Deep Learning:

Regularization & Generalization

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Deep Learning VO - WS 23/24

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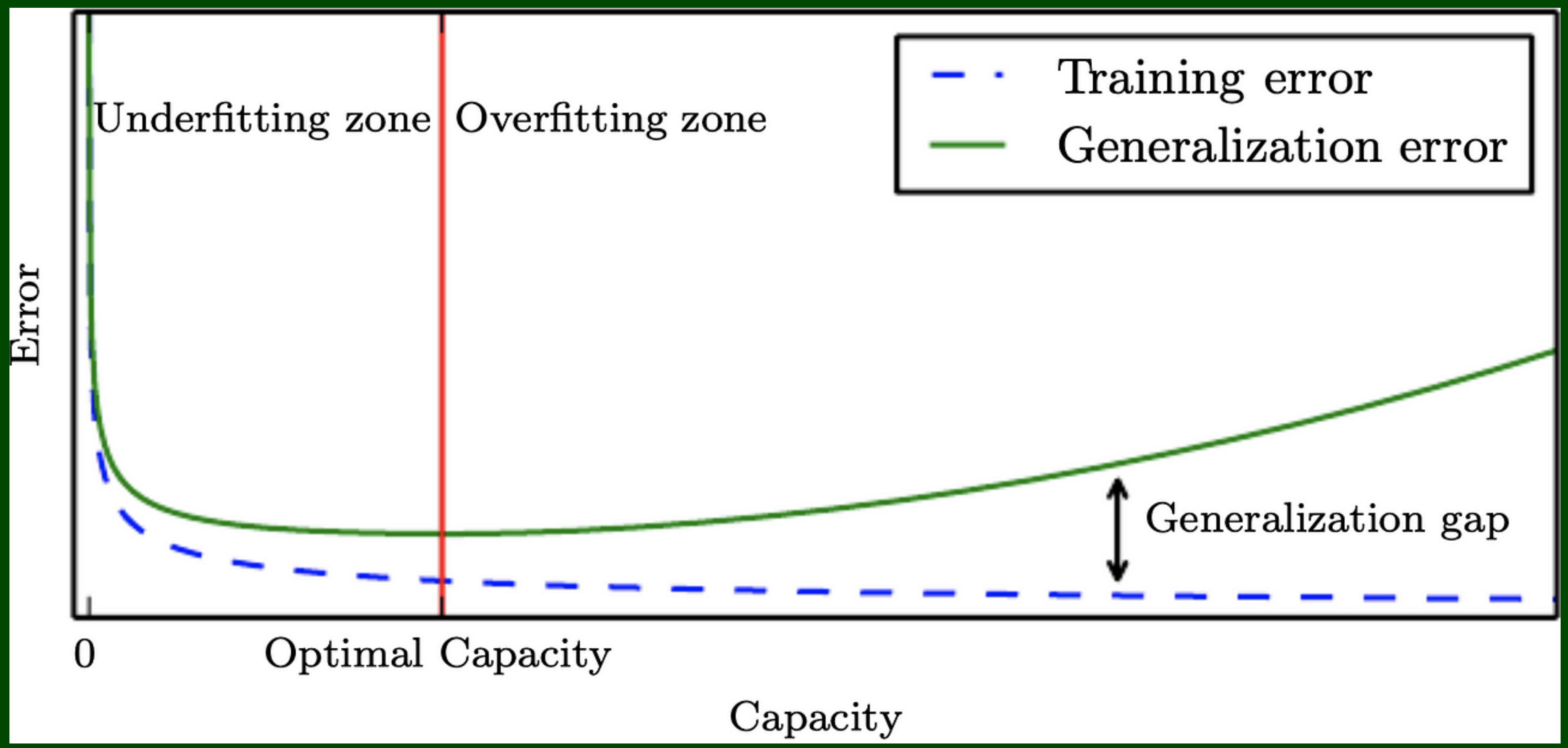
Today

- ☐ Regularization
  - ☐ Parameter Norm Penalties
  - ☐ Early Stopping
  - ☐ Dropout
  - ☐ Dataset Augmentation
  - ☐ Further Techniques

Recap

***Regularization** is any modification we make to a learning algorithm that is intended to reduce its **generalization** error but not its training error.*



(1) Parameter Norm Penalties

Adding a parameter norm penalty $\Omega(\mathbf{w})$ to the error E.

$$\tilde{E}(\mathbf{w}; \mathscr{D}) = E(\mathbf{w}; \mathscr{D}) + \lambda\, \Omega(\mathbf{w})$$

- Typically only regularize weights, leave biases unregularized.
- Sometimes it is desirable to use different λ for different layers.

$\mathbf{w}$: network parameters

$\mathscr{D}$: data

$\lambda \in [0,\infty)$: relative contribution of the regularizer

L_2 regularization (weight decay)

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L_2 regularization:

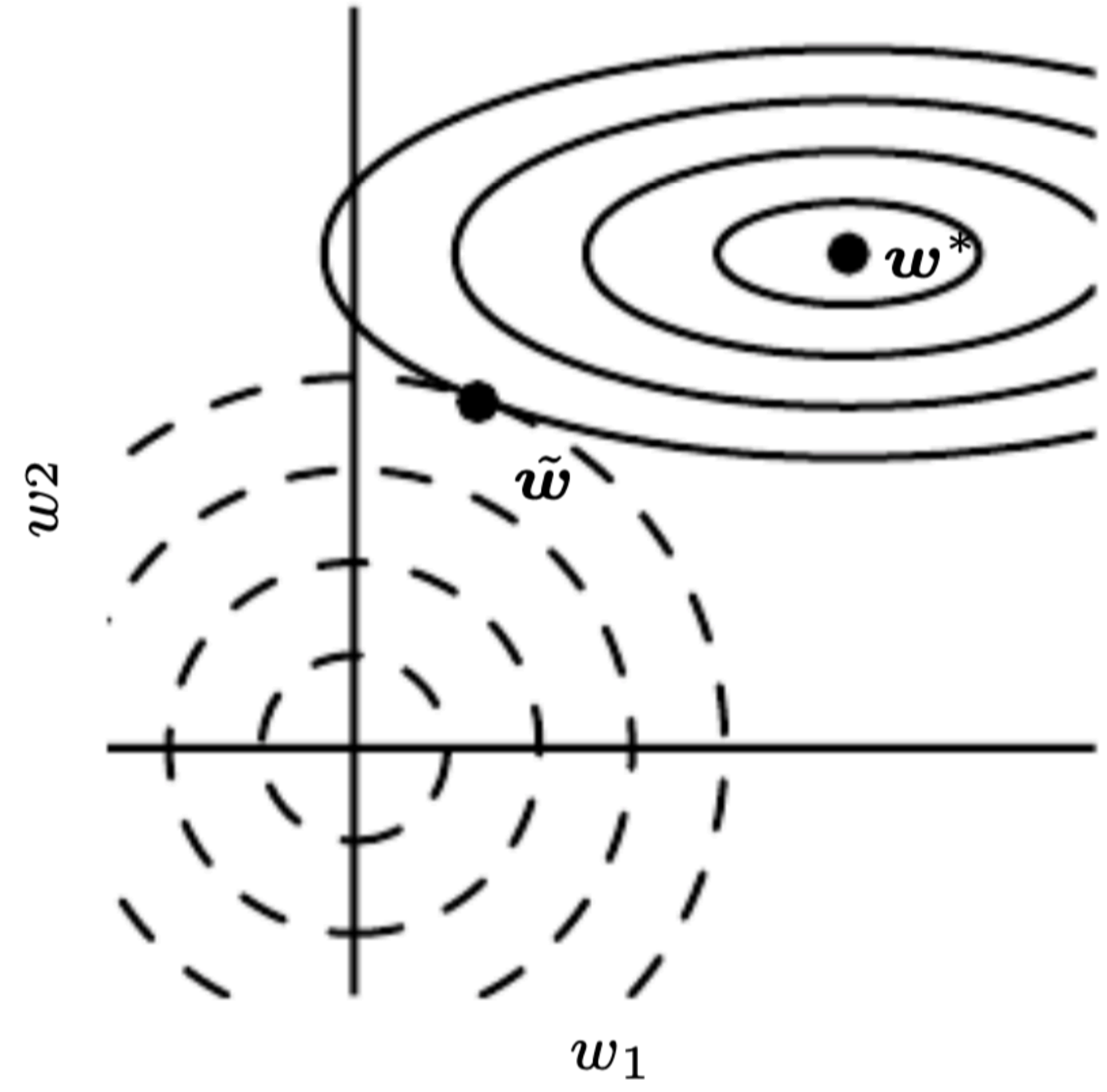
$$\Omega(\mathbf{w}) = \frac{1}{2}||\mathbf{w}||_2^2 = \frac{1}{2}\mathbf{w}^T\mathbf{w}$$

$$\nabla_{\mathbf{w}}\tilde{E}(\mathbf{w};\mathscr{D}) = \nabla_{\mathbf{w}}E(\mathbf{w};\mathscr{D}) + \lambda\,\nabla_{\mathbf{w}}\Omega(\mathbf{w})$$

$$= \nabla_{\mathbf{w}}E(\mathbf{w};\mathscr{D}) + \lambda\,\mathbf{w}$$

$$\mathbf{w} \leftarrow \mathbf{w} - \epsilon\left(\lambda\mathbf{w} + \nabla_{\mathbf{w}}E(\mathbf{w};\mathscr{D})\right)$$

leads to **weight decay**



- Can be interpreted as MAP inference: it would correspond to a zero-mean Gaussian prior over weights.

L_1 regularization

Adding a parameter norm penalty $\Omega(\mathbf{w})$ to the error E.

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$\mathbf{w}$: network parameters

$\mathcal{D}$: data

$\lambda \in [0, \infty)$: relative contribution of the regularizer

$\boxed{\textbf{L}_1\textbf{ regularization:}}$ $\quad \Omega(\mathbf{w}) = ||\mathbf{w}||_1 = \sum_i |w_i|$

Weight updates using the sub-gradient: $\nabla_{\mathbf{w}} ||\mathbf{w}||_1 = \mathrm{sign}(\mathbf{w})$

$$\mathbf{w} \leftarrow \mathbf{w} - \epsilon \left(\lambda\, \mathrm{sign}(\mathbf{w}) + \nabla_{\mathbf{w}} E(\mathbf{w}; \mathcal{D})\right) \longrightarrow$$

leads to **sparse** parameter vectors (many entries are 0).

- As MAP inference: corresponds to a Laplacian prior over weights.

$$p(w_i) = \frac{1}{2\sigma} e^{-\frac{|w_i|}{\sigma}}$$

- A linear model with least squares error and L_1 norm regularization is known as LASSO (least absolute shrinkage and selection operator).

L_1 regularization

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$$p(w_i) = \frac{1}{2\sigma} e^{-\frac{|w_i|}{\sigma}}$$

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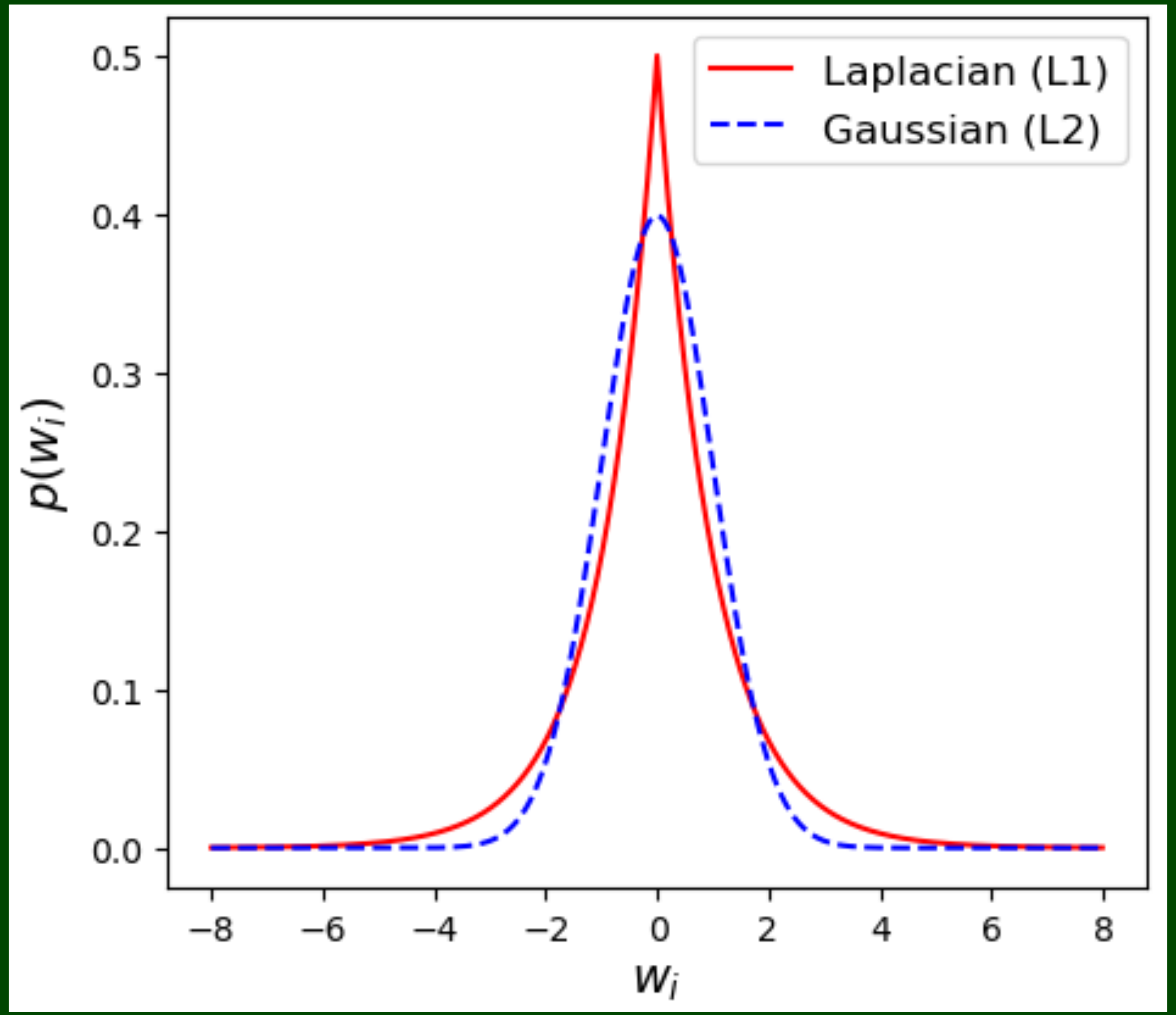
Impact of L_1 vs L_2 regularization on weights:



With L_1 regularization:

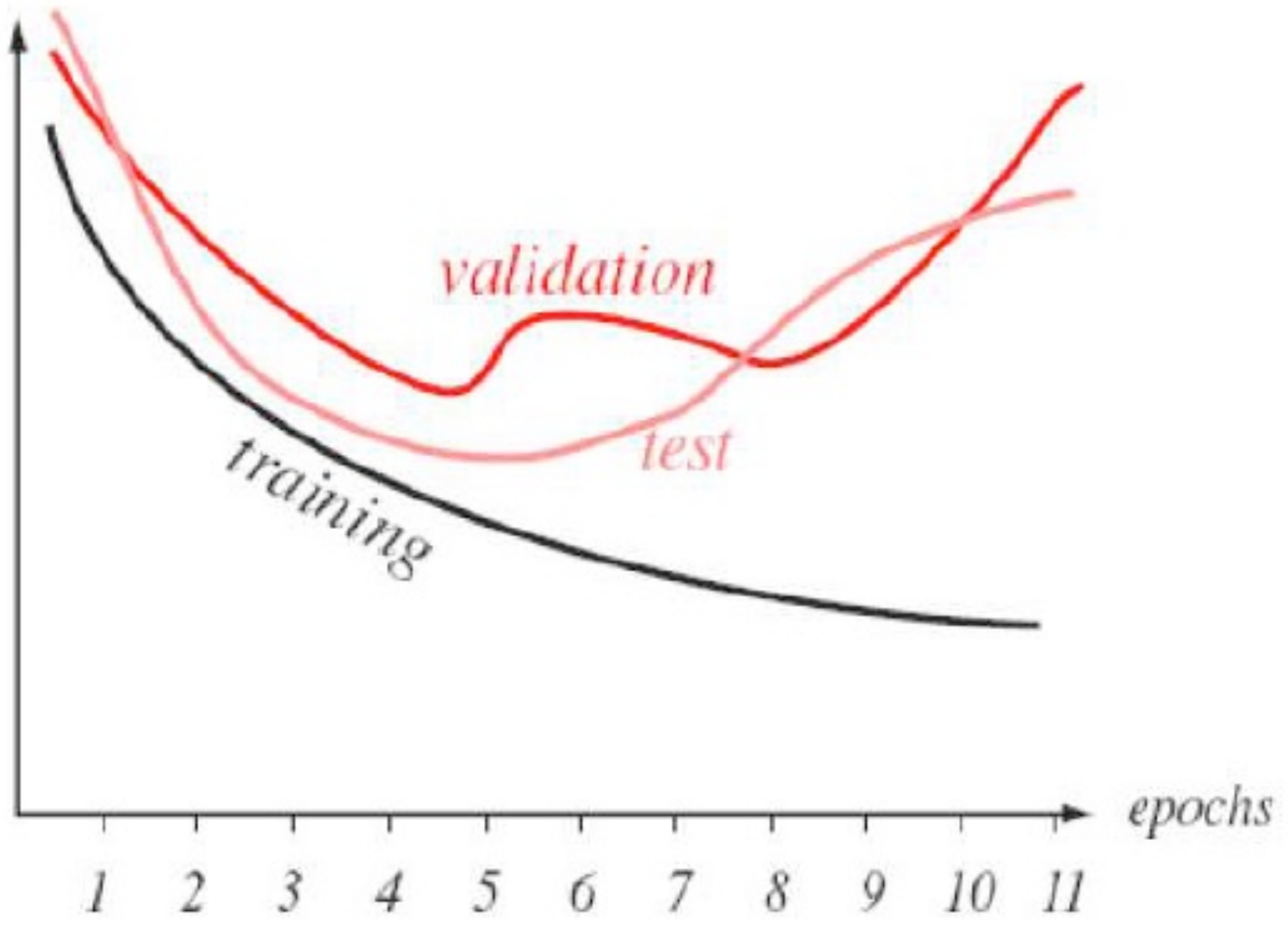
- zero weights are more probable (sparse)
- remaining weights get higher values (w.r.t. L_2)
  - > since Laplacian dist. is heavier tailed

(2) Early Stopping

- Training error decreases over training. However, test error first decreases, then increases.

Early stopping:

- Monitor error on a validation set.
- Store parameters whenever validation error decreases.
- Use parameters of best validation error as final setting.



Alternative (to make better use of data):

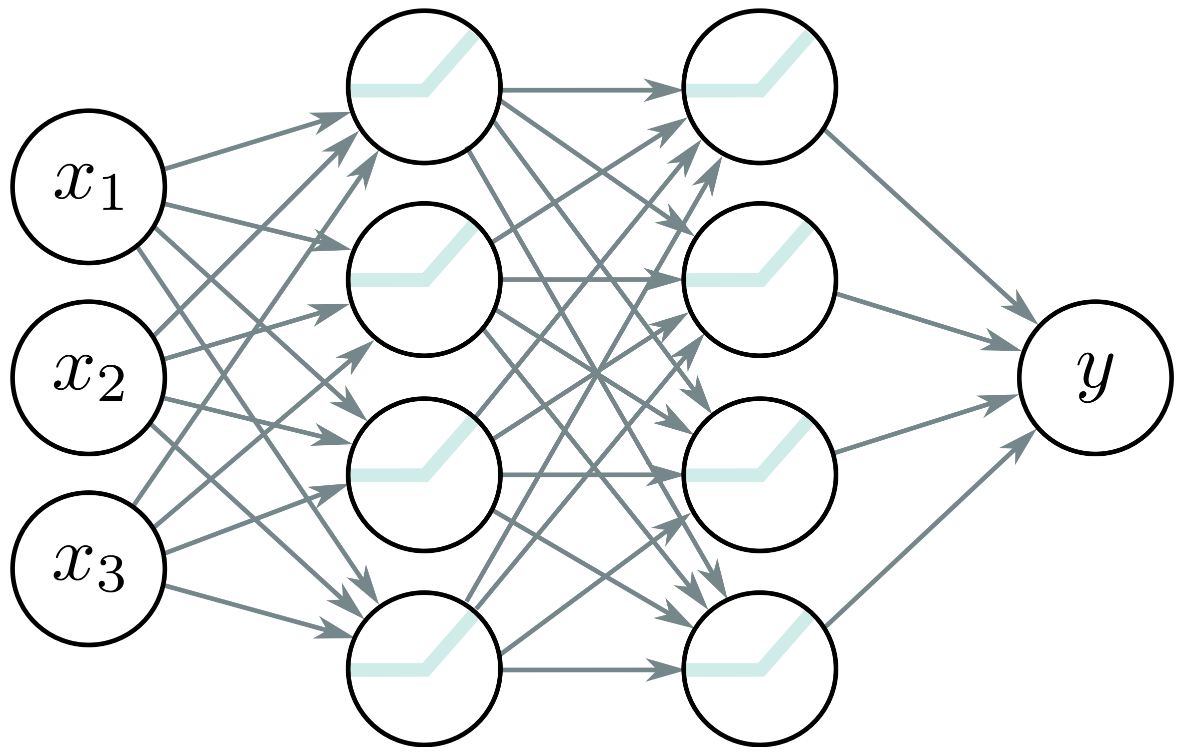
- Use early stopping to determine number of epochs.
- Then retrain with validation set included with the determined number of epochs.

How early stopping acts as a regularizer:

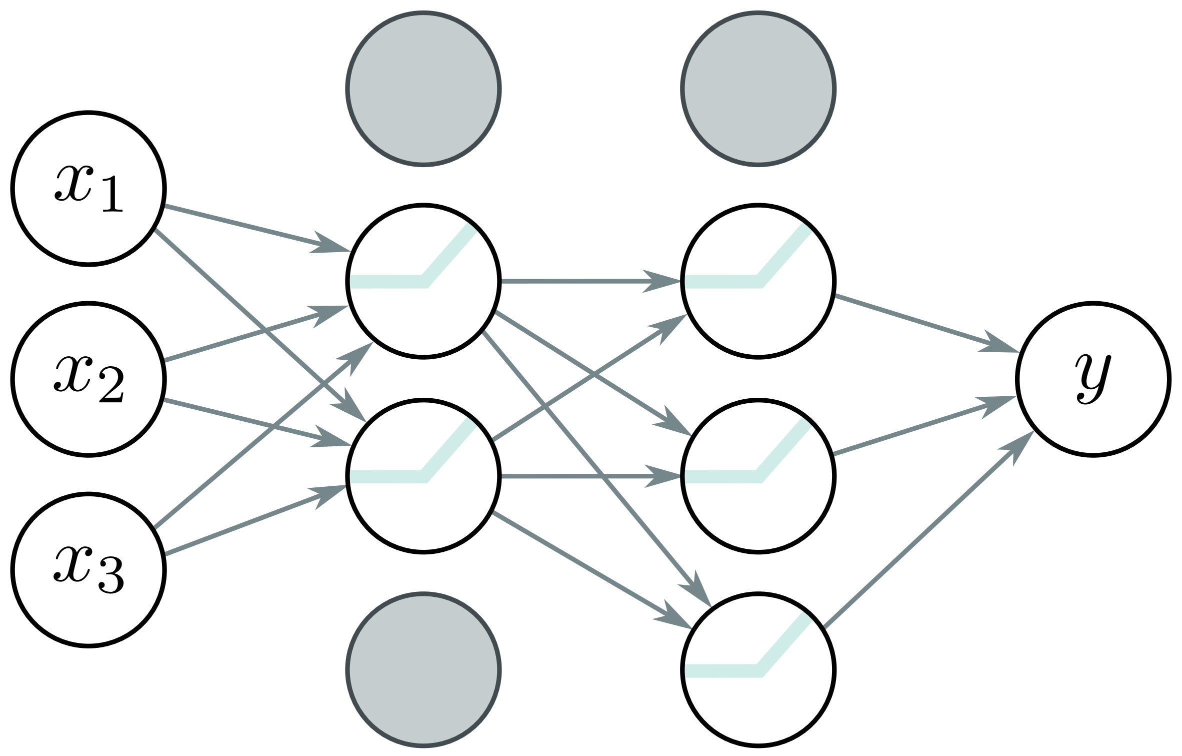
- We start training with small parameters.
- As training continues, parameters grow. Hence, the effective model capacity (complexity) grows.
- Since we monitor validation error, we can stop at a particularly good point.

(3) Dropout

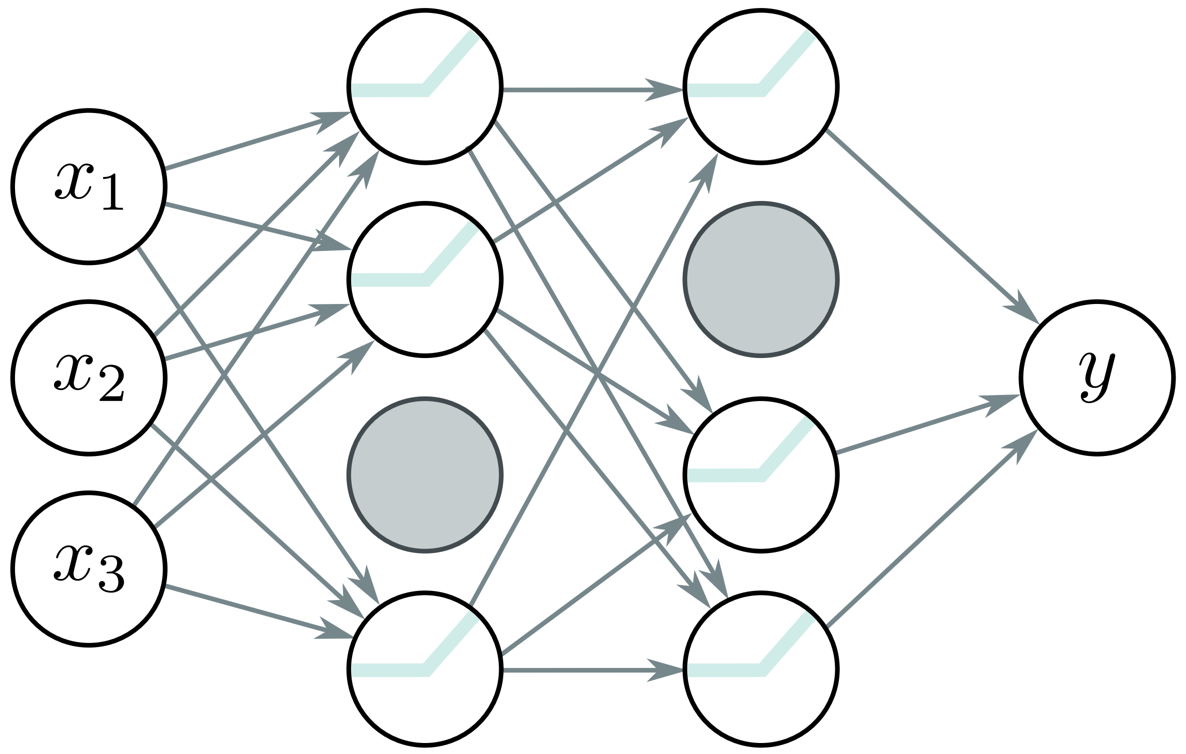
- During training with minibatches, in each minibatch, drop each neuron with probability $1 - p$ (e.g., $p = 0.5$).
  - "dropping" means: In both the forward and backward-pass, the neuron is ignored and its output is set to 0.



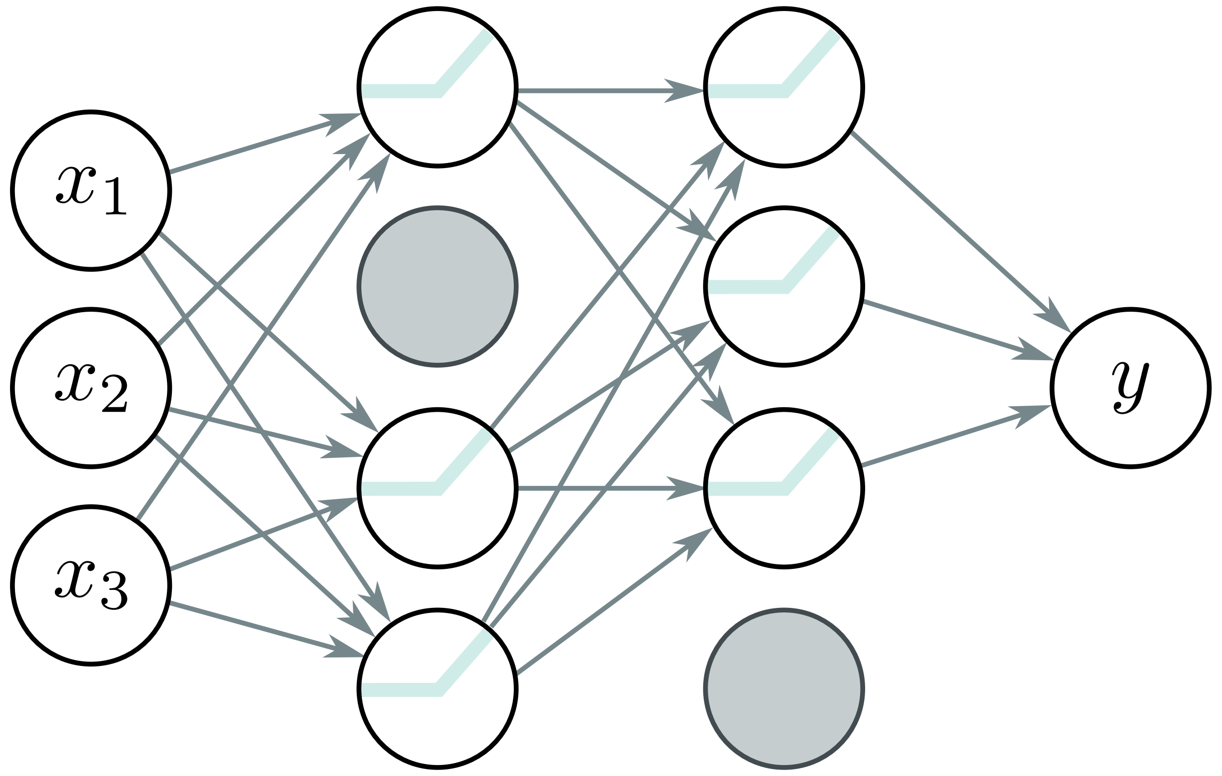
original network



iteration i



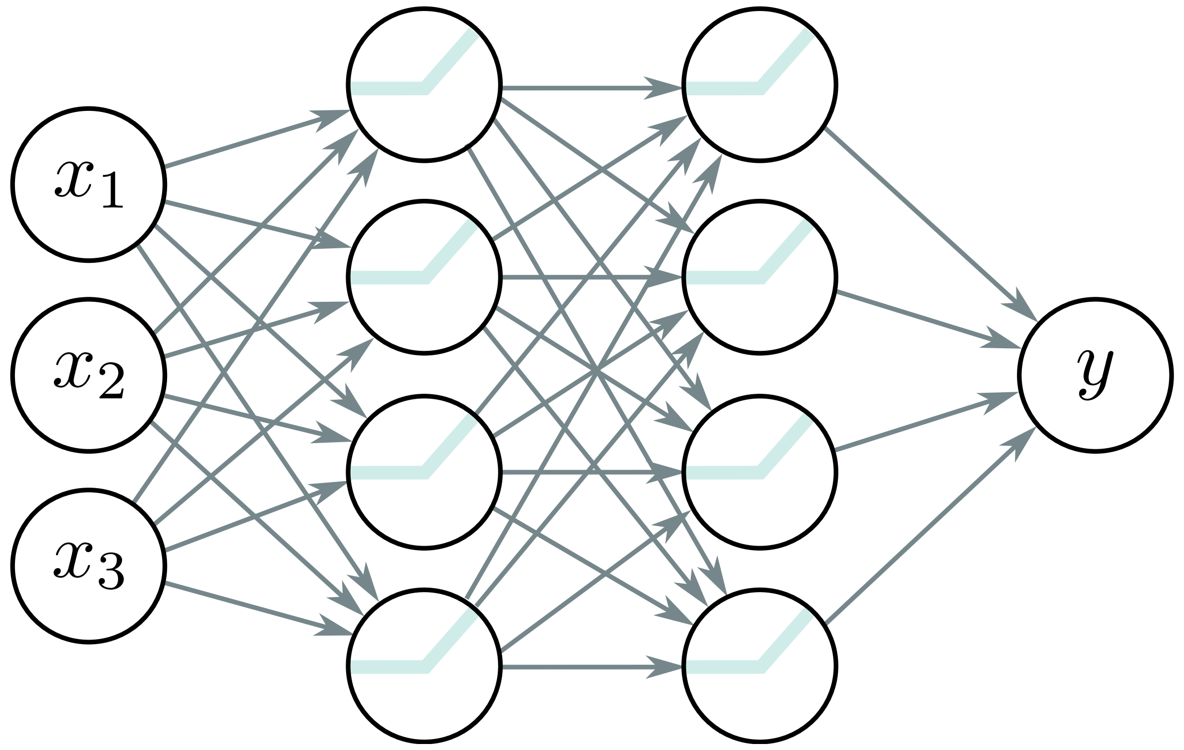
iteration $i + 1$



iteration $i + 2$

[Hinton et al., 2012]: "Improving neural networks by preventing co-adaptation of feature detectors"

(3) Dropout



- During training with minibatches, in each minibatch, drop each neuron with probability $1 - p$ (e.g., $p = 0.5$).
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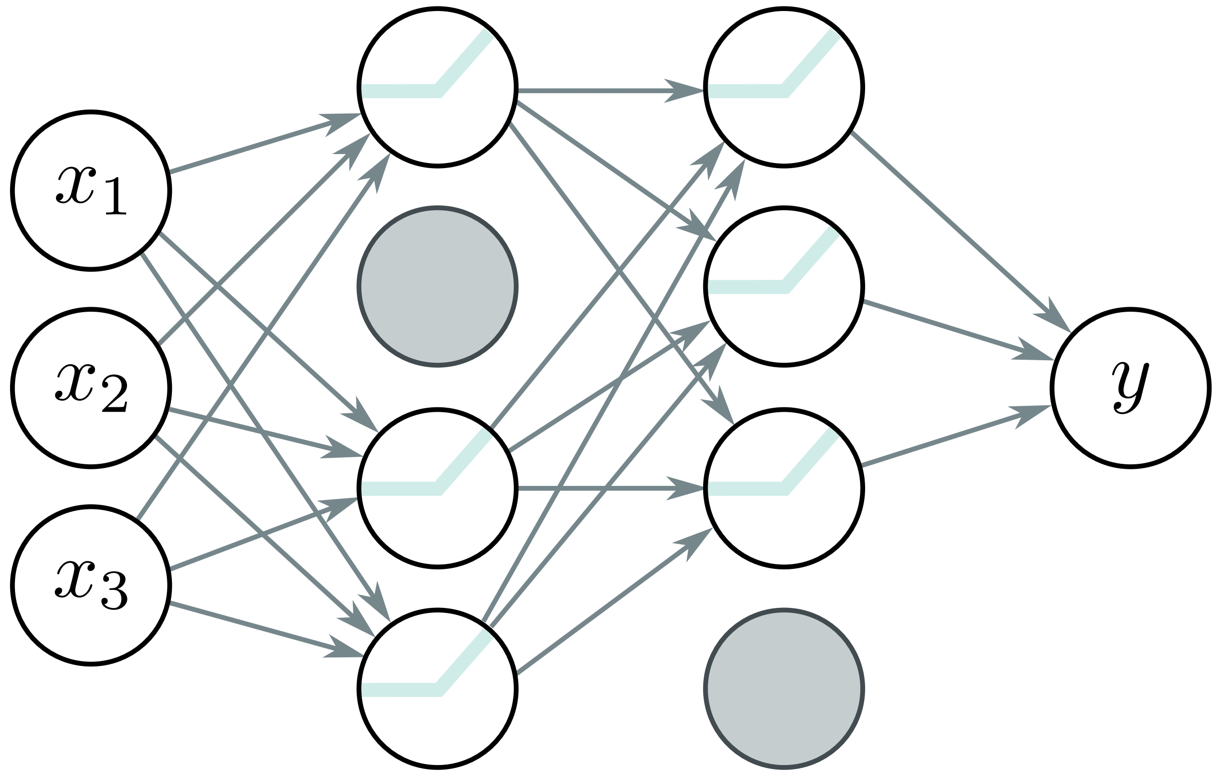
Idea:

- Neurons cannot fully rely on the output of other neurons.
- Co-specialization is not possible.



- Sometimes, also inputs are dropped out during training.

Final network (application after training):

- Use all weights (and neurons), but rescale: $w_{ij}^{final} = p\, w_{ij}$

[Hinton et al., 2012]: "Improving neural networks by preventing co-adaptation of feature detectors"

(3) Dropout - Why does it work well?

Model Averaging:

- Train several models separately on the data.
- All models vote for the output on test examples.

Dropout is an efficient way to implement model averaging:

- 2^N different thinned networks are possible (N : number of neurons).
- Many of them are trained, but with shared weights.

Final network (application after training):

- Rescaling of weights $w_{ij}^{final} = p\, w_{ij}$ approximates the geometric mean of the thinned models.

[Hinton et al., 2012]: "Improving neural networks by preventing co-adaptation of feature detectors"

(4) Dataset Augmentation

Augment training data with transformed instances of the original data.

Boost the size of training set by deformation of input samples.

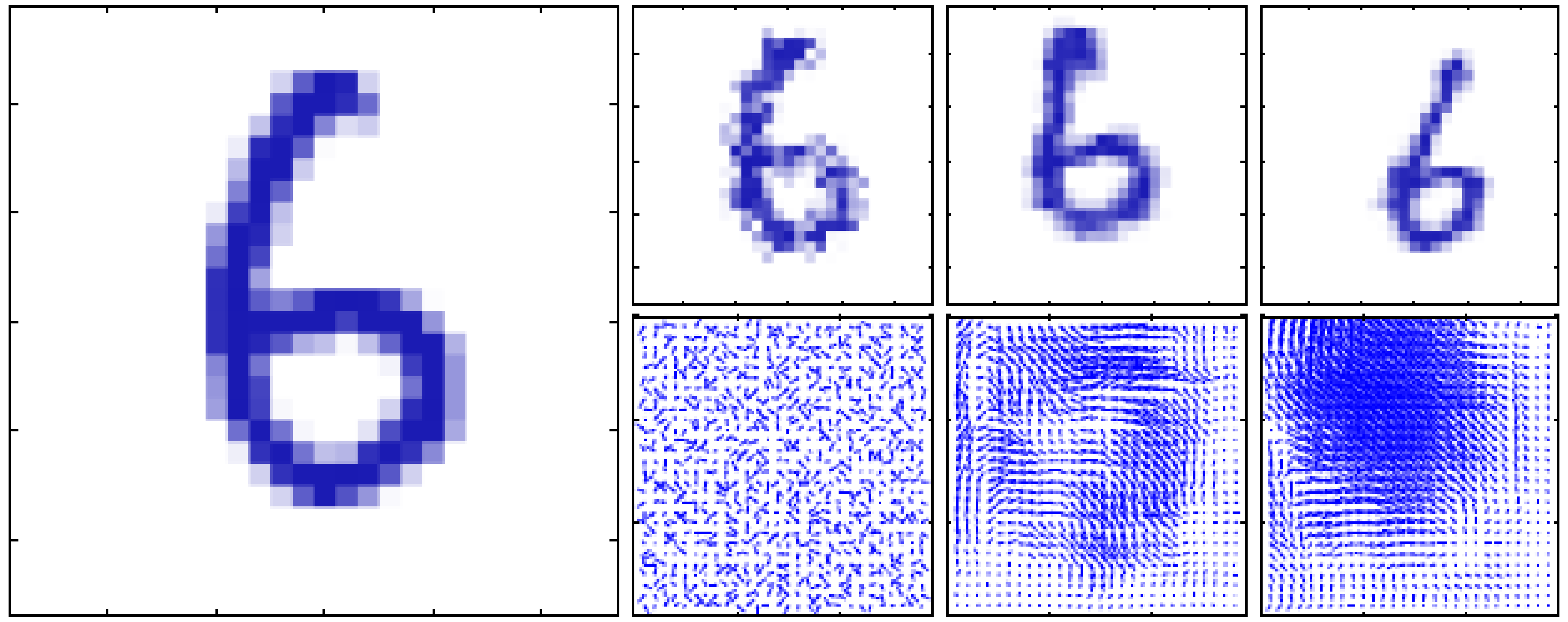


Table 1:

Error Rates on MNIST Test Set.

	Architecture				
	(Number of Neurons	Test Error for	Best Test	Simulation	Weights
ID	in Each Layer)	Best Validation (%)	Error (%)	Time (h)	(Millions)
1	1000, 500, 10	0.49	0.44	23.4	1.34
2	1500, 1000, 500, 10	0.46	0.40	44.2	3.26
3	2000, 1500, 1000, 500, 10	0.41	0.39	66.7	6.69
4	2500, 2000, 1500, 1000, 500, 10	0.35	0.32	114.5	12.11
5	9 × 1000, 10	0.44	0.43	107.7	8.86

[DC Ciresan, U Meier, LM Gamberdella, J Schmidhuber. “Deep Big Simple Neural Nets For Handwritten Digit Recognition”. Neural Computation, 2010]

(4) Dataset Augmentation

Augment training data with transformed instances of the original data.

e.g., image classification: boost the size of training set with common image transformations.

original input

horizontal flip

vertical stretch

rotate and crop

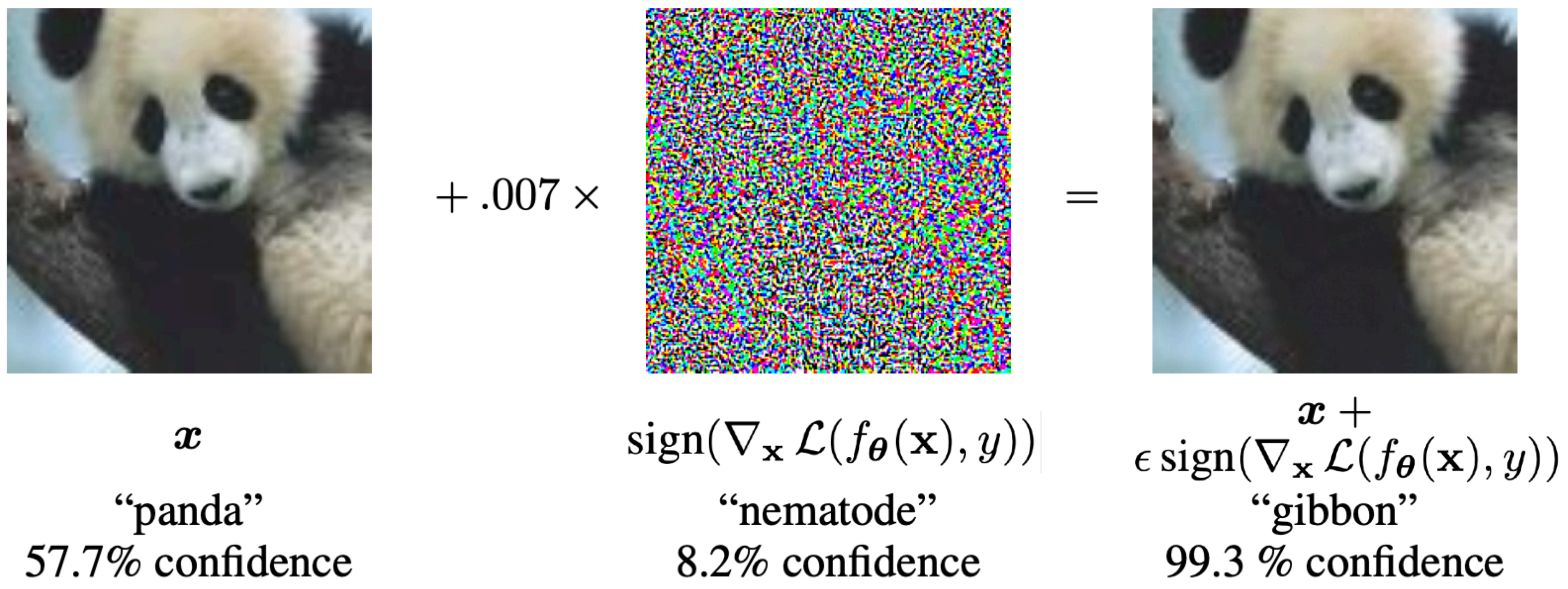
color balance

blur

Adversarial Training

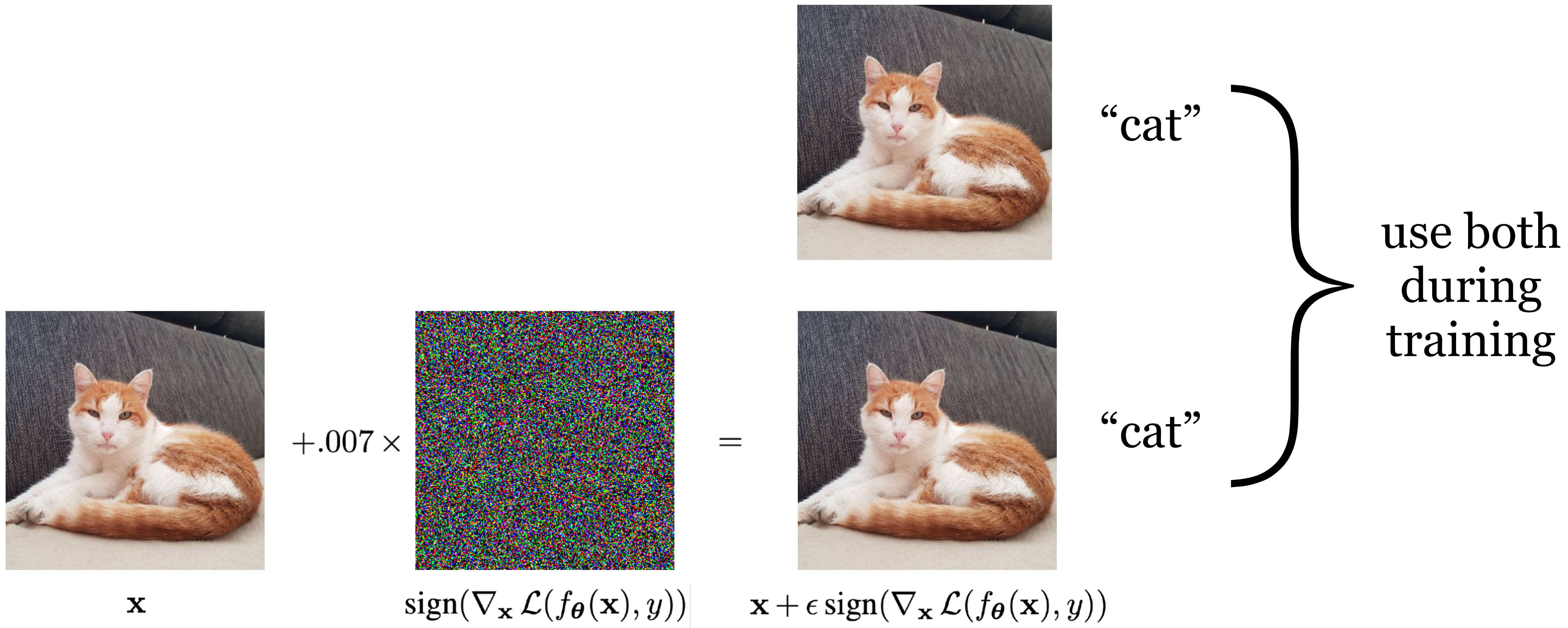
Adversarial example

- Small (and human-imperceptible) changes in inputs can produce different outputs.



Adversarial training

- During training, seek for adversarial examples (i.e., examples $\mathbf{x}'$ nearby a training example $\mathbf{x}$ where $y' \neq y$).
- Train with input $\mathbf{x}'$ and target y.



(5) Further Techniques

Label smoothing

- Training labels are also often noisy → We can assume that a training label is correct with probability $1 - \epsilon$
- Simple implementation: Replace $\{0,1\}$ targets for k-softmax output with $\left\{ \frac{\epsilon}{k-1}, 1 - \epsilon \right\}$ targets.

Semi-supervised learning

- Use unlabeled data to obtain good representation of examples.
- Use labeled examples for classification.

Multi-task learning (auxiliary training)

- Pooling examples out of several tasks (e.g., train lower layers on several tasks, upper layers are task-specific)

Parameter sharing

- Some parameters can be constrained to have the same value.
- *(more on Convolutional Neural Networks…)*

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Questions?