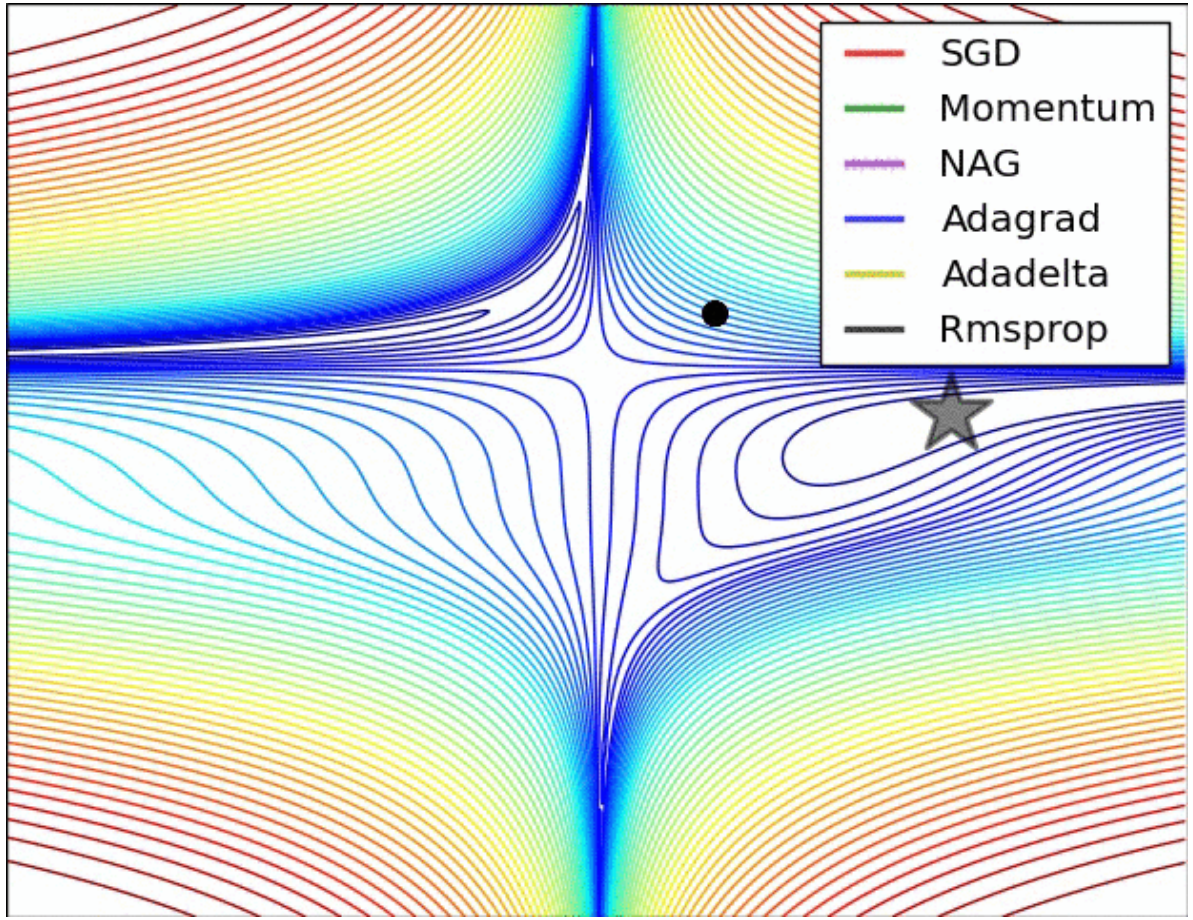
- RMSProp (problem solved ☺)

```
scale_factor = 0
for iter in range(0, MAX_ITER):
    dx = backpropagate(x)   # compute gradient
    scale_factor = decay_rate*scale_factor + (1-decay_rate)*dx*dx
    x -= learning_rate * dx / (np.sqrt(scale_factor) + epsilon)
```

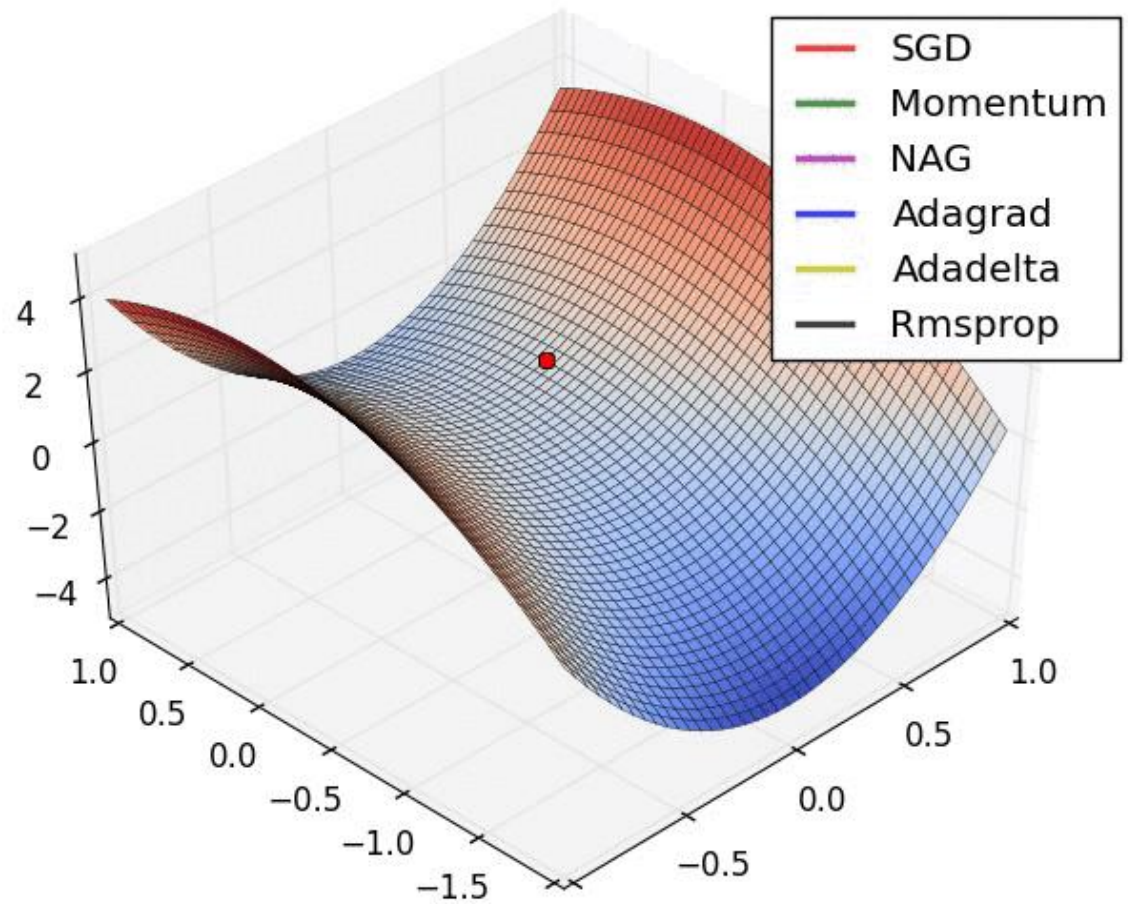
Comparison of Optimization Methods



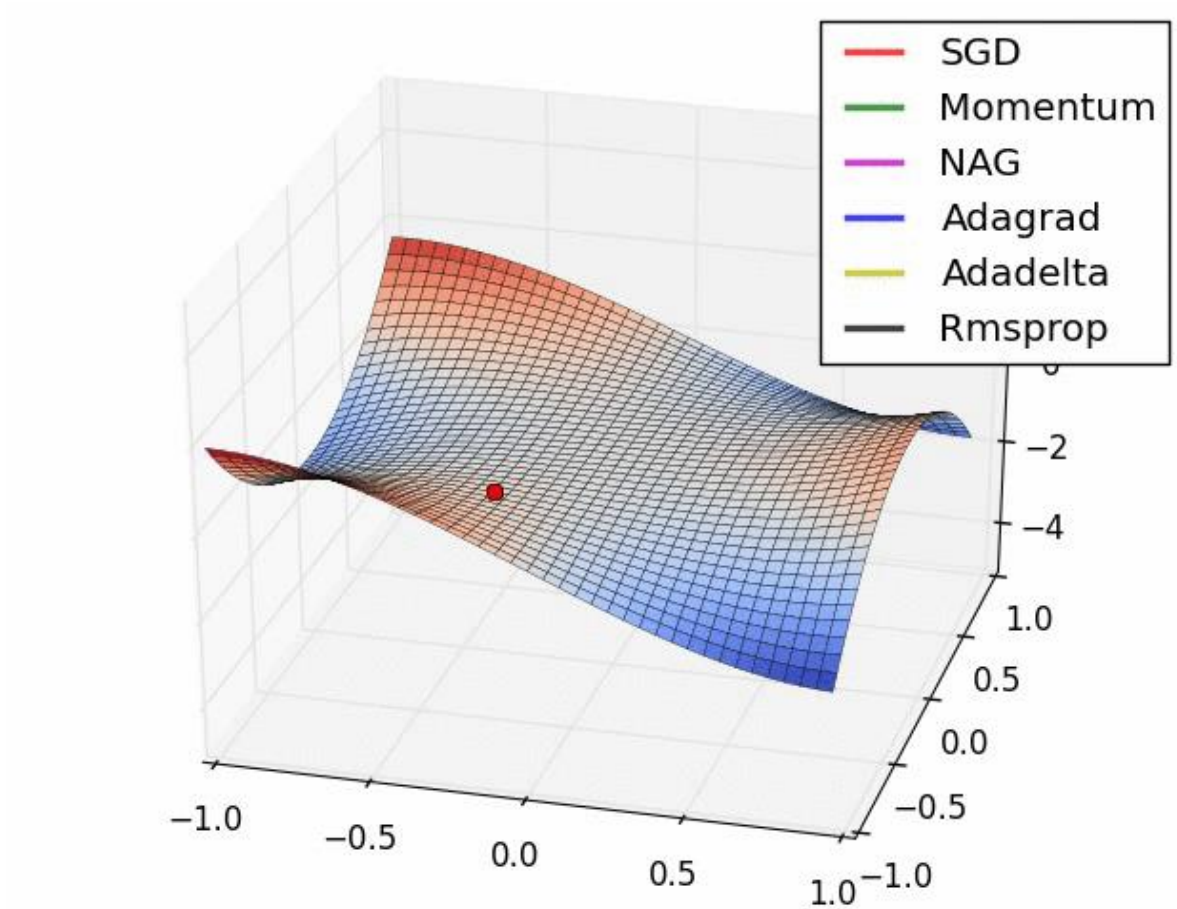
Comparison of Optimization Methods



Comparison of Optimization Methods



Comparison of Optimization Methods



Adam (All of the above!)

- Why not take the advantage of both momentum and adaptive gradient methods?

```
moment = [0, 0]
for iter in range(0, MAX_ITER):
    dx = backpropagate(x)   # compute gradient
    moment[0] = beta[0]*moment[0] + (1-beta[0])*dx                    # momentum
    moment[1] = beta[1]*moment[1] + (1-beta[1])*dx*dx                 # RMSProp
    x -= learning_rate * moment[0] / (np.sqrt(moment[1]) + epsilon)
```

- Problem with the idea: what happens when iter = 0?
  - moments = 0 → bias!

Adam (All of the above!)

```
moment = [0, 0]
for iter in range(0, MAX_ITER):
    dx = backpropagate(x)   # compute gradient
    moment[0] = beta[0]*moment[0] + (1-beta[0])*dx                  # momentum
    moment[1] = beta[1]*moment[1] + (1-beta[1])*dx*dx               # RMSProp
    x -= learning_rate * moment[0] / (np.sqrt(moment[1]) + epsilon)
```

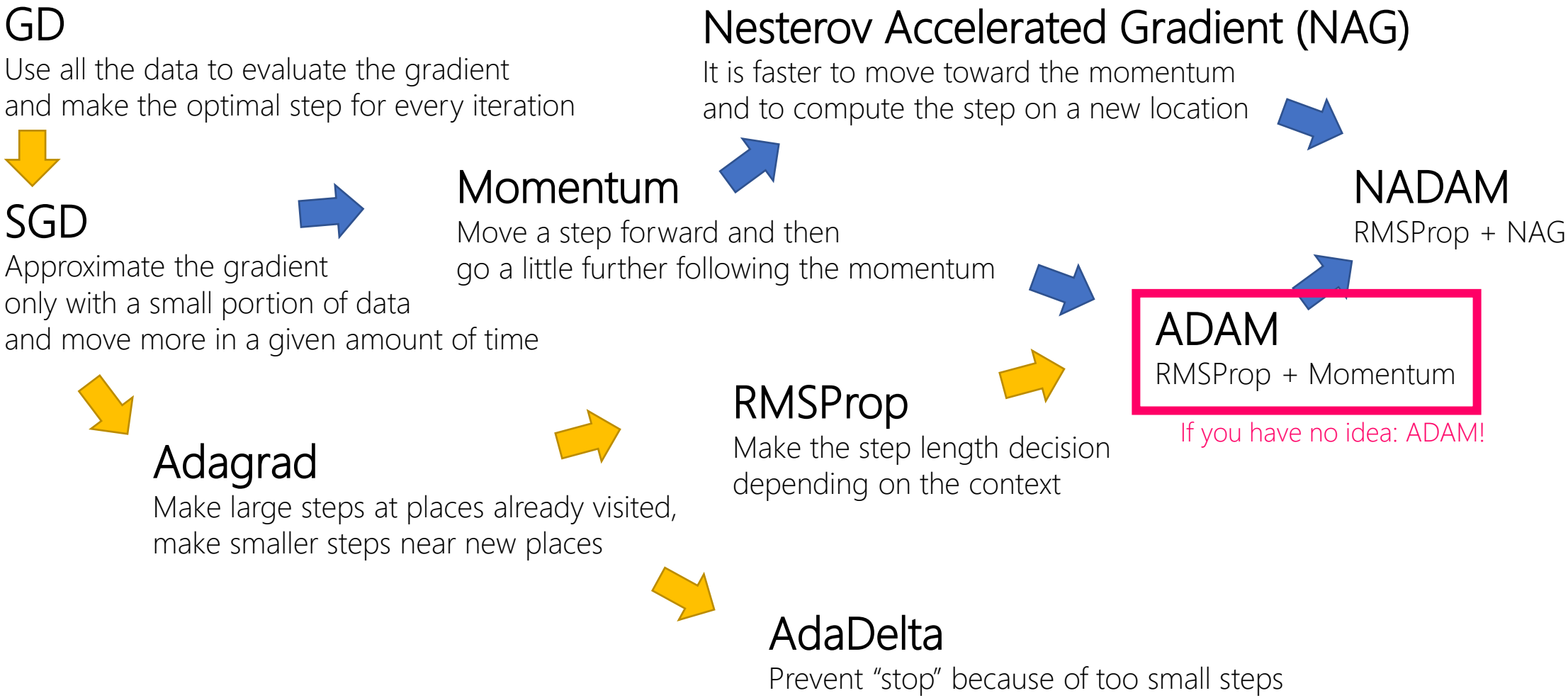
- Modified version:

In typical scenarios, a good starting point:

- beta = some big number close to 1 (e.g. 0.9, 0.99)
- learning_rate = 1e-3

```
moment = [0, 0]
for iter in range(0, MAX_ITER):
    dx = backpropagate(x)   # compute gradient
    moment[0] = beta[0]*moment[0] + (1-beta[0])*dx                  # momentum
    moment[1] = beta[1]*moment[1] + (1-beta[1])*dx*dx               # RMSProp
    unbiased[0] = moment[0] / (1 - beta[0]**iter)                   # bias correction
    unbiased[1] = moment[1] / (1 - beta[1]**iter)
    x -= learning_rate * unbiased[0] / (np.sqrt(unbiased[1]) + epsilon)
```

History of NN Optimizers



Tips on Learning Process & Hyperparameter Tuning

Training Process, Step-by-step

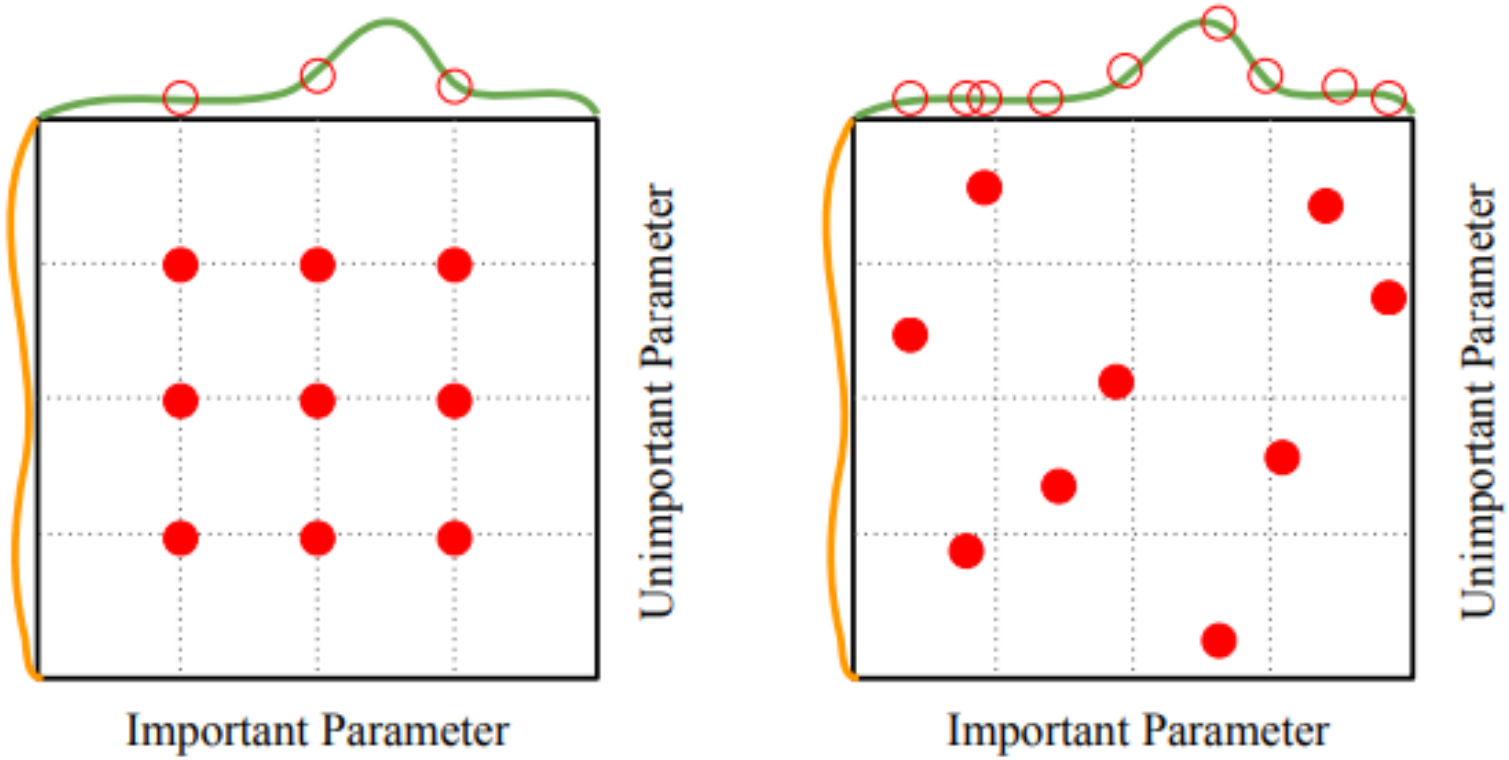
1. Preprocess the data (normalize/whiten, or at least zero-center them)
2. Design the network architecture (start with a simple one if possible)
3. Train with a small amount of data (a subset of your data). Make sure the model can overfit (i.e. loss go down to 0 and accuracy goes 1).
4. Now, the actual training, find the learning rate
   - LR too low: loss won't go down, LR too high: loss will explode.
   - Start with a small number and find the learning rate that makes some observable change.
5. Hyperparameter Tuning!

Hyperparameters Tuning

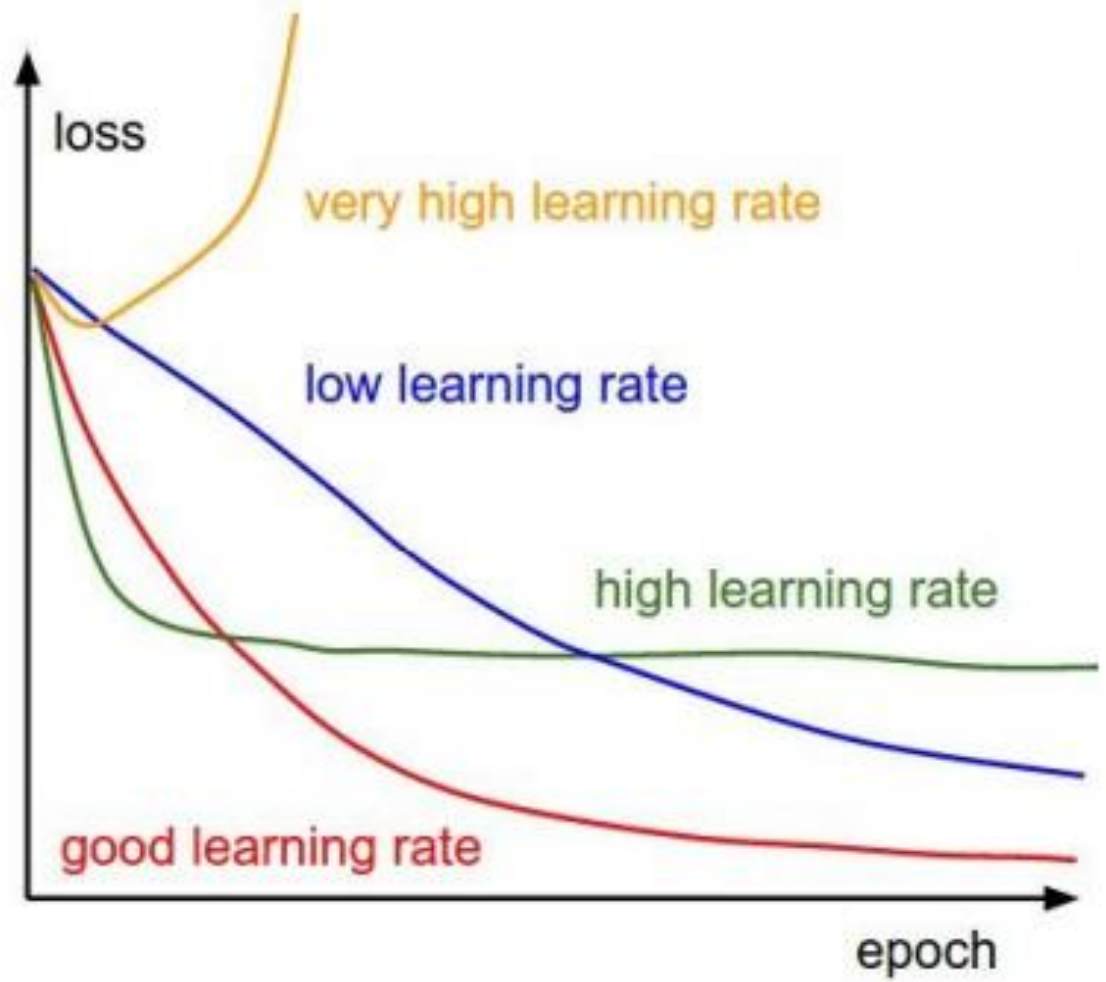
- Major hyperparameters: depth and breadth (or network architecture)
- Others: regularization terms, learning rate and its decay schedule, etc.

- Coarse-to-fine Strategy:
  - First, only a few epochs to get a rough idea of how parameters play
  - Second, longer epochs, do finer search
  - Repeat this as architecture changes.

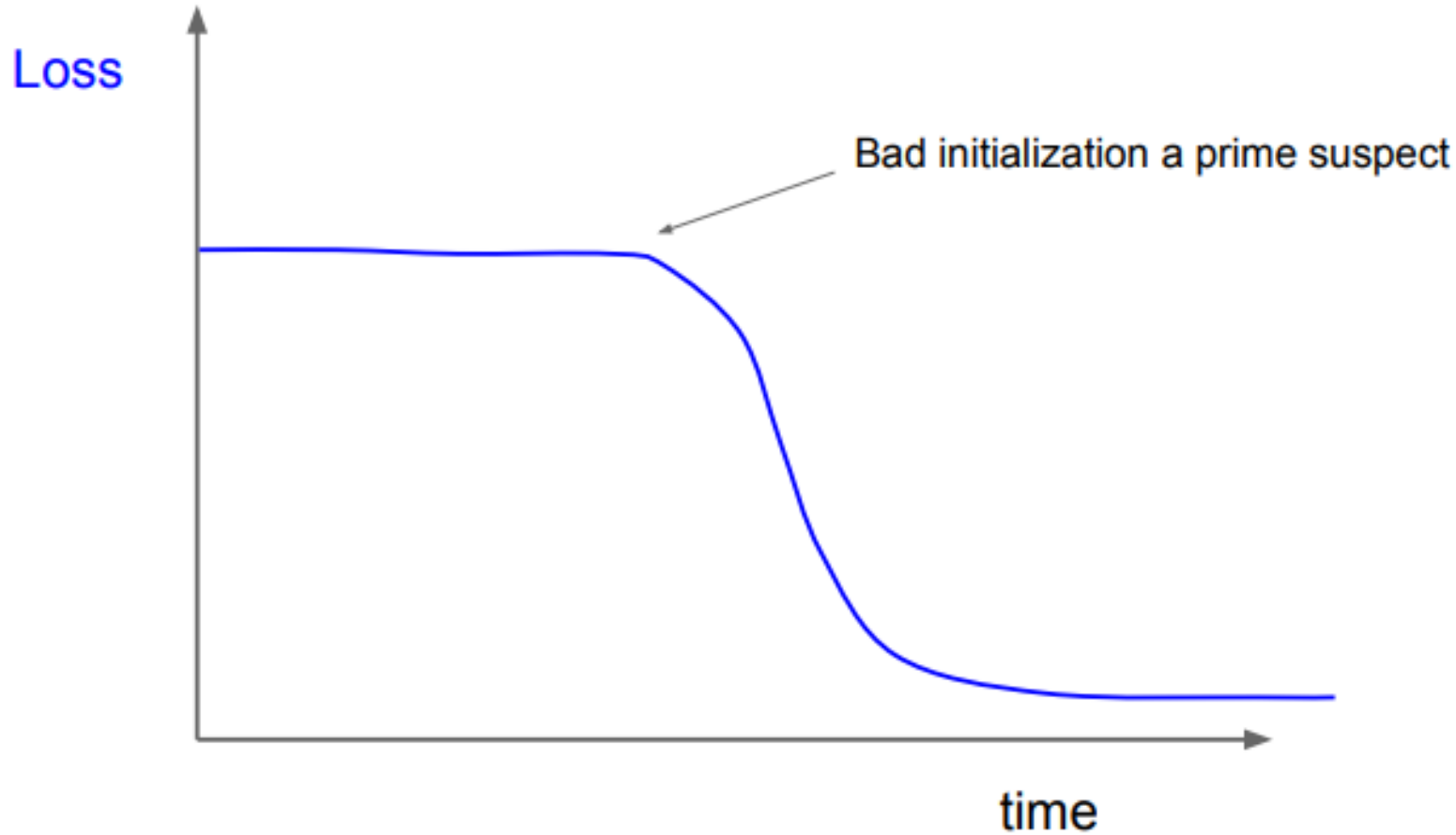
Grid Search vs. Random Search



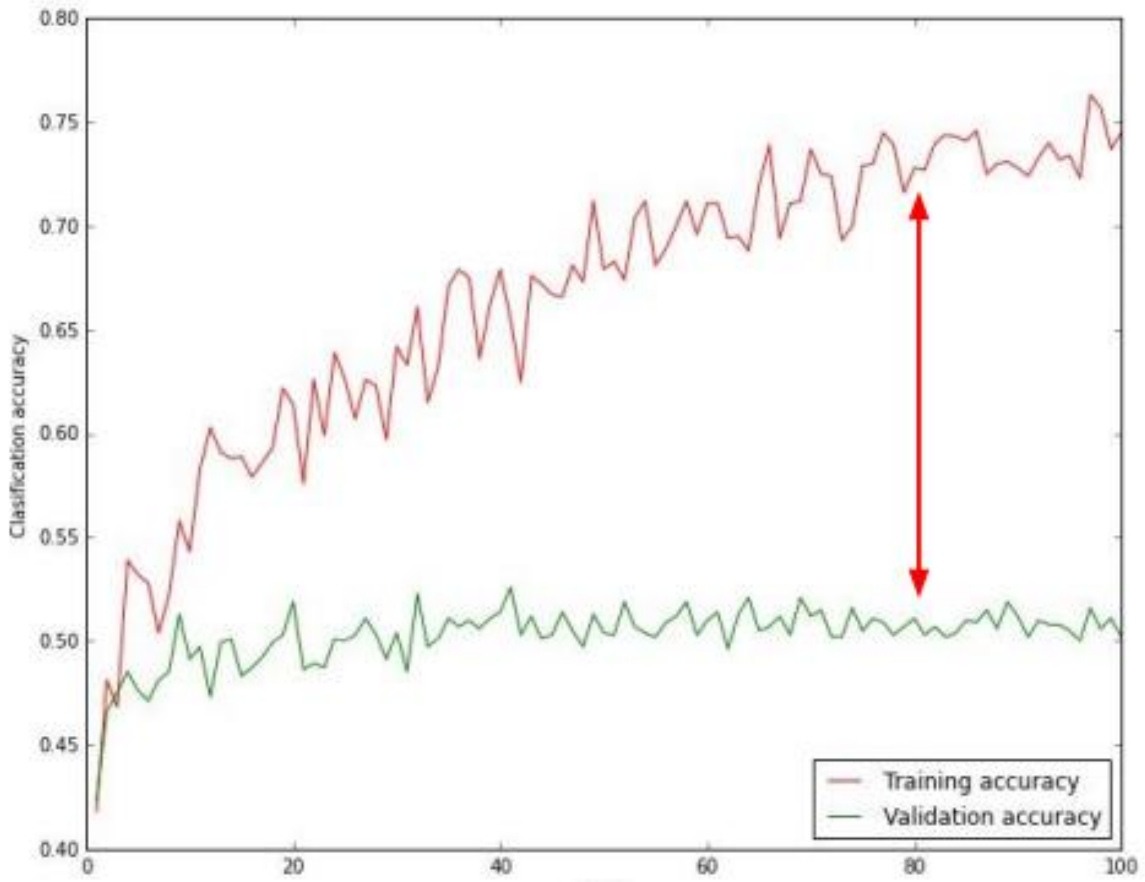
Always monitor and visualize the loss/accuracy!



Always monitor and visualize the loss/accuracy!



Always monitor and visualize the loss/accuracy!



big gap = overfitting

=> increase regularization strength?

no gap

=> increase model capacity?

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Tracking the weights also helps

- Percentage of weight update over weight magnitudes
  - Around 0.001 is ideal
  - Around 0.01 is about okay

```
# assume parameter vector W and its gradient vector dW
param_scale = np.linalg.norm(W.ravel())
update = -learning_rate*dW # simple SGD update
update_scale = np.linalg.norm(update.ravel())
W += update # the actual update
print update_scale / param_scale # want ~1e-3
```

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