Applied Deep Learning

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Learning objectives of today

Goals: Understand the difficulties in using neural networks in practice, and the more advanced concepts to overcome these difficulties

- Bias and variance, as well as regularization tools
- The problem of vanishing and exploding gradients, as well as slow learning
- Hyperparameter tuning

How will we do this?

- We look at the theoretical foundations of both the issues and the solutions
- In class, we will then introduce the TensorFlow code to implement a range of different solutions

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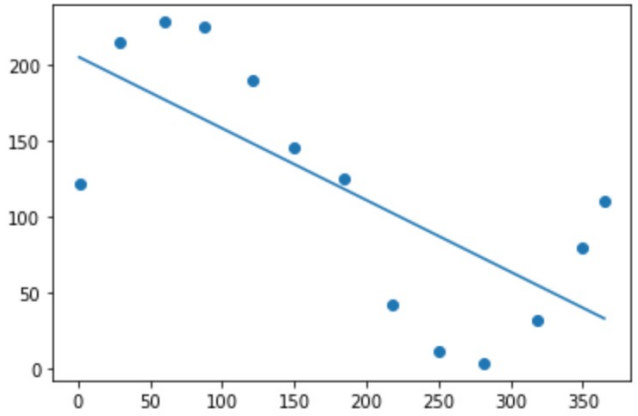
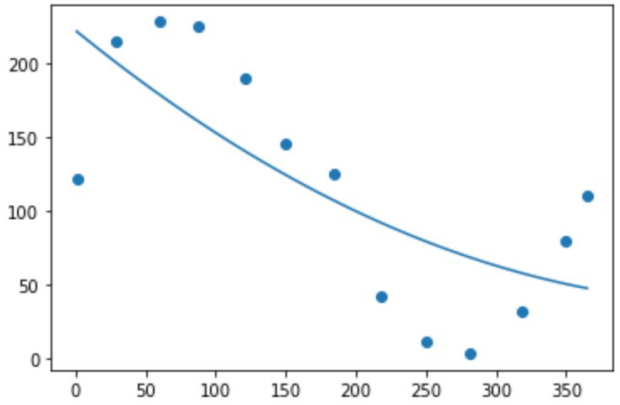
Bias-variance trade-off

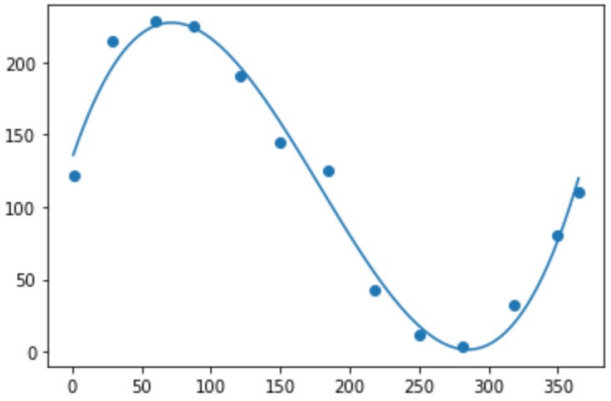
Looking back: predicting sales using polynomial regression and the problem of overfitting



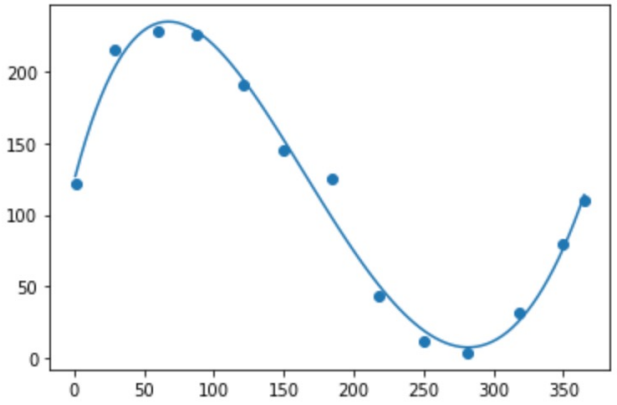
d=1, R^2=0.516



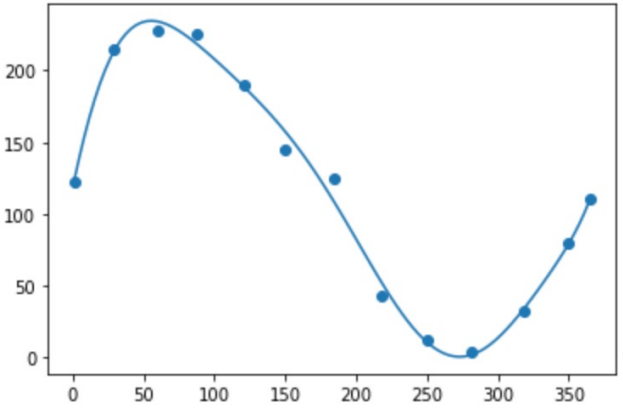
d=2, R^2=0.531



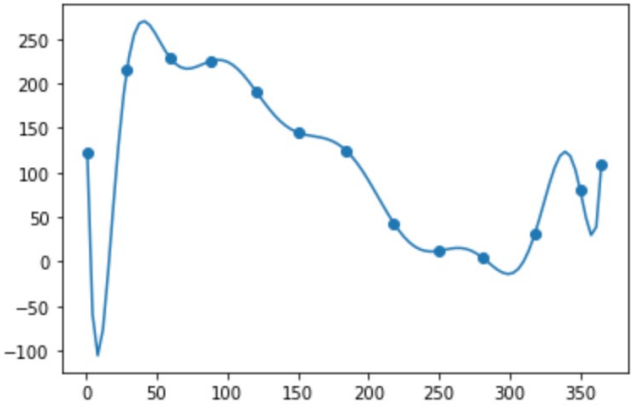
d=3, R^2=0.979



d=5, R^2=0.985



d=8, R^2=0.992



d=12, R^2=1

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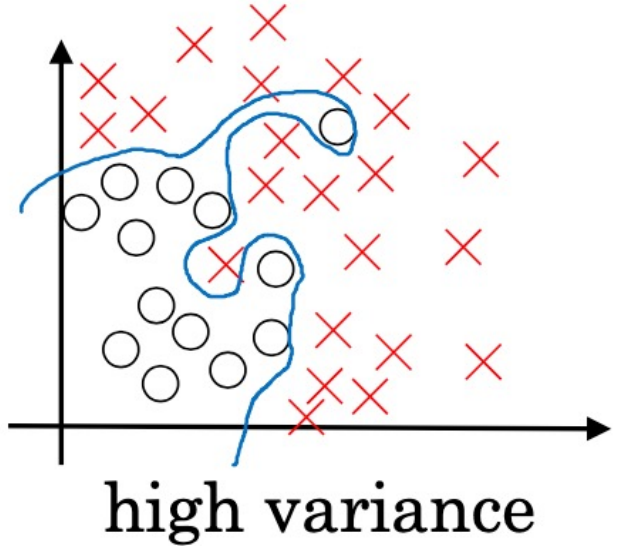
Bias and variance



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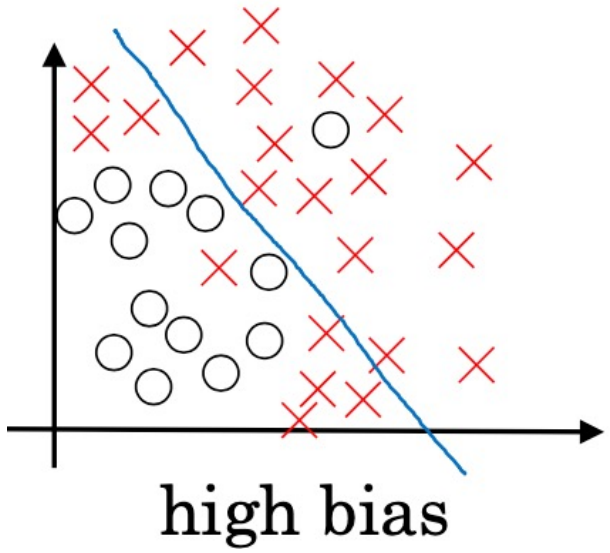
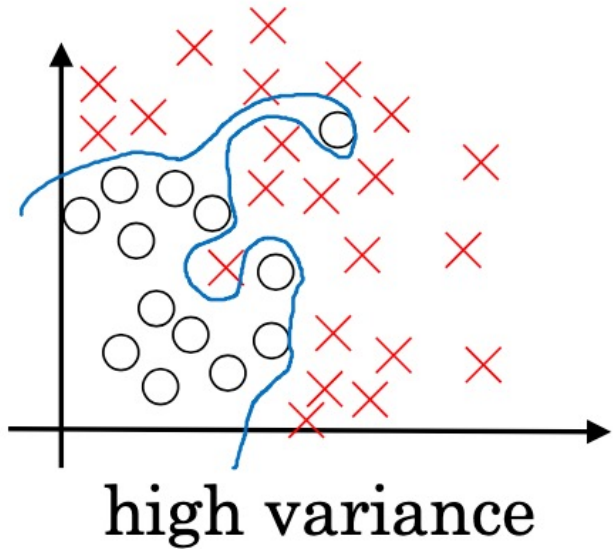
Bias and variance





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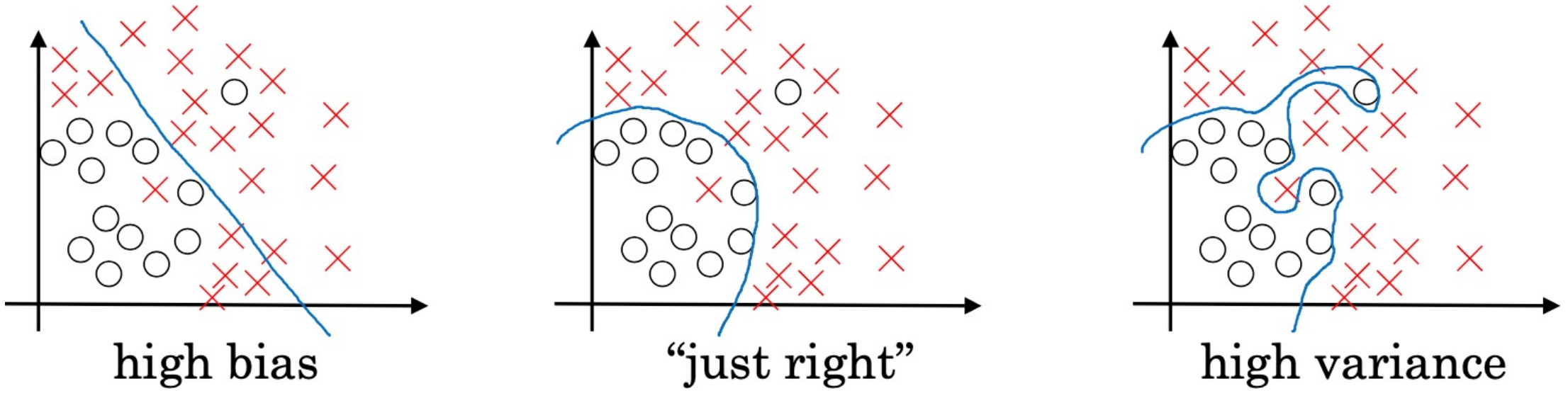
Bias and variance



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Recognizing bias and variance

"Bayes error"	(Avoidable) bias	1%	1%
Error on training set	Variance	2%	10%
Error on validation set		10%	12%
		High variance	High bias

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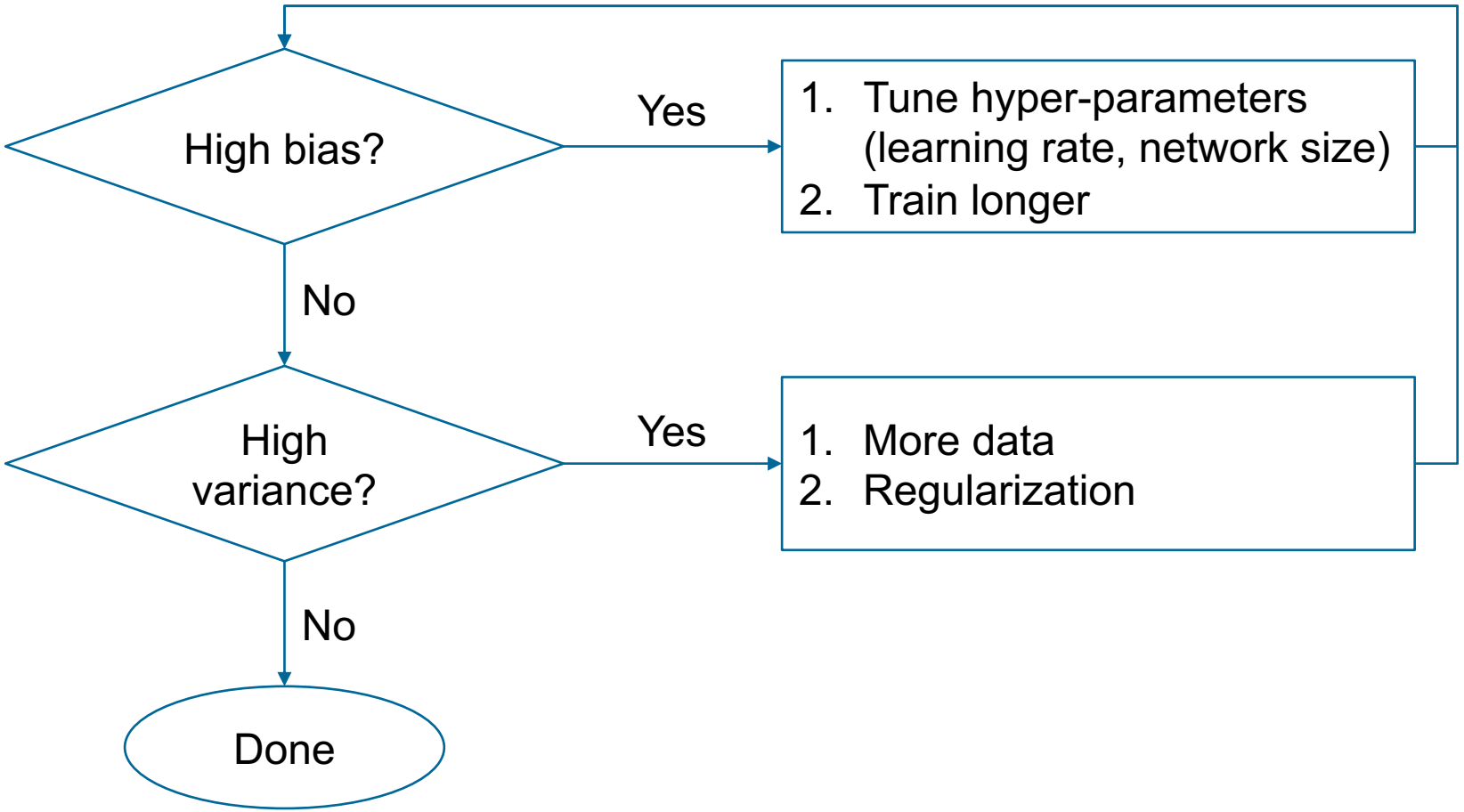
How to deal with bias and variance



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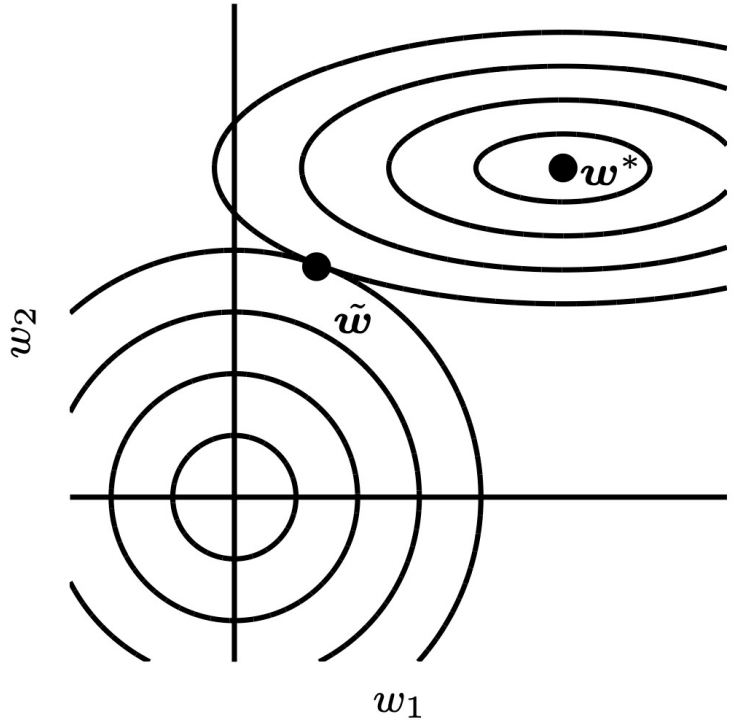
L2-regularization ("Ridge regression")

$$J(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} L^{(i)} \quad \Longleftrightarrow \quad J_R(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} L^{(i)} + \frac{\lambda}{2}\|\boldsymbol{\theta}\|_2 = \frac{1}{n}\sum_{i=1}^{n} L^{(i)} + \frac{\lambda}{2}\sqrt{\theta_1^2 + \theta_2^2 + \cdots + \theta_m^2}$$

- Gradient: $\nabla_\theta J_R(\boldsymbol{\theta}) = \nabla_\theta J(\boldsymbol{\theta}) + \lambda\boldsymbol{\theta}$
- Gradient descent update:

$$\begin{aligned}\boldsymbol{\theta} &:= \boldsymbol{\theta} - \alpha\nabla_\theta J_R \\ &= \boldsymbol{\theta} - \alpha\nabla_\theta J(\boldsymbol{\theta}) - \alpha\lambda\boldsymbol{\theta} \\ &= (1 - \alpha\lambda)\boldsymbol{\theta} - \alpha\nabla_\theta J(\boldsymbol{\theta})\end{aligned}$$

→ "weight decay"



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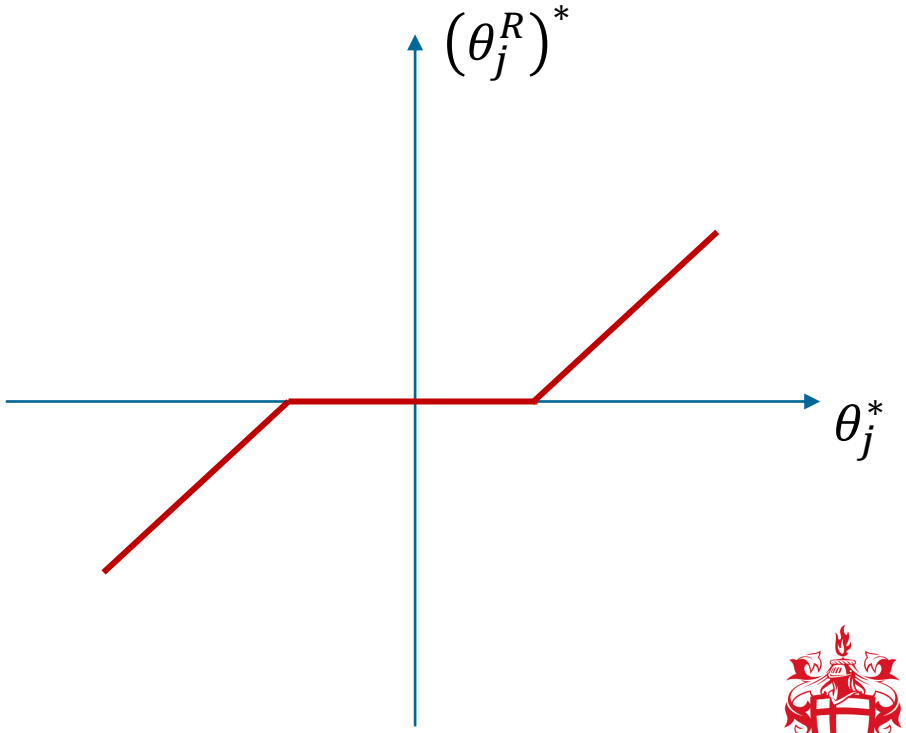
L1-regularization (“Lasso regression”)

$$J(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} L^{(i)} \quad \Longleftrightarrow \quad J_R(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} L^{(i)} + \lambda\|\boldsymbol{\theta}\|_1 = \frac{1}{n}\sum_{i=1}^{n} L^{(i)} + \lambda\sum_{j=1}^{m}|\theta_j|$$

- Gradient: $\nabla_\theta J_R(\boldsymbol{\theta}) = \nabla_\theta J(\boldsymbol{\theta}) + \lambda\, sign(\boldsymbol{\theta})$
- Gradient descent update:

$$\boldsymbol{\theta} := \boldsymbol{\theta} - \alpha\nabla_\theta J_R$$
$$= \boldsymbol{\theta} - \alpha\nabla_\theta J(\boldsymbol{\theta}) - \alpha\lambda\, sign(\boldsymbol{\theta})$$

→ “sparsity”



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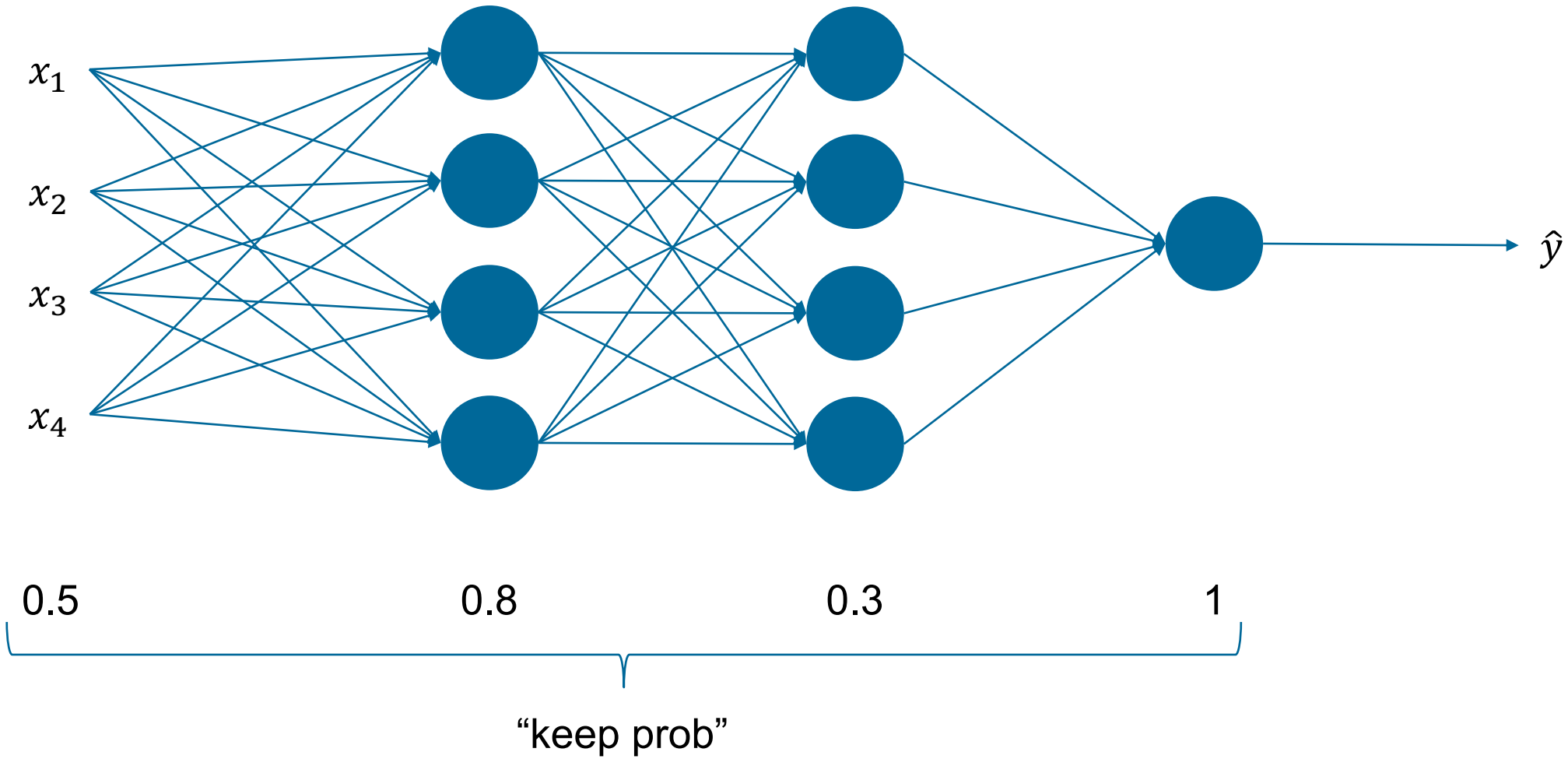
Dropout regularization



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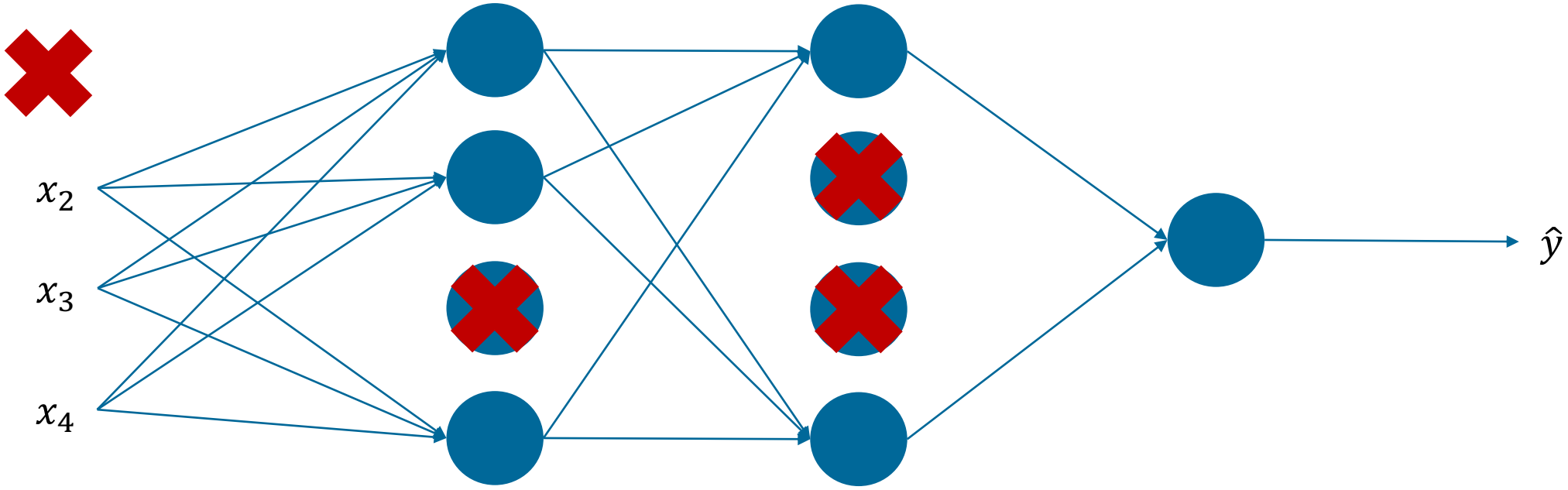
Dropout regularization



0.5 0.8 0.3 1

"keep prob"

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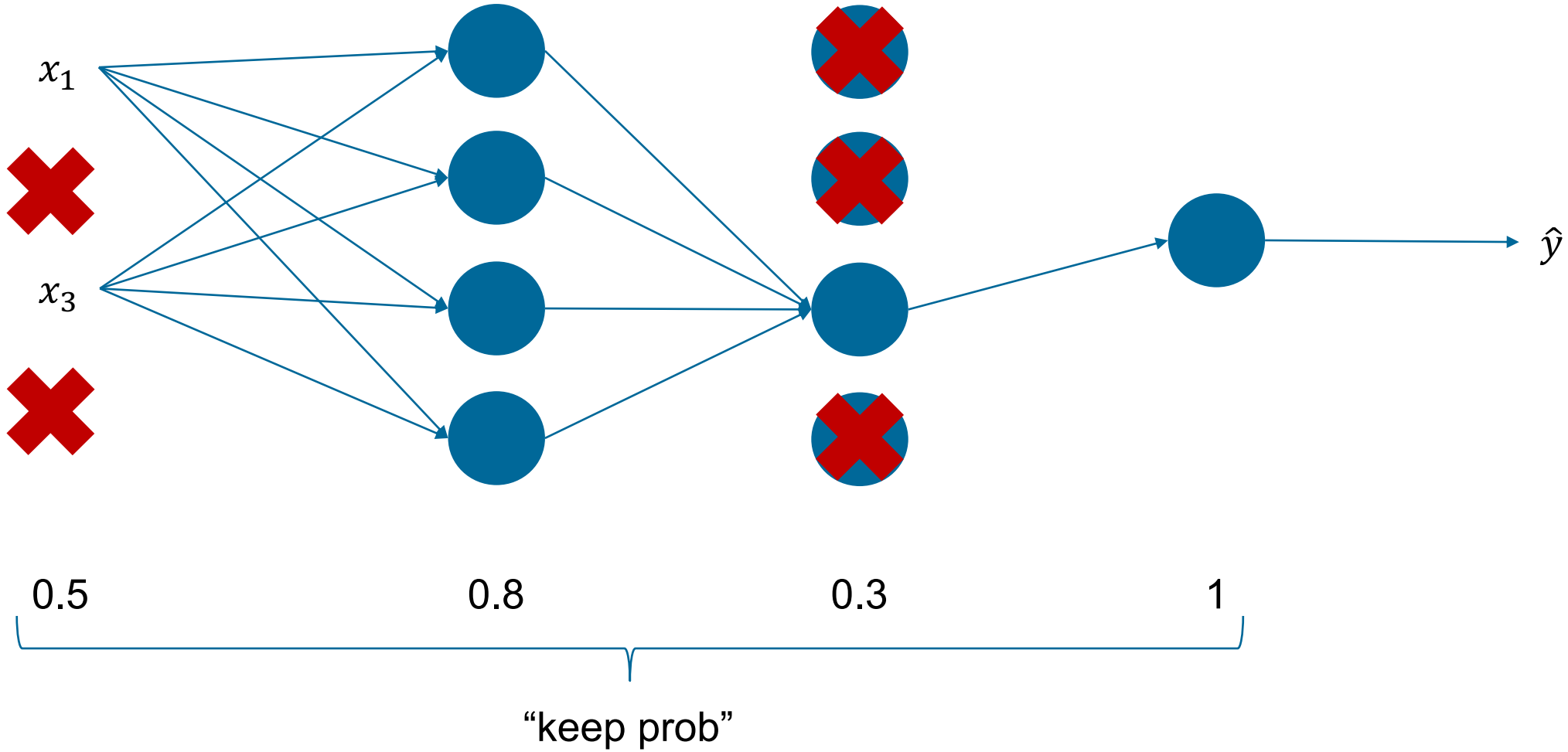
Dropout regularization



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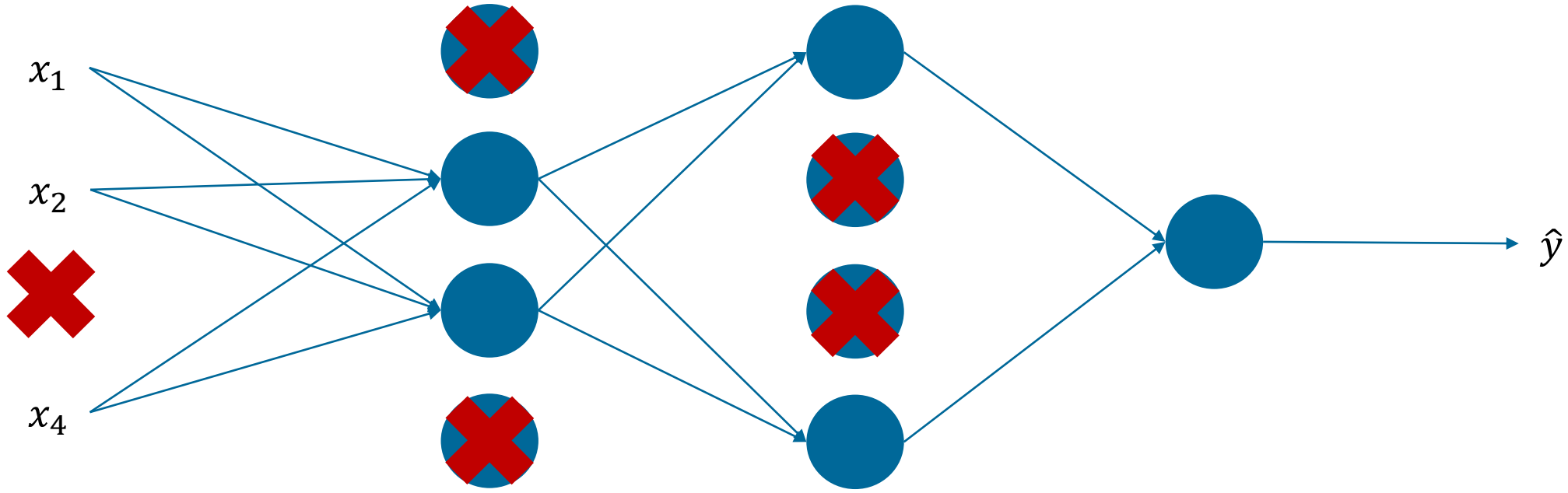
Dropout regularization



0.5 0.8 0.3 1

"keep prob"

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The idea behind dropout regularization

We cannot rely on any one feature (or previous neuron's activation), so the weights need to be spread out.

Effectively, we train multiple smaller networks in an ensemble.

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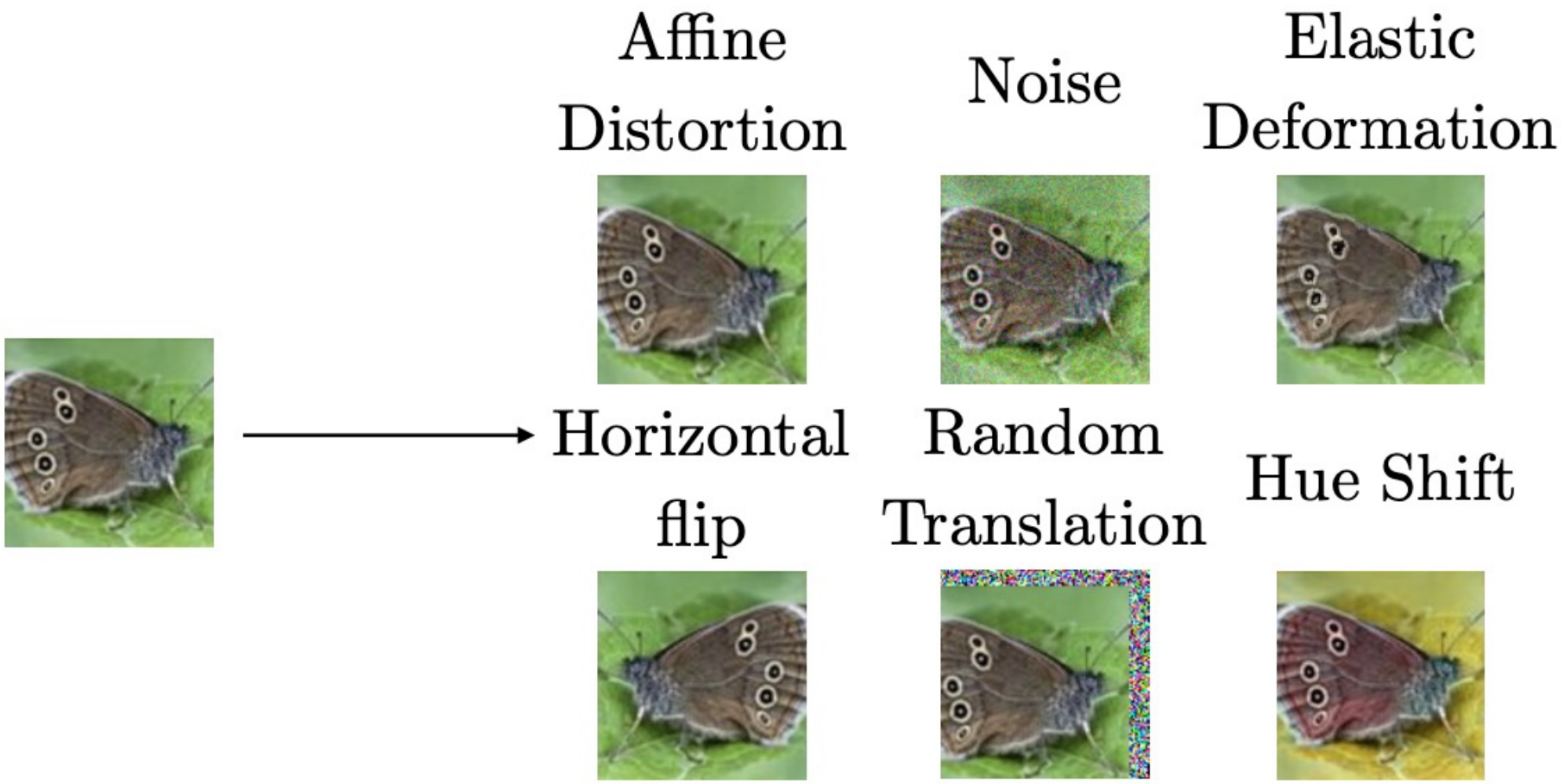
Dataset augmentation



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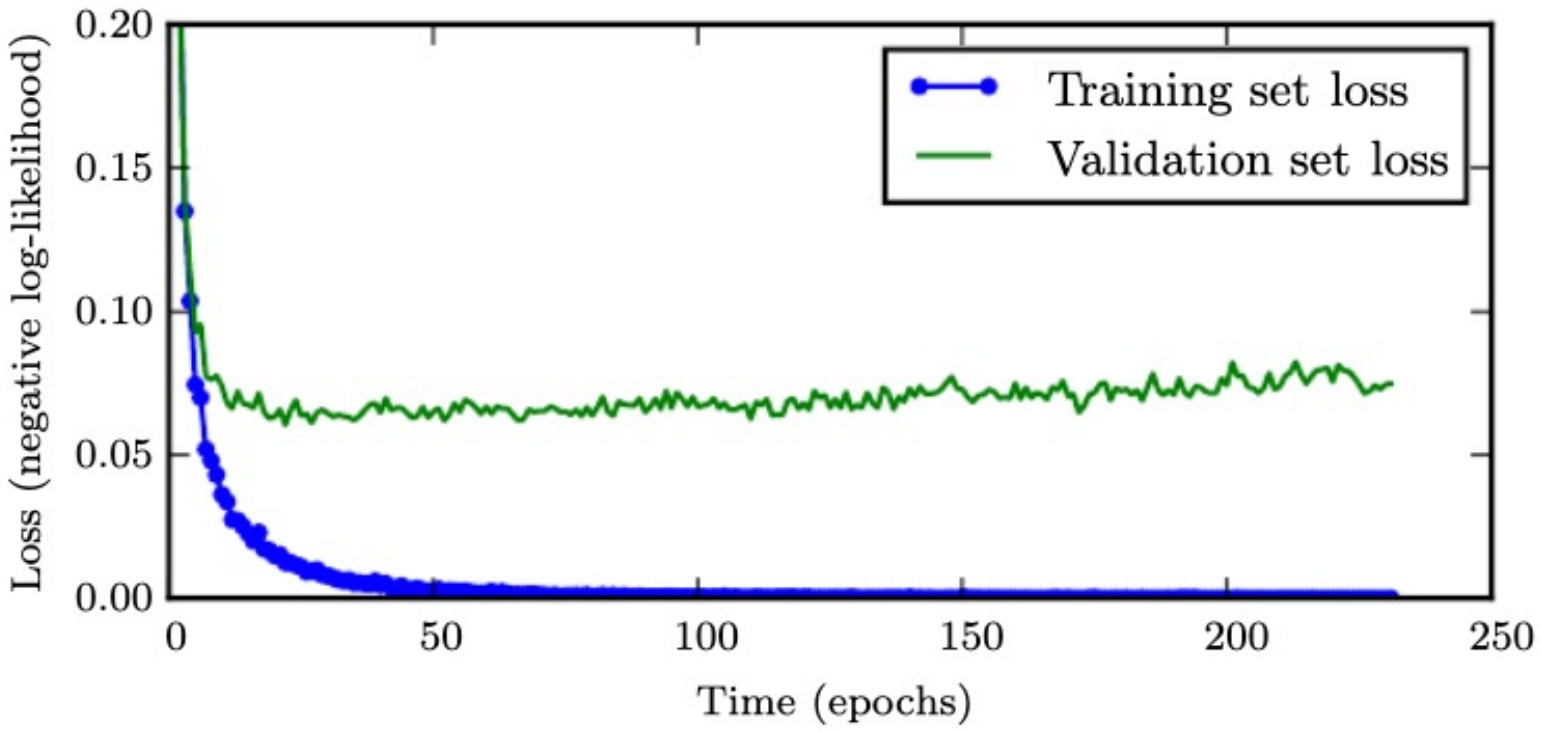
Early stopping



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Improving learning

Other possible issues we might come across in training

- Vanishing and exploding gradients
  - → Initialization
  - → Activation functions
  - → Data normalization
  - → Batch normalization

- Very slow training
  - → Mini-batch gradient descent
  - → Momentum optimization, RMSprop, Adam
  - → Reusing pretrained layers

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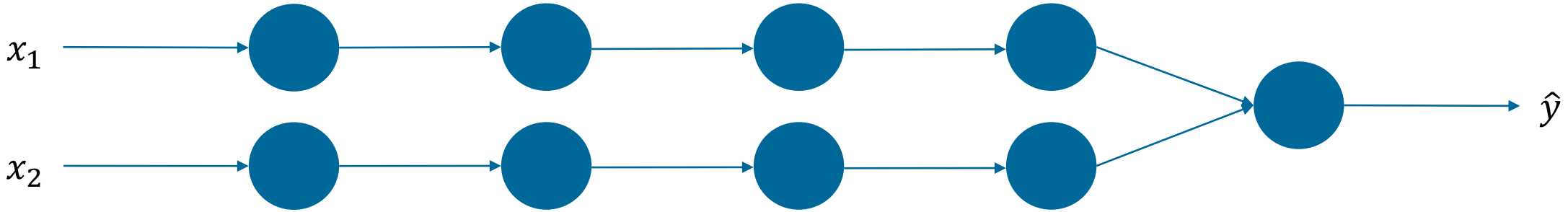
Improving learning – vanishing and exploding gradients

Why gradients vanish and explode



For simplicity, assume a linear activation function, as well as $b = 0$. We then have that

$$\nabla_{W^{[l]}} J = \left(A^{[l-1]}\right)^T \left(W^{[l+1]} \dots W^{[L]}\right)^T$$

$$= \left(A^{[l-1]}\right)^T \begin{pmatrix} w_{1,1}^{[l+1]} w_{1,1}^{[l+2]} \dots w_{1,1}^{[L]} & 0 \\ 0 & w_{2,2}^{[l+1]} w_{2,2}^{[l+2]} \dots w_{2,2}^{[L]} \end{pmatrix}^T$$

If we assume the weights are w everywhere, we have

$$= \left(A^{[l-1]}\right)^T \begin{pmatrix} w^{L-l} & 0 \\ 0 & w^{L-l} \end{pmatrix}^T$$

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Possible counter: the “right” initialization

- Glorot-initialization (assuming logistic sigmoid, tanh, softmax activation):
  - variance of inputs ≈ variance of outputs
  - variance of gradients before layer ≈ variance of gradients after layer

  - Idea: given a layer with in inputs and out neurons, distribute weights either
    - normally, with mean 0 and variance $\frac{1}{\frac{in+out}{2}}$, or (kernel_initializer=“glorot_normal”)
    - uniformly between $\left[-\sqrt{\frac{3}{\frac{in+out}{2}}}, \sqrt{\frac{3}{\frac{in+out}{2}}}\right]$ (default)

- He-initialization (assuming ReLU and its variants):
  - Idea: given a layer with in inputs and out neurons, distribute weights either
    - normally, with mean 0 and variance $\frac{2}{in}$, or (kernel_initializer=“he_normal”)
    - uniformly between $\left[-\sqrt{\frac{6}{in}}, \sqrt{\frac{6}{in}}\right]$ (kernel_initializer=“he_uniform”)

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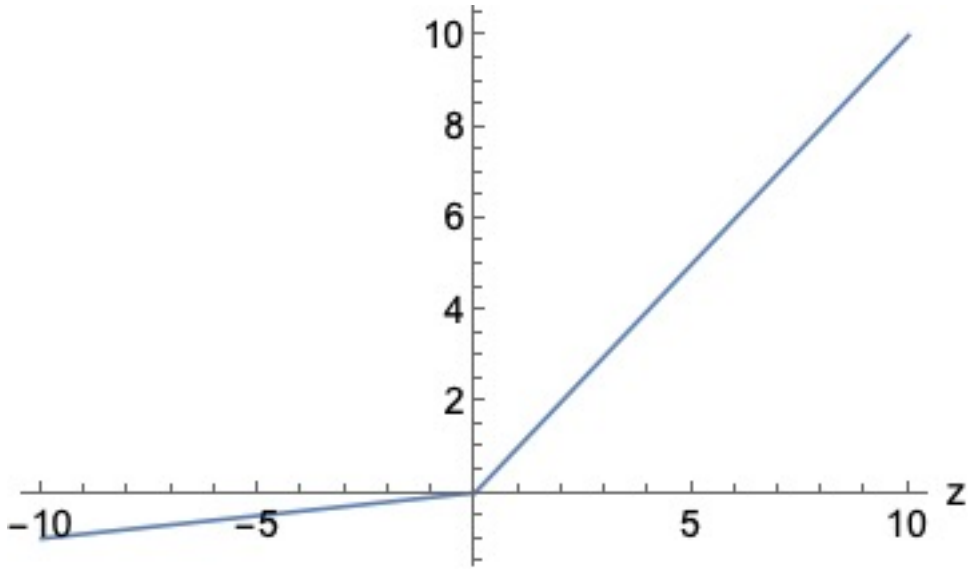
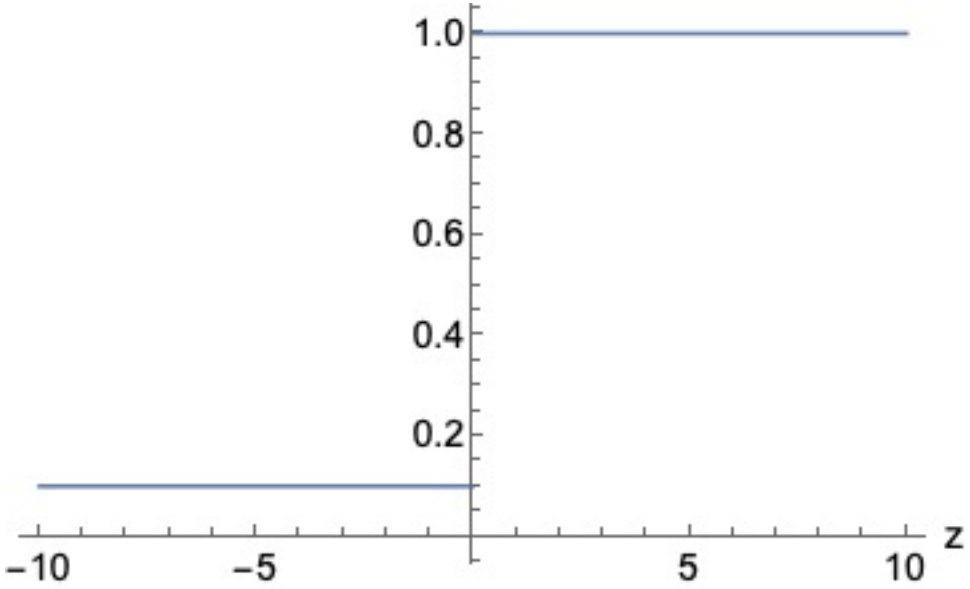
Another possible counter: non-saturating activation functions

Leaky ReLU



$$f(z) = \max\{0.1z, z\}$$

"Derivative"



$$f'(z) = \begin{cases} 0.1, if\ z < 0 \\ 1, if\ z > 0 \end{cases}$$

Consider also: ELU

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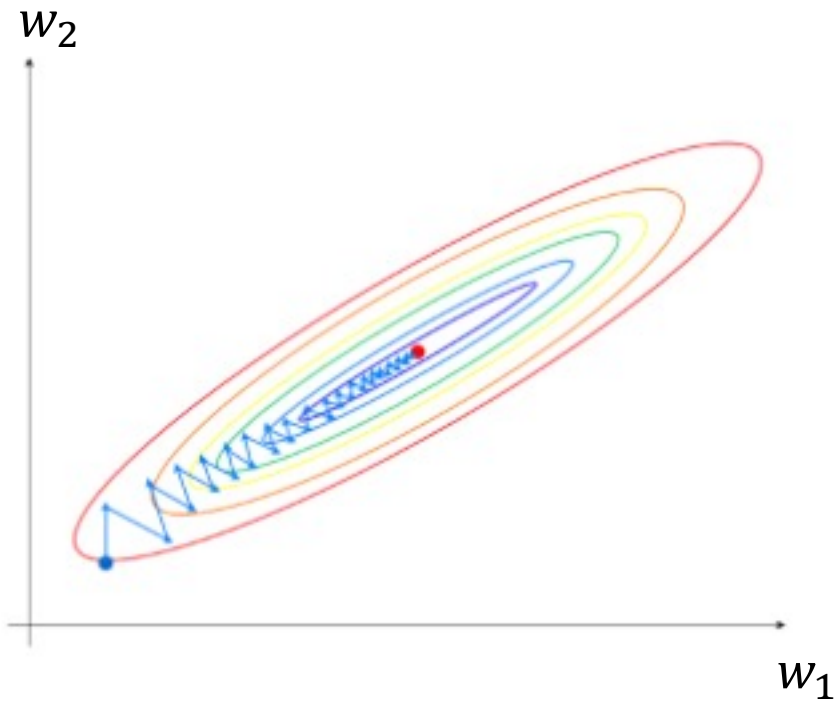
Finally: normalizing the inputs

E.g., $x_1 \in (0,100)$
$x_2 \in (0,1)$



Source: Erdem

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E.g., $x_1 \in (0,100)$
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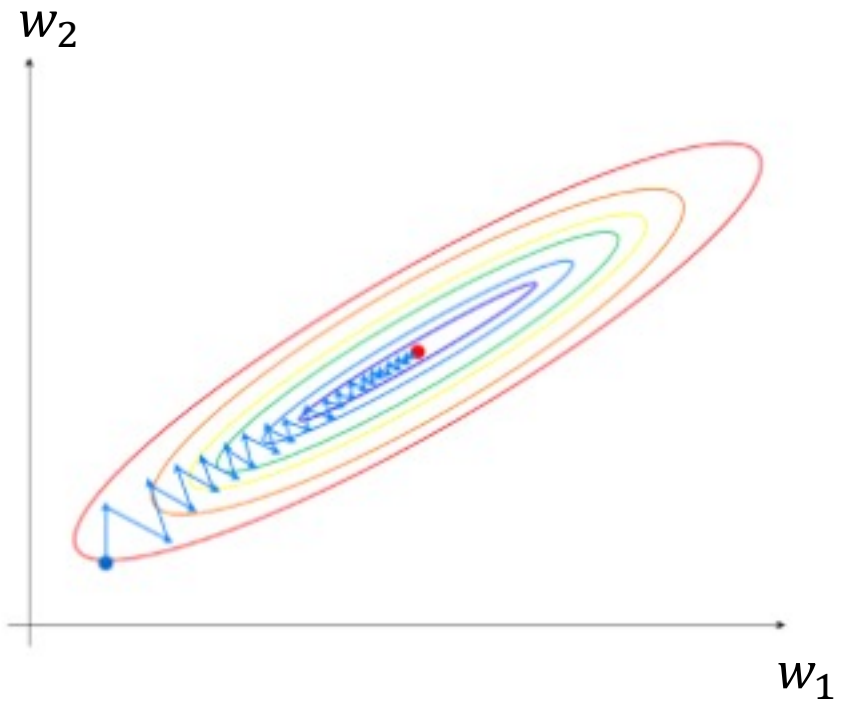
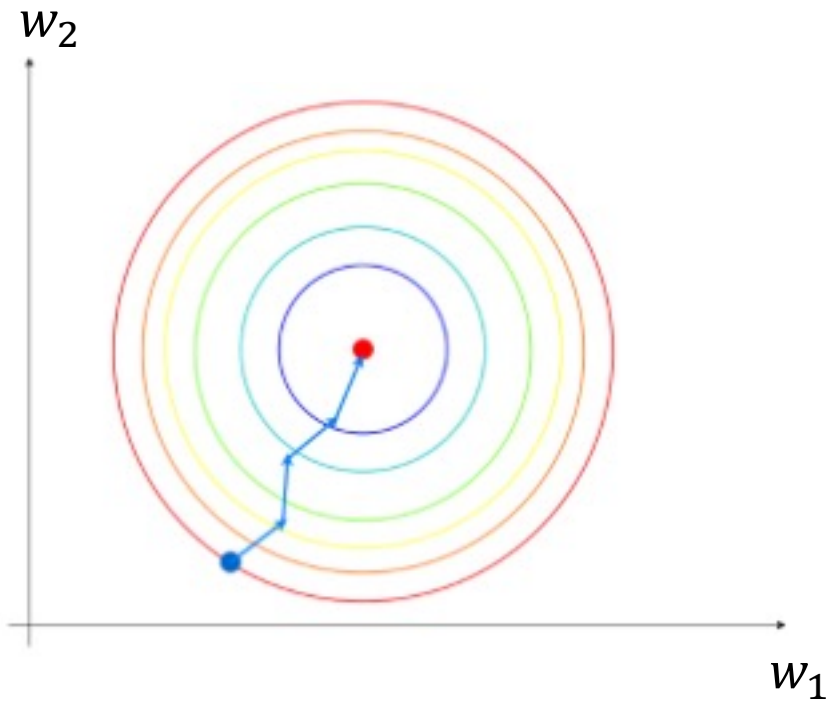


E.g., $x_1 \in (0,1)$
$x_2 \in (0,1)$



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Normalizing the inputs also for deeper layers: batch normalization

- Add an operation before/after activation function. For each input:
  - Standardize it (zero-centering, and division by standard deviation)
  - Then, scale it by a parameter γ and add a shift β (we **learn** these parameters)

- When we use the neural network to compute predictions, we don't necessarily have means and standard deviations, however (or the new observations might not be independent, …)
  → also keep track of a running mean μ and variance σ (we keep track of a moving average, but we are not learning, so these are **non-trainable** parameters)

- Overall, for each layer that is batch-normalized, we have $4 \times neurons$ additional parameters

- Batch normalization tends to make the network less sensitive to the initialization, and also helps to regularize it, but adds to the runtime

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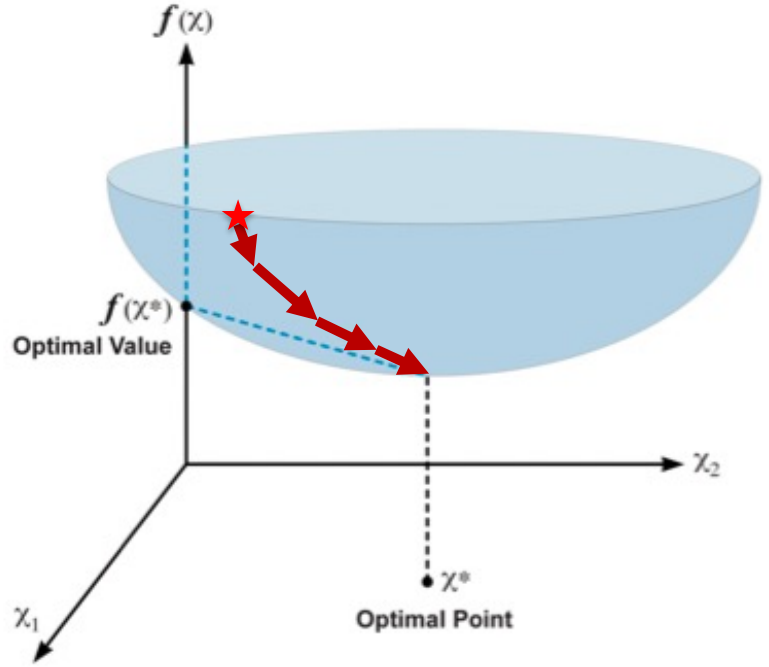
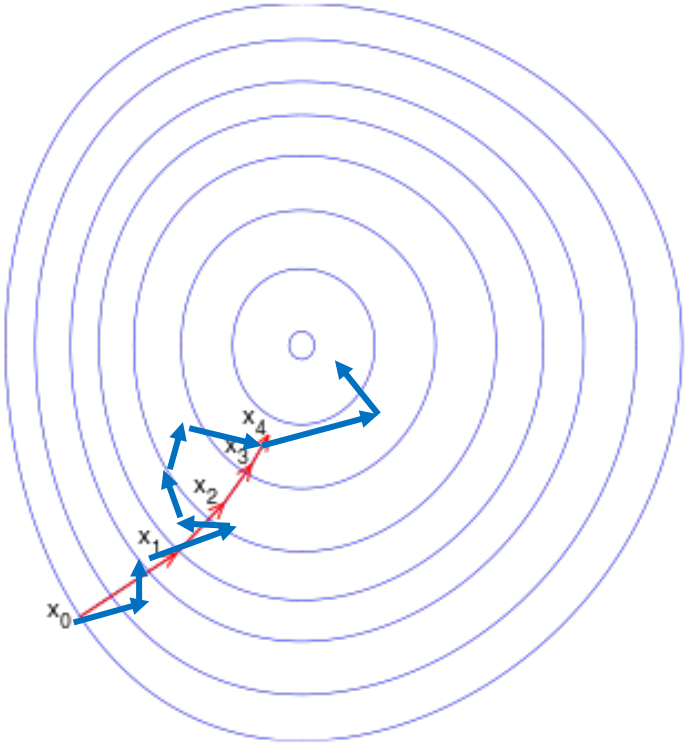
Improving learning – slow training

Gradient descent versus stochastic gradient descent





1. Decide a "learning rate" α
2. Start with some parameters $\boldsymbol{\theta}$
3. For a certain number of iterations
   - Compute $J(\boldsymbol{\theta})$
   - Compute $\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \nabla_{\boldsymbol{\theta}} \left(\frac{1}{n} \sum_{i=1}^{n} L^{(i)} \right)$
   - Let $\boldsymbol{\theta} := \boldsymbol{\theta} - \alpha \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

1. Decide a "learning rate" α
2. Start with some parameters $\boldsymbol{\theta}$
3. For a certain number of iterations
   - Compute $J(\boldsymbol{\theta})$
   - Compute $\nabla_{\boldsymbol{\theta}} L^{(i)}$ for a random (i)
   - Let $\boldsymbol{\theta} := \boldsymbol{\theta} - \alpha \nabla_{\boldsymbol{\theta}} L^{(i)}$

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Mini-batch gradient descent

- Core idea: don’t take the derivative over all observations, but over a bit more than just one

- Trading off between normal gradient descent (“batch gradient descent”) and stochastic gradient descent
  - Batch gradient descent: too slow per iteration
  - Stochastic gradient descent: loses benefits of vectorization

- For small training sets: batch gradient descent
  - Otherwise, use typical batch sizes such as 64, 128, 256, 512, 1024 …

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Gradient descent with momentum

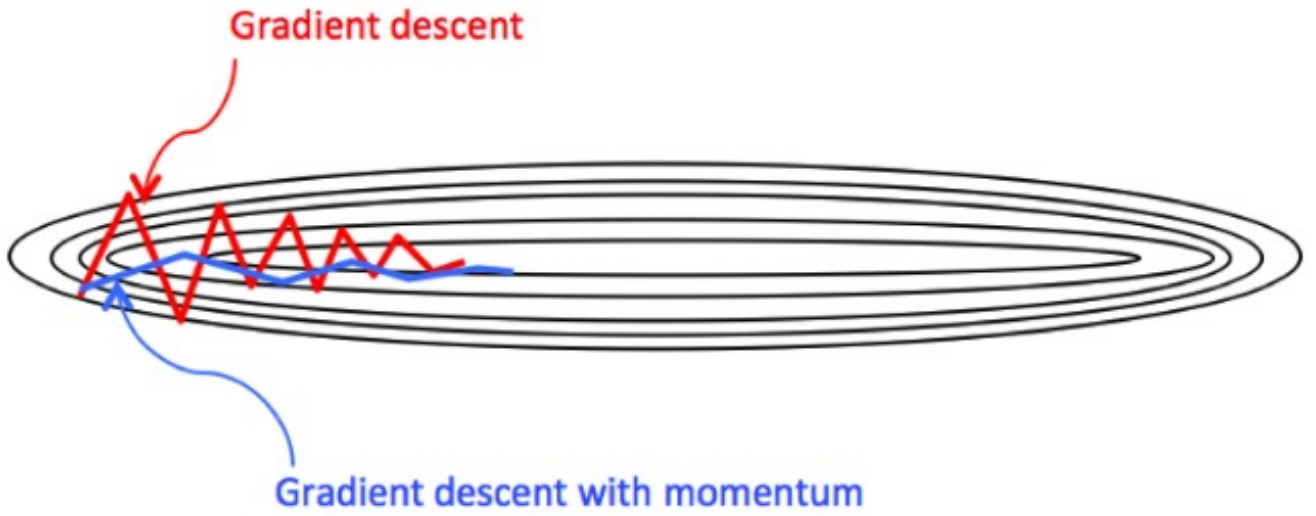
- In gradient descent, we take small, regular steps down a slope
- But if you think of a ball rolling down a slope, it will start slowly, but build up speed (and, thus, momentum) → the "steps" depend not just on the current slope, but on the slope so far!

Gradient descent:

$$\boldsymbol{\theta} \coloneqq \boldsymbol{\theta} - \alpha \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$$

Momentum optimization:

$$\boldsymbol{m} \coloneqq \beta \boldsymbol{m} - \alpha \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$$
$$\boldsymbol{\theta} \coloneqq \boldsymbol{\theta} + \boldsymbol{m}$$



- We can also escape faster from plateaus

Source: Trehan

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RMSprop (“Root mean square prop”)

- We normalize the gradient (using the moving average of the square of the gradients)
  - If there is a direction with a lot of oscillation, we penalize the update in this direction
  - If there is a direction with little oscillation, we help along the update in this direction

$$s := \beta s + (1 - \beta)\left(\frac{\partial J}{\partial \theta}\right)^2$$

$$\theta := \theta - \alpha \frac{\frac{\partial J}{\partial \theta}}{\sqrt{s + \varepsilon}}$$

- Used to be the standard algorithm to use until Adam

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Adam ("Adaptive moment estimation")

- Combining momentum and RMSprop

$$m \coloneqq \beta_1 m - (1 - \beta_1)\frac{\partial J}{\partial \theta}$$

$$s \coloneqq \beta_2 s + (1 - \beta_2)\left(\frac{\partial J}{\partial \theta}\right)^2$$

$$\hat{m} \coloneqq \frac{m}{1 - \beta_1^t}$$

$$\hat{s} \coloneqq \frac{s}{1 - \beta_2^t}$$

$$\theta \coloneqq \theta + \alpha \frac{\hat{m}}{\sqrt{\hat{s} + \varepsilon}}$$

- Like RMSprop, the algorithm is adaptive → less tuning of the learning rate α is required

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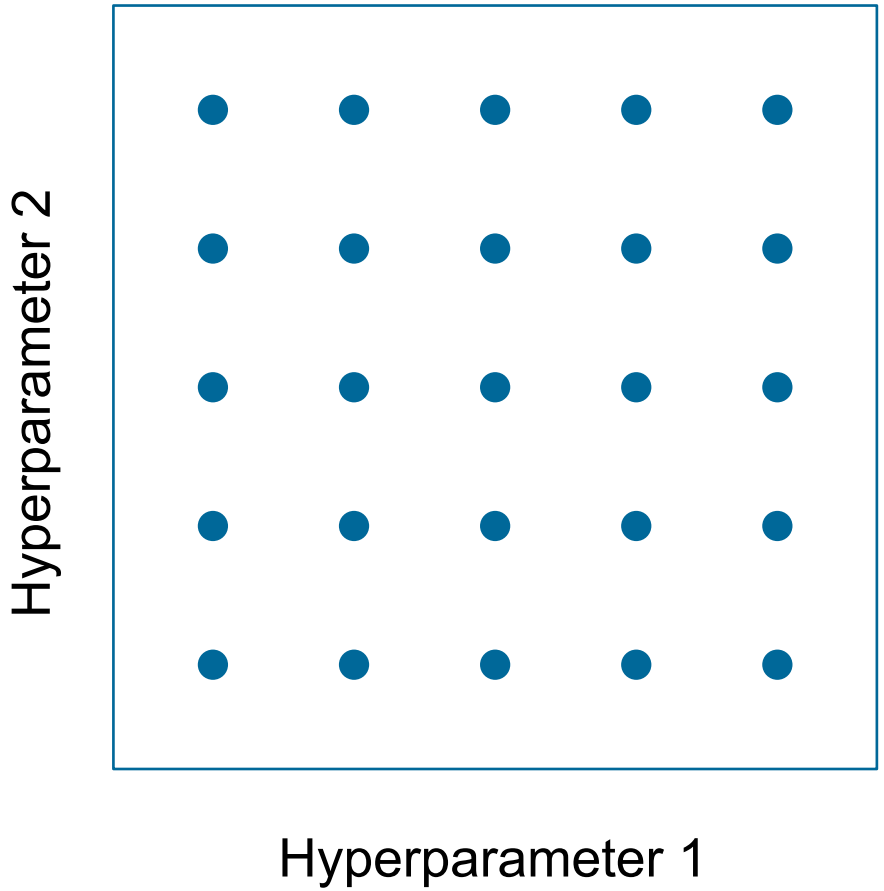
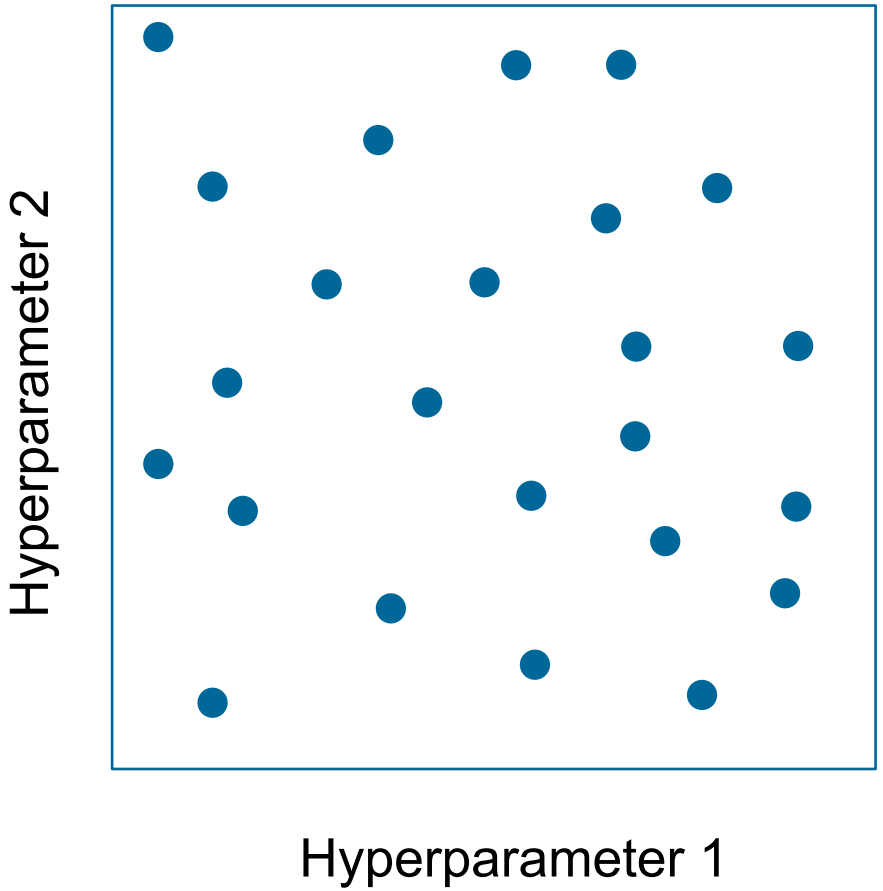
Hyperparameter tuning

Hyperparameter tuning process rule 1: Choose random combinations





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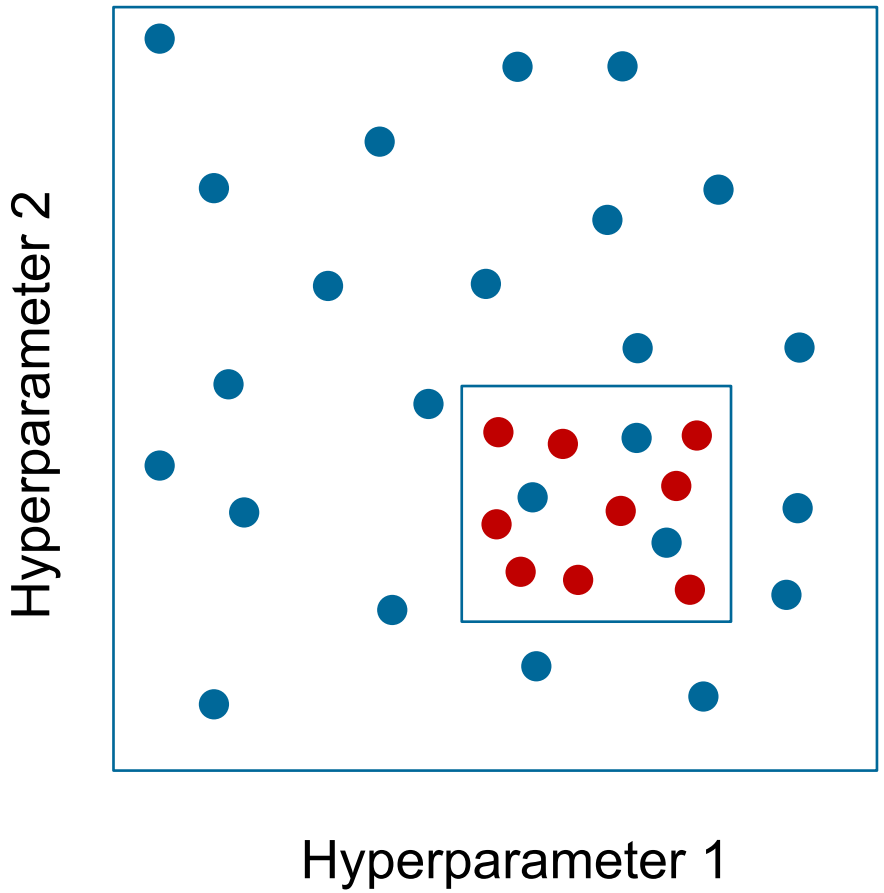
Hyperparameter tuning process rule 2: Go from coarse to fine



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Hyperparameter tuning process rule 3: Pick the right scale

- Say you want to set hyperparameter α in the range $0.001, \ldots, 1$
- You can try out your model 5 times

- The naïve option: uniform distribution between 0.001 and 1
  → $\alpha = np.random.rand(0.001,1)$

- The smarter option: logarithmic spacing
  → $r = -3 \times np.random.rand(0,1)$
  → $\alpha = 10^r$

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Hyperparameter tuning process rule 4: Use purpose-built libraries

- Hyperopt
- Keras Tuner
- Scikit-Optimize
- …

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Hyperparameter tuning process rule 5: Prioritize

A typical (but no way always optimal) prioritization:

1. Learning rate
2. Mini-batch size
3. Number of hidden units (mostly, the same number per layer works just fine – with some exceptions, such as a larger first hidden layer)
4. Number of hidden layers (usually, start with just a few hidden layers, unless you are dealing with complex tasks such as image classification. But then, you usually don't train your own model)
5. Learning rate decay
6. Other algorithm parameters (but the defaults often work fine)

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Learning rate scheduling and decay

- Generally, can find a good learning rate by training a bit, then increasing the rate (on a log-scale), then training a bit, …, until the loss goes up again.
  - A decent learning rate is slightly less than that

- Better: adjusting the learning rate during training (with a “learning schedule”)

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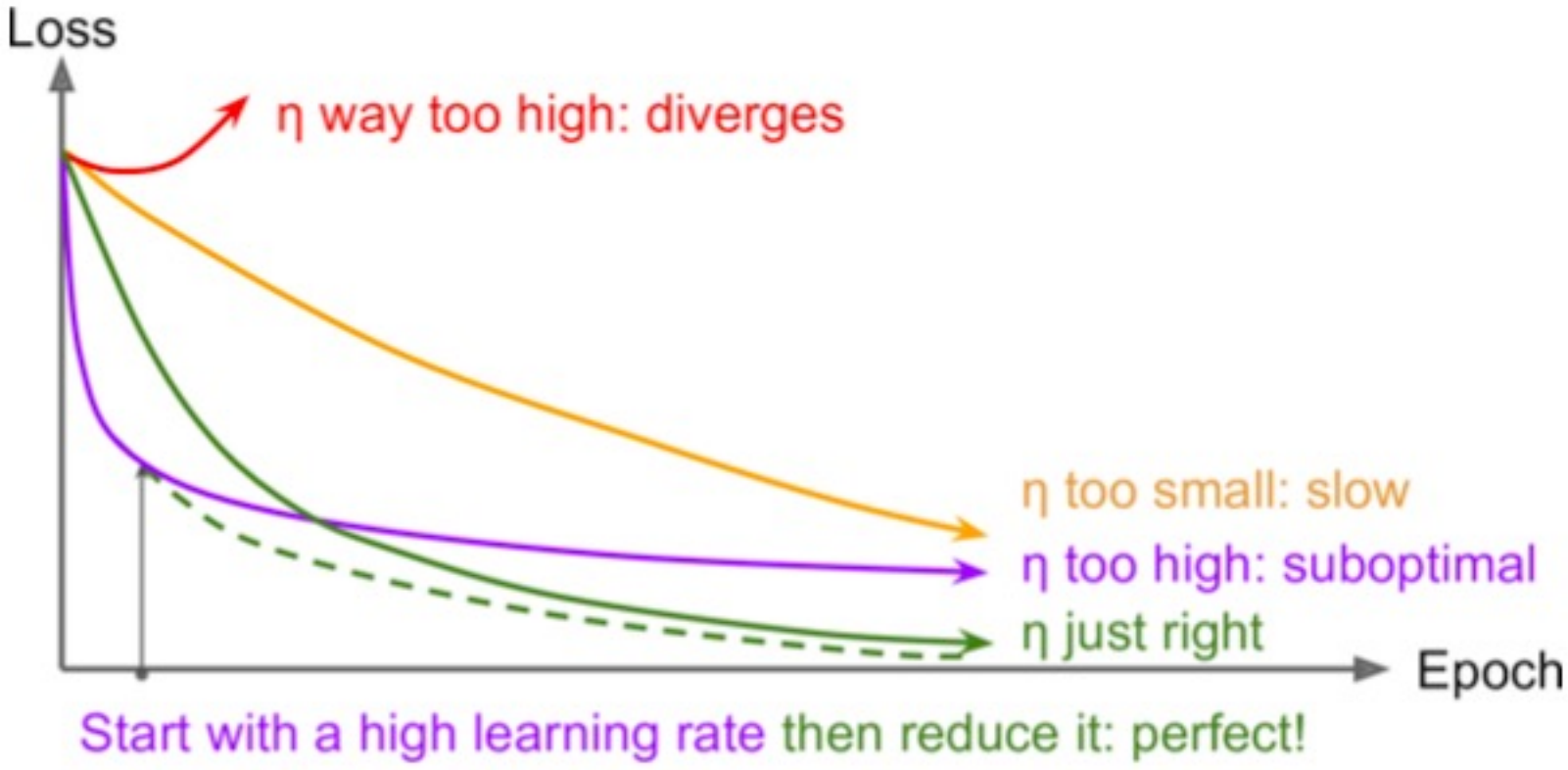
Learning rate scheduling and decay



Source: Géron

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Typical learning rate schedules

Power scheduling

- $\alpha_t = \frac{\alpha_0}{1+\frac{t}{s}}$, where t is the epoch and s is the number of epochs until we reach $\frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \frac{1}{5}, \ldots$
- Can also take a power of the denominator
- Very easy to implement directly within the tf.keras optimization routine

Exponential scheduling

- $\alpha_t = \alpha_0 0.1^{t/s}$, so now we indicate with s the number of epochs until we reach $0.1, 0.01, 0.001, \ldots$
- To use in TensorFlow, need to implement a callback

1cycle scheduling

- Start to increase from α_0 to α_1 (linearly for the first half), then decrease it (again, linearly)

…

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See you in class!

Sources

- Bhaskhar, 2021, Introduction to Deep Learning: https://cs229.stanford.edu/syllabus.html
- DeepLearning.AI, n.d.: deeplearning.ai
- Erdem, 2020, DengAI — Data preprocessing: https://towardsdatascience.com/dengai-data-preprocessing-28fc541c9470
- Géron, 2019, Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow
- Goodfellow, Bengio, Courville, 2016, The Deep Learning Book: http://www.deeplearningbook.org
- Liang, 2016, Introduction to Deep Learning: https://www.cs.princeton.edu/courses/archive/spring16/cos495/
- Trehan, 2020, Gradient Descent Explained: https://towardsdatascience.com/gradient-descent-explained-9b953fc0d2c