Mathematics of AI

Error sources, bias-variance, and regularisation for deep learning

Prince, *Understanding Deep Learning* & Bishop, *PRML* & Goodfellow *et al*, *Deep Learning*

Connections to previous weeks

Matt’s class last week

Beyond PCA

Underlying each of these is often an optimisation problem. There are two main parts that determine what you are doing:

1. The objective of the optimisation, which defines what the method is trying to achieve, and
2. Often there is an additional *regularisation* term that prevents overfitting (and has other positive affects like inducing a variance-bias tradeoff).

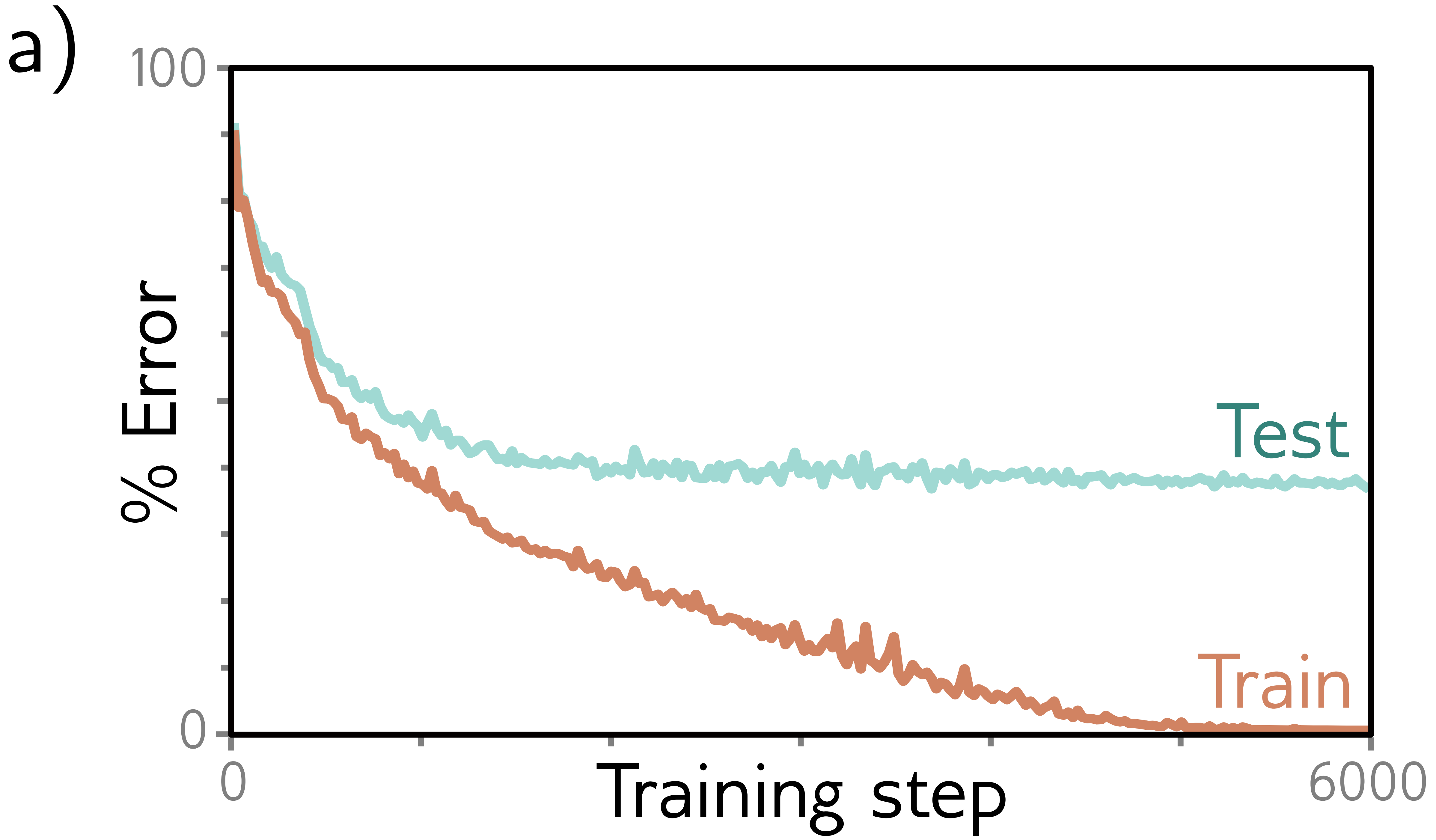
Lewis already talked about regularisation, but here we are often regularising towards a lower-dimensional space.

SIMON J. D. PRINCE

Understanding Deep Learning

There’s a bit of a problem with over-training

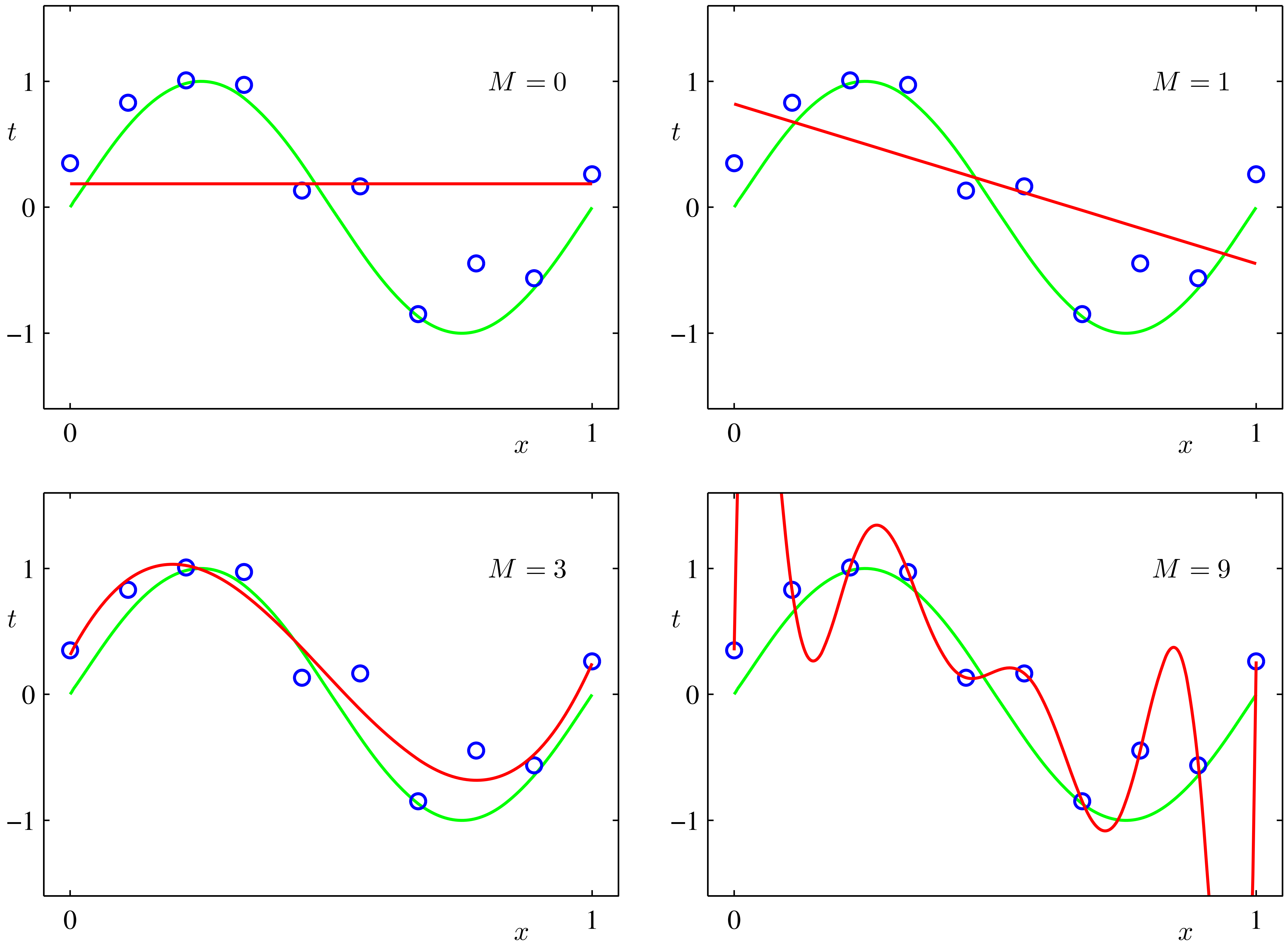
MNIST-1D

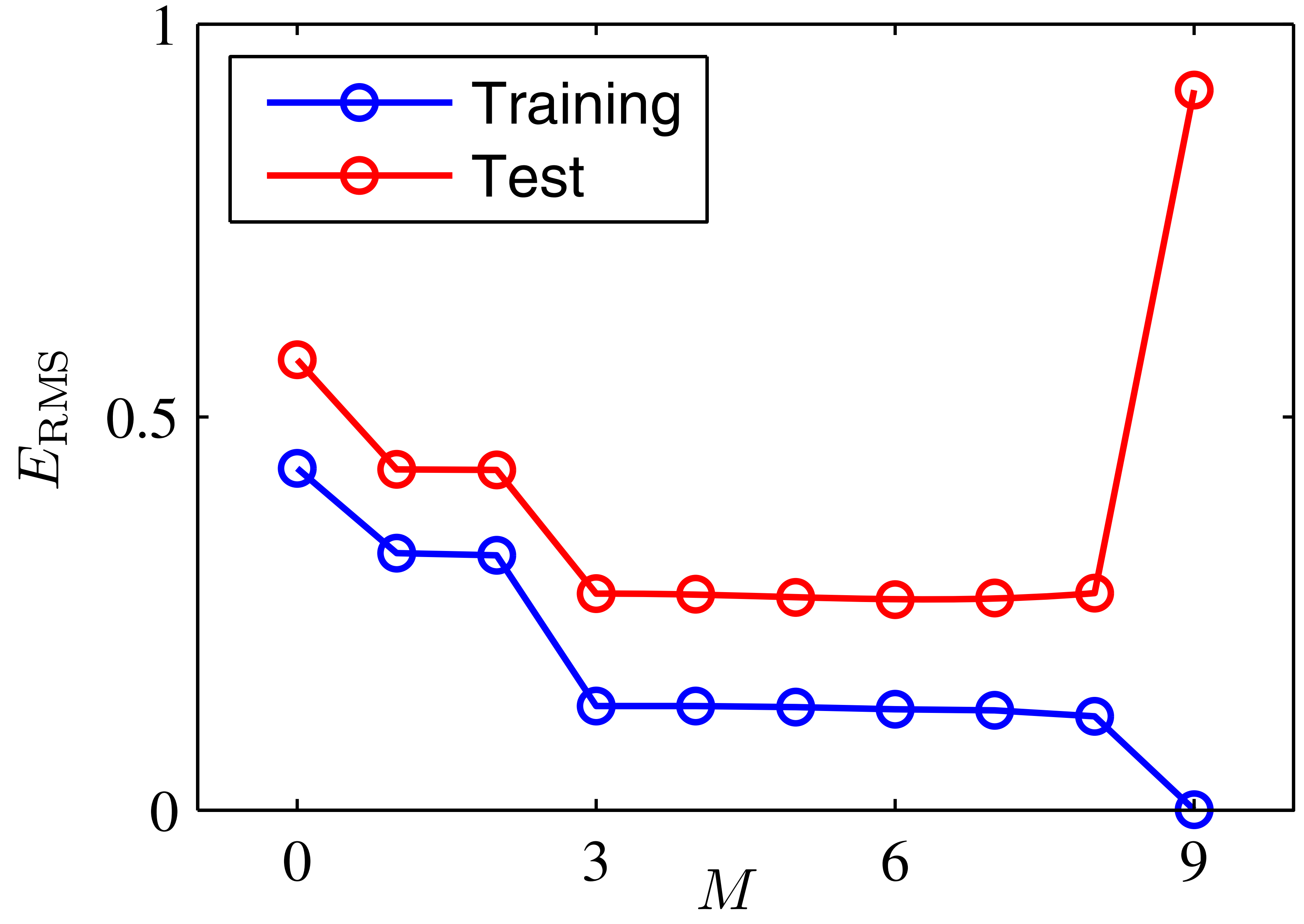


Prince (2023), *Understanding Deep Learning*

Overfitting

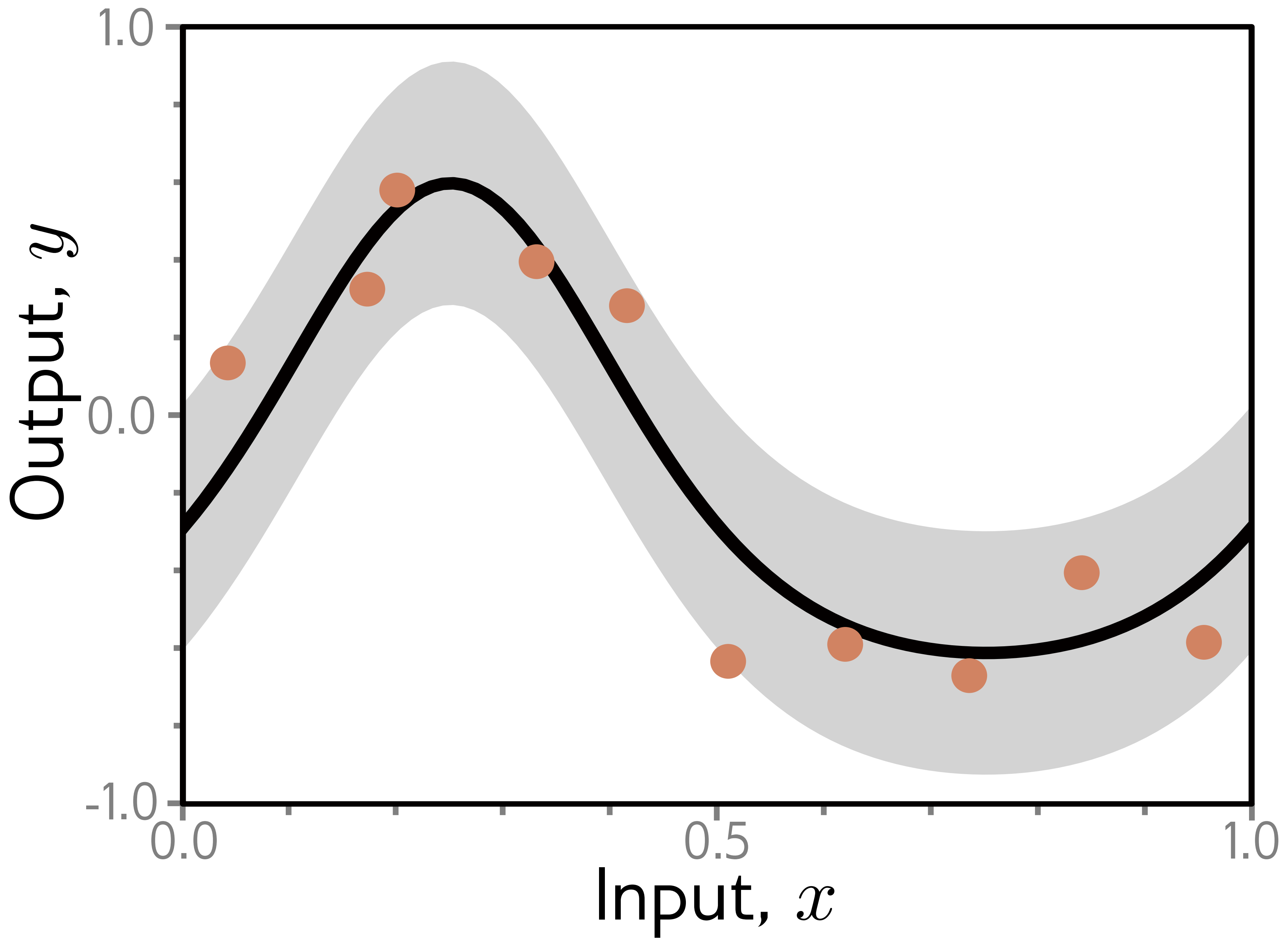
When too many parameters are barely enough

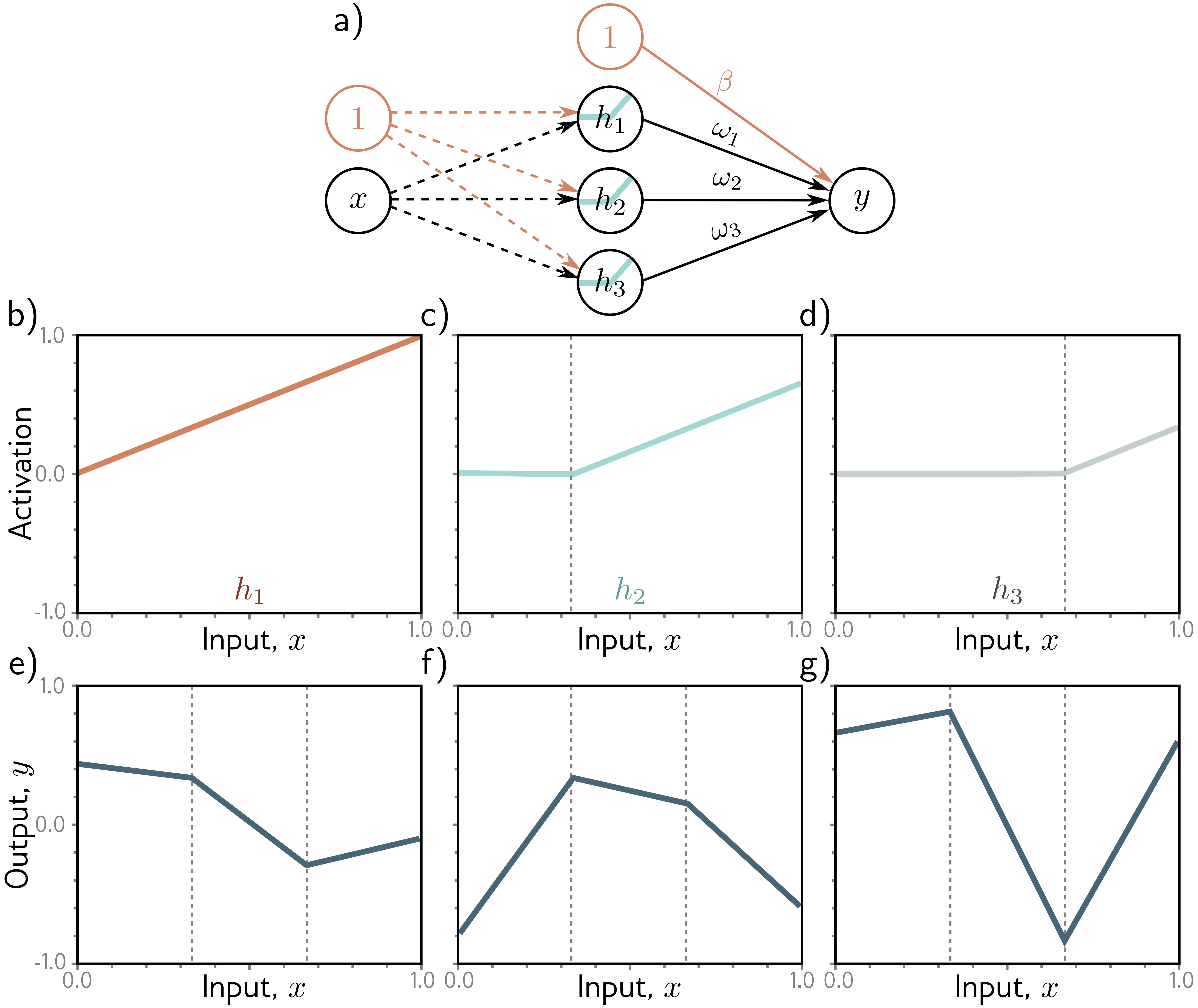




Bishop (2006), *PRML* & (2023) *Deep Learning*

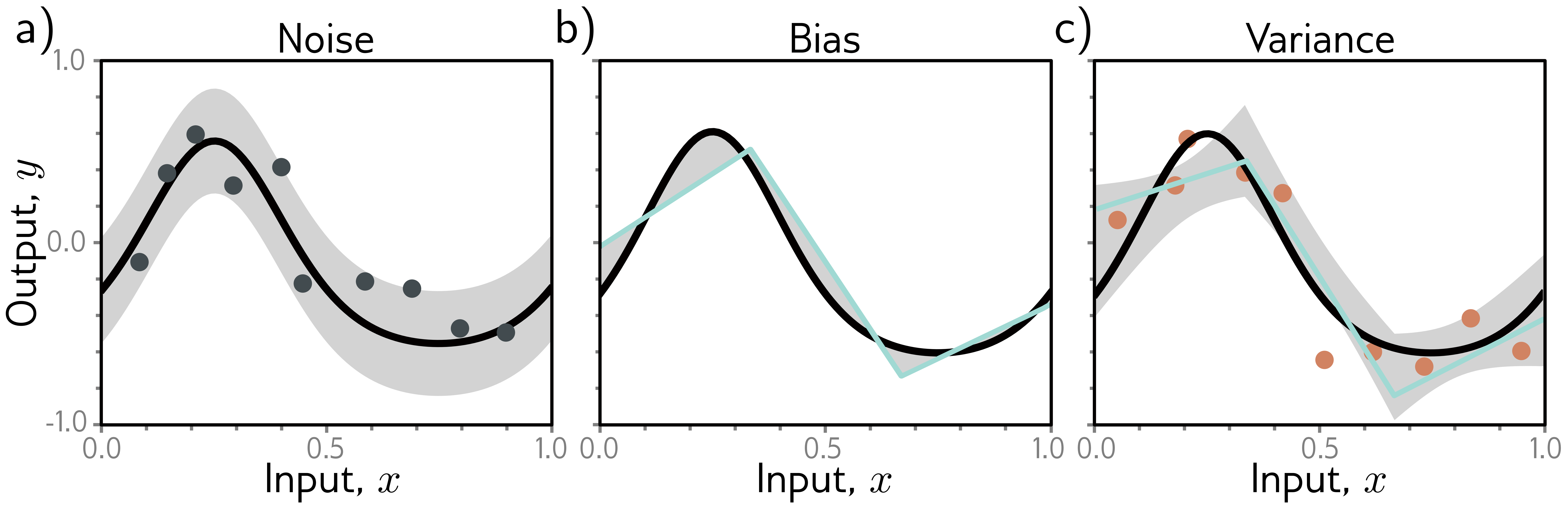
A toy example





Prince (2023), *Understanding Deep Learning*

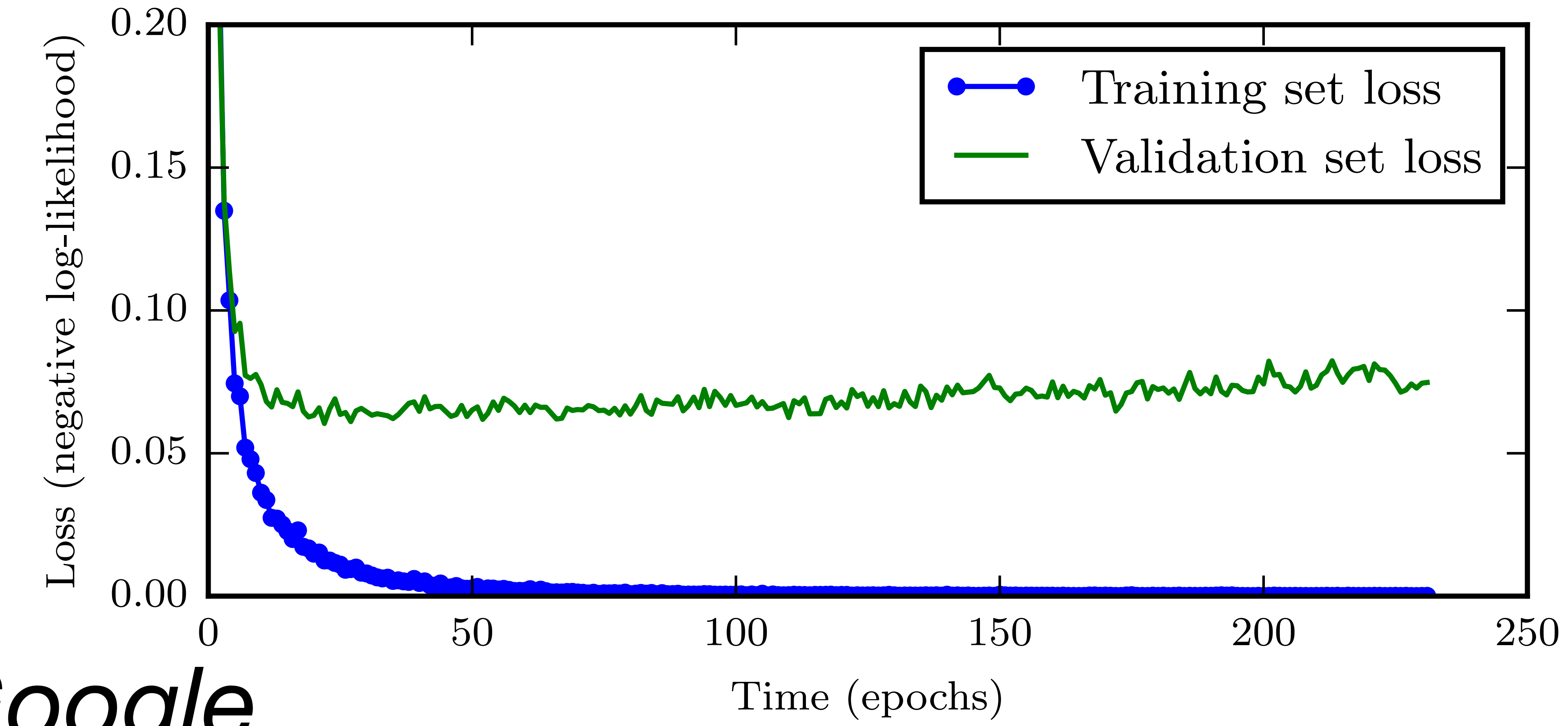
Three sources of error



Prince (2023), *Understanding Deep Learning*

Reducing error

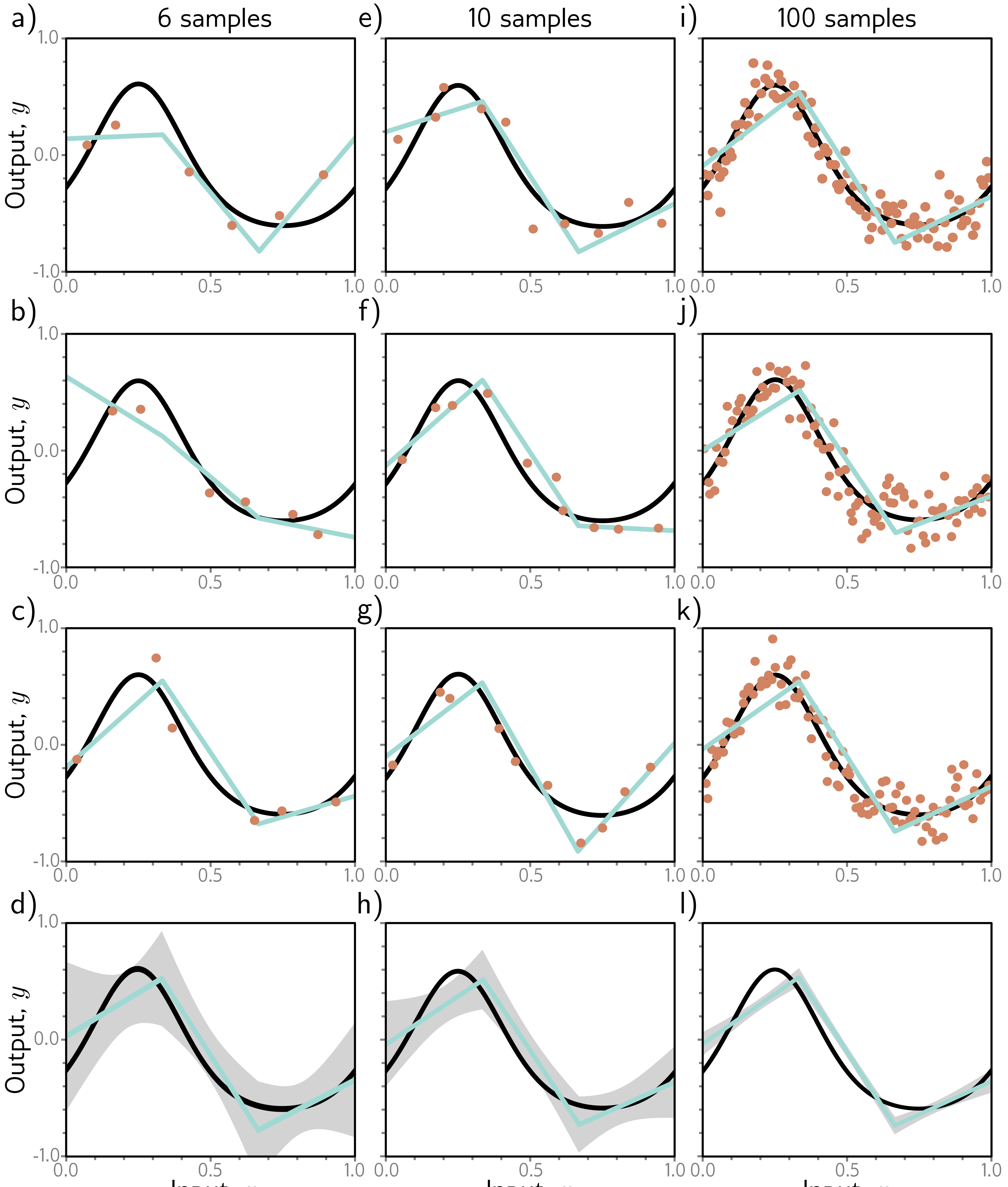
And regularisation



- **Variance: “Just get more data”** *—Guy from Google*
- **Bias: “We need to go deeper”**
- Early stopping, i.e., “cheating”
- … (bagging, multi-task learning, …)
- Sparse representations! (cf. compressive sensing…)
- Dropout

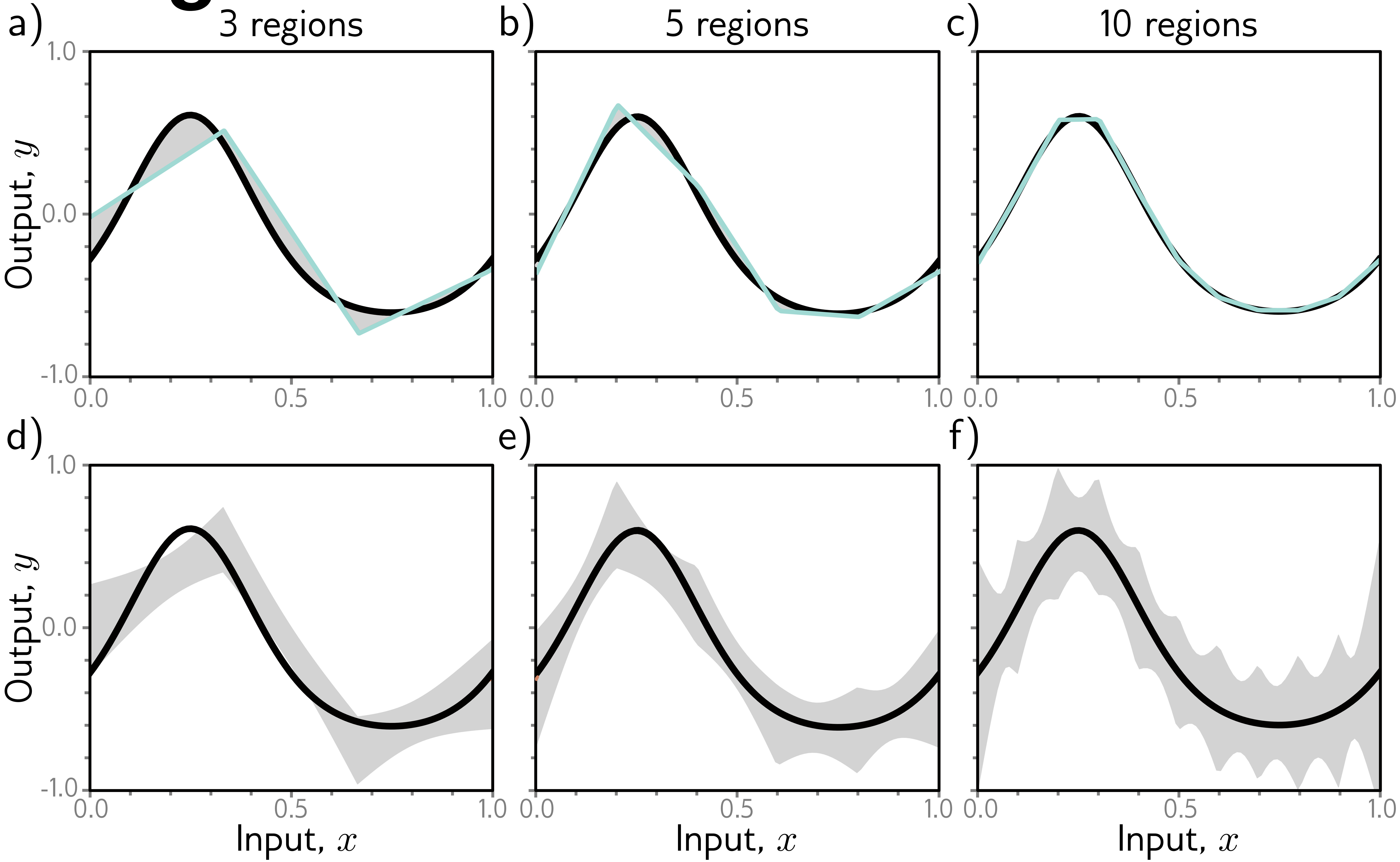
Goodfellow *et al* (2016), *Deep Learning*

Reducing variance



Prince (2023), *Understanding Deep Learning*

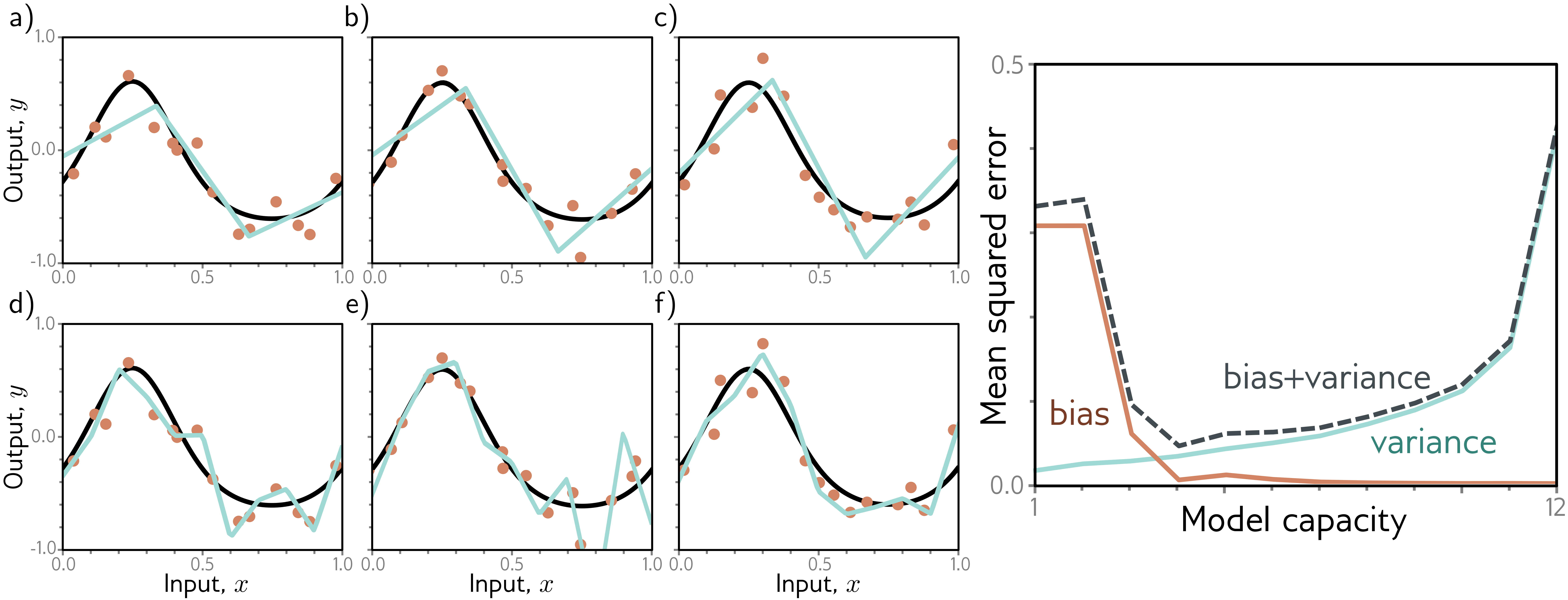
Reducing bias



Prince (2023), *Understanding Deep Learning*

Overfitting

Bias-variance tradeoff

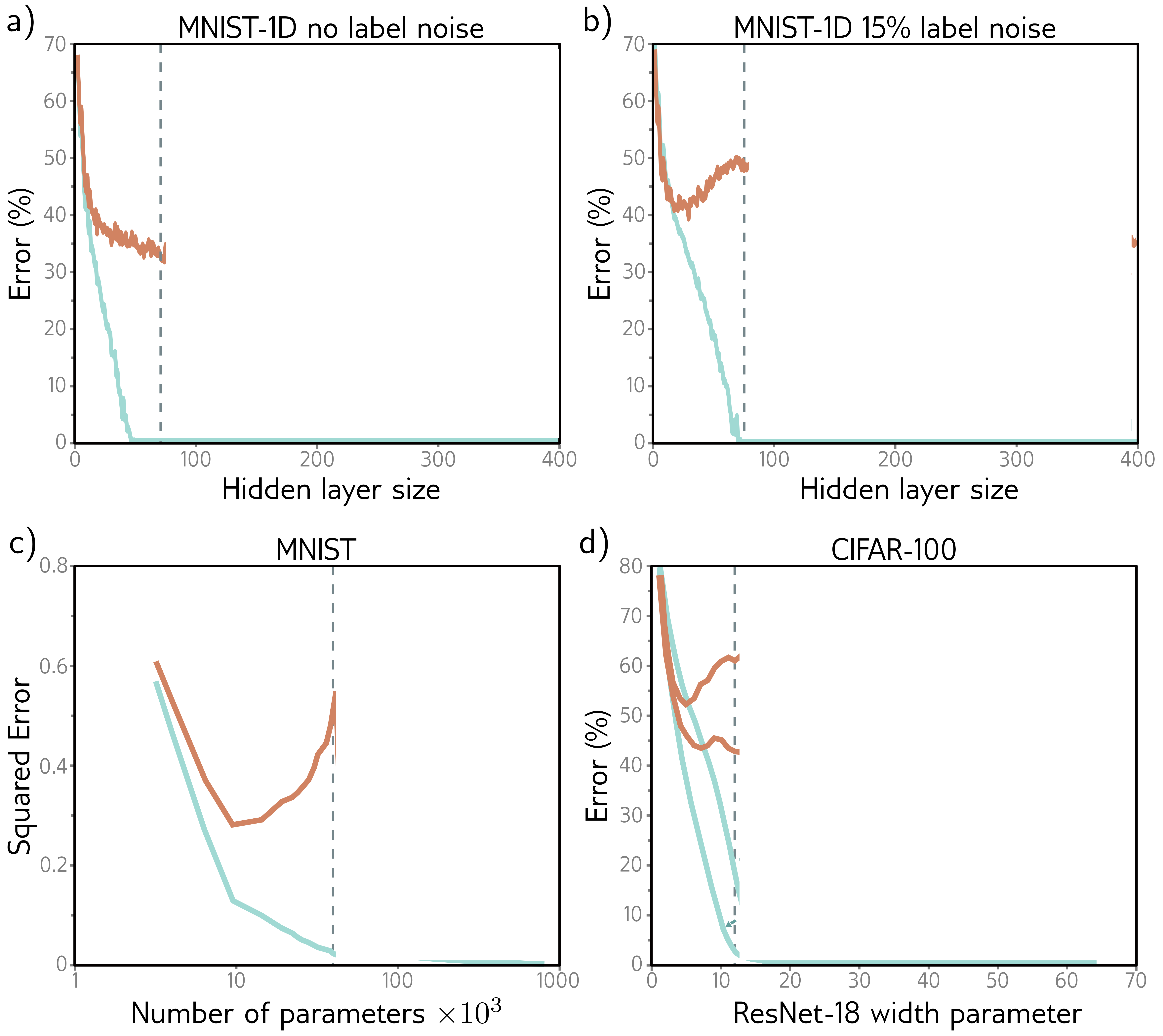


Prince (2023), *Understanding Deep Learning*

Double descent

Test

Train



Prince (2023), *Understanding Deep Learning*

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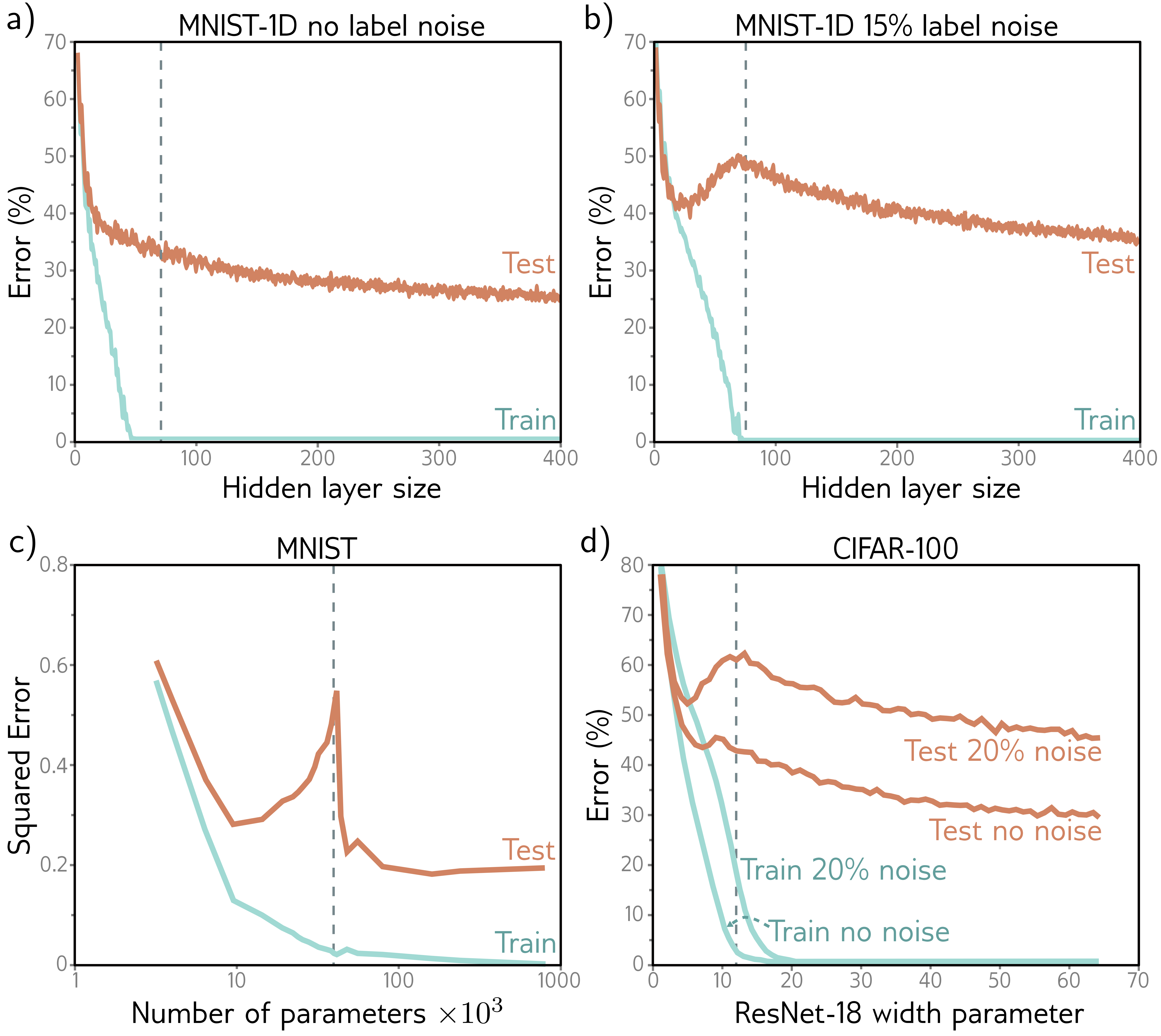
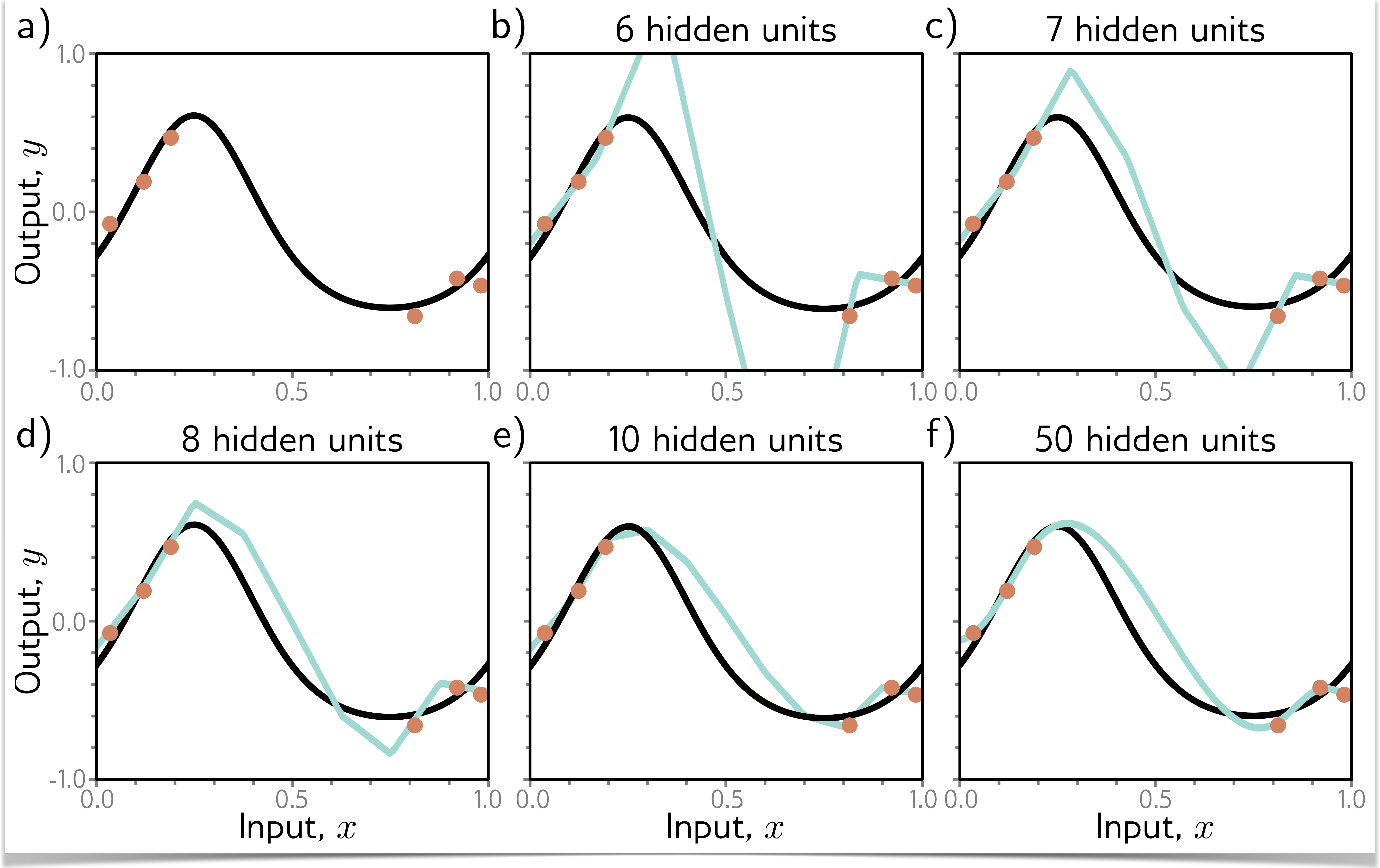
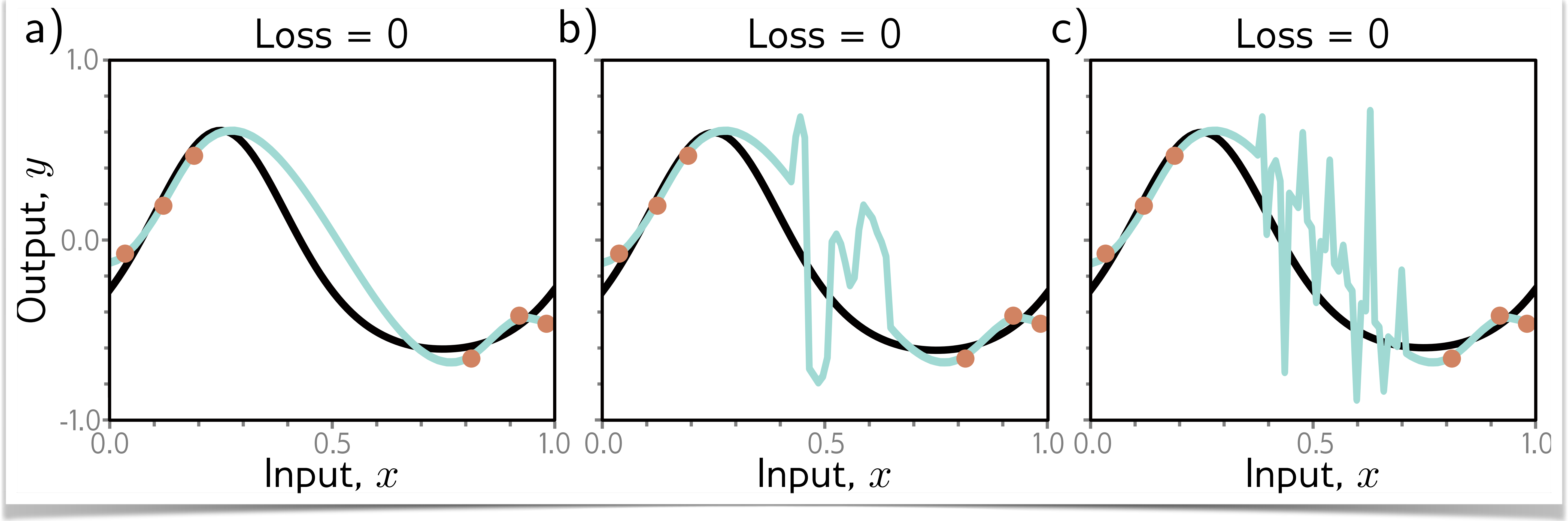


Prince (2023), *Understanding Deep Learning*

Why?



Capacity == smoothness



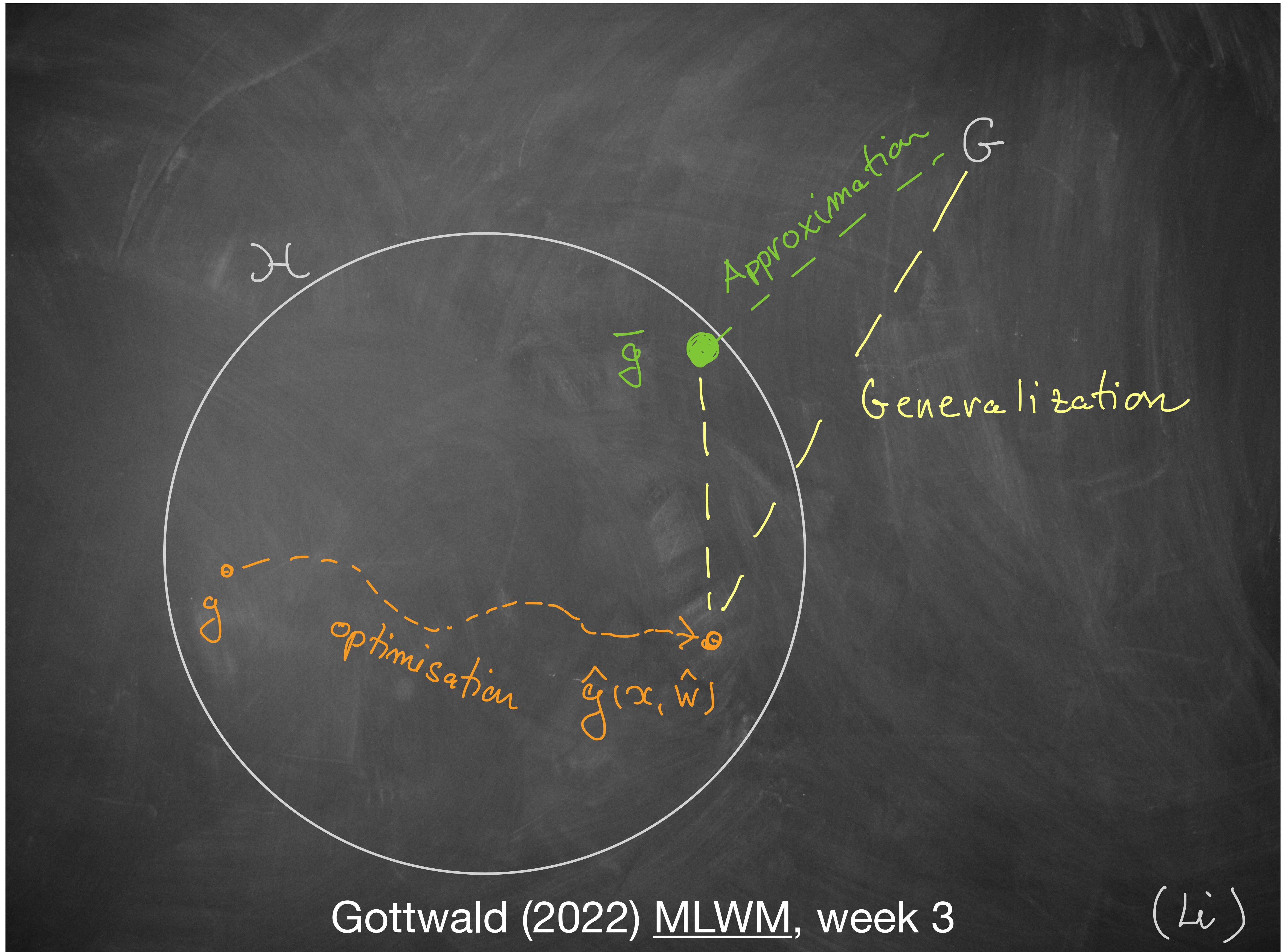
Regularisation == smoothness

Regularisation

Regularisation

- In traditional statistics: “explicit terms in the loss function to favour certain parameter choices” (e.g., L1, L2, ridge regression, LASSO, …)

- In deep learning: “any strategy that improves generalisation”

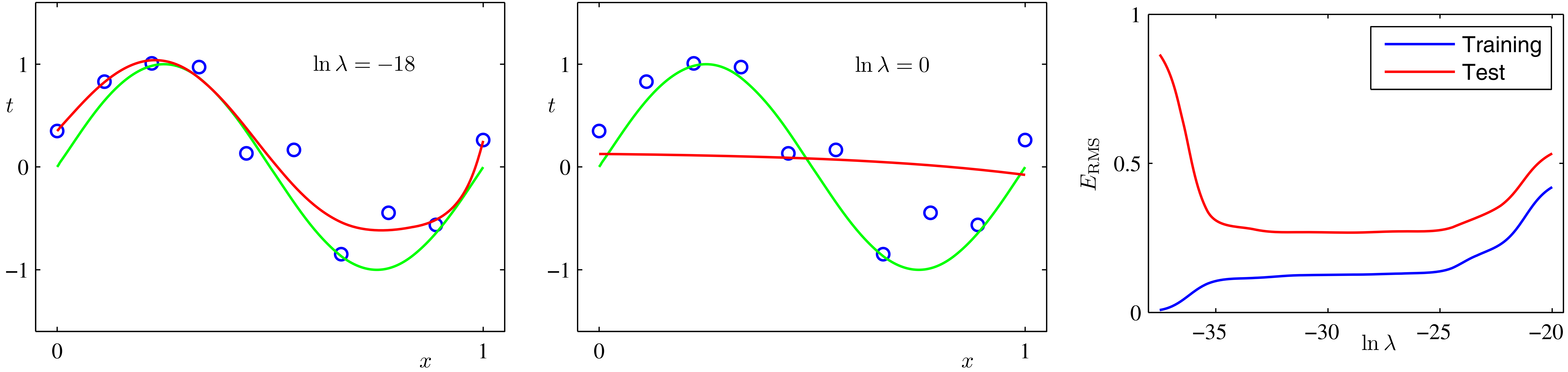


Gottwald (2022) MLWM, week 3

Regularisation

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n,\mathbf{w}) - t_n\}^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

(ridge regression)



Regularisation

In general

L1 (LASSO): $$\tilde{J}(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y}) = \frac{\alpha}{2}\boldsymbol{w}^{\top}\boldsymbol{w} + J(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y}),$$

$$w_i = \operatorname{sign}(w_i^*) \max\left\{|w_i^*| - \frac{\alpha}{H_{i,i}}, 0\right\}.$$

(note bias-variance)

L2 (ridge): $$\tilde{J}(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y}) = \frac{\alpha}{2}\boldsymbol{w}^{\top}\boldsymbol{w} + J(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y}),$$

Regularisation

In general

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$$\tilde{J}(\boldsymbol{w};\boldsymbol{X},\boldsymbol{y}) = \frac{\alpha}{2}\boldsymbol{w}^\top\boldsymbol{w} + J(\boldsymbol{w};\boldsymbol{X},\boldsymbol{y}),$$

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(note bias-variance)

L2 (ridge):

$$\tilde{J}(\boldsymbol{w};\boldsymbol{X},\boldsymbol{y}) = \frac{\alpha}{2}\boldsymbol{w}^\top\boldsymbol{w} + J(\boldsymbol{w};\boldsymbol{X},\boldsymbol{y}),$$

This is constrained optimisation! (i.e., KKT)

$$\min_{\boldsymbol{x}}\max_{\boldsymbol{\lambda}}\max_{\boldsymbol{\alpha},\boldsymbol{\alpha}\geq 0} -f(\boldsymbol{x}) + \sum_i \lambda_i g^{(i)}(\boldsymbol{x}) + \sum_j \alpha_j h^{(j)}(\boldsymbol{x}).$$

Weight Decay as Constrained Optimization

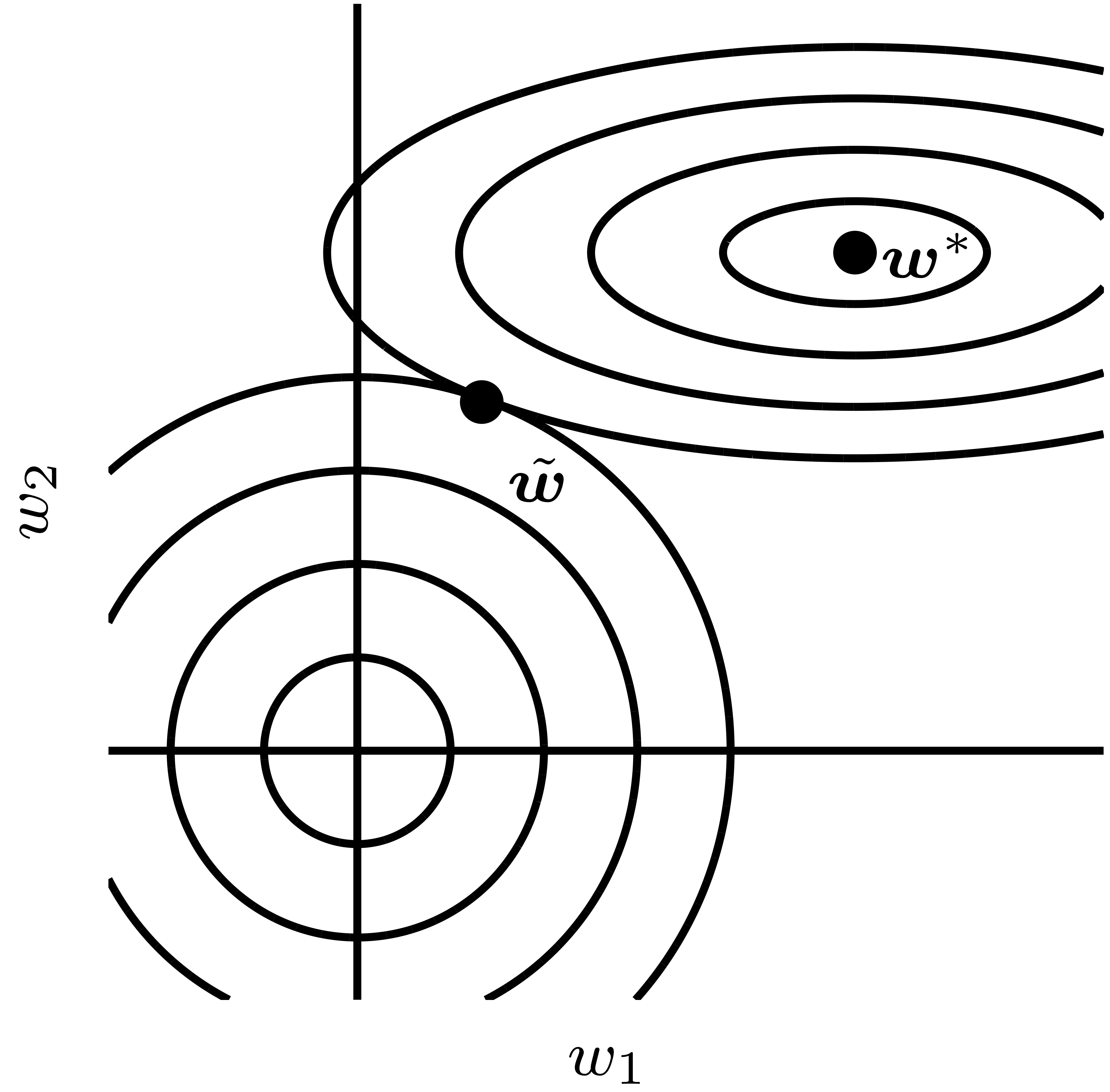


Figure 7.1

(Goodfellow 2016)

the problem is not convex (but some other regularity conditions hold), then these KKT conditions still characterise a local minima.

Theorem 4.12 (KKT: Slater's condition version)**.** *Let $f : \mathbb{R}^n \to \mathbb{R}$ be a convex, continuously differentiable function on the set $\Omega = \{\boldsymbol{x} \in \mathbb{R}^n : g_i(\boldsymbol{x}) \leq 0,$ for all $i = 1, \ldots, m\}$, where the $g_i : \mathbb{R}^n \to \mathbb{R}$ are convex and continuously differentiable for all $i = 1, \ldots, m$, such that $\operatorname{int} \Omega \neq \emptyset$. A necessary and sufficient condition that $\boldsymbol{x}^* \in \Omega$ minimises f over Ω is that there exists a solution to the system*

$$\nabla f(\boldsymbol{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla g_i(\boldsymbol{x}^*) = \boldsymbol{0}, \tag{4.7a}$$

$$\lambda_i g_i(\boldsymbol{x}^*) = 0 \text{ for all } i = 1, 2, \ldots, m, \tag{4.7b}$$

$$\boldsymbol{g}(\boldsymbol{x}^*) \leq \boldsymbol{0}, \tag{4.7c}$$

$$\boldsymbol{\lambda} \geq \boldsymbol{0}. \tag{4.7d}$$

Section 4.2.1 proves this theorem.

The condition (4.7b) is sometimes called a complementary slackness condition because it expresses that either the constraint is active (and the Lagrange multiplier is potentially positive) or the Lagrange multiplier is zero (and potentially the constraint is not active).

The conditions (4.7) are called the **KKT conditions**. Conditions (4.7a) and (4.7b) may be equivalently replaced with

$$\nabla f(\boldsymbol{x}^*) + \sum_{i \in I(\boldsymbol{x}^*)} \lambda_i \nabla g_i(\boldsymbol{x}^*) = \boldsymbol{0}, \tag{4.8}$$

and for all $i \notin I(\boldsymbol{x}^*)$ we set $\lambda_i = 0$.

Theorem 4.12 is an extension of the Lagrange multiplier idea. That is, for the active constraints $I(\boldsymbol{x}^*)$[5] we would write a new objective function

$$h(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) + \sum_{i \in I(\boldsymbol{x}^*)} \lambda_i g_i(\boldsymbol{x}),$$

including Lagrange multipliers as in (4.4) for the active constraints, and then ∇h is just the left-hand side of condition (4.8). So we are basically solving a problem including Lagrange multipliers to enforce the appropriate set of constraints (the active ones).

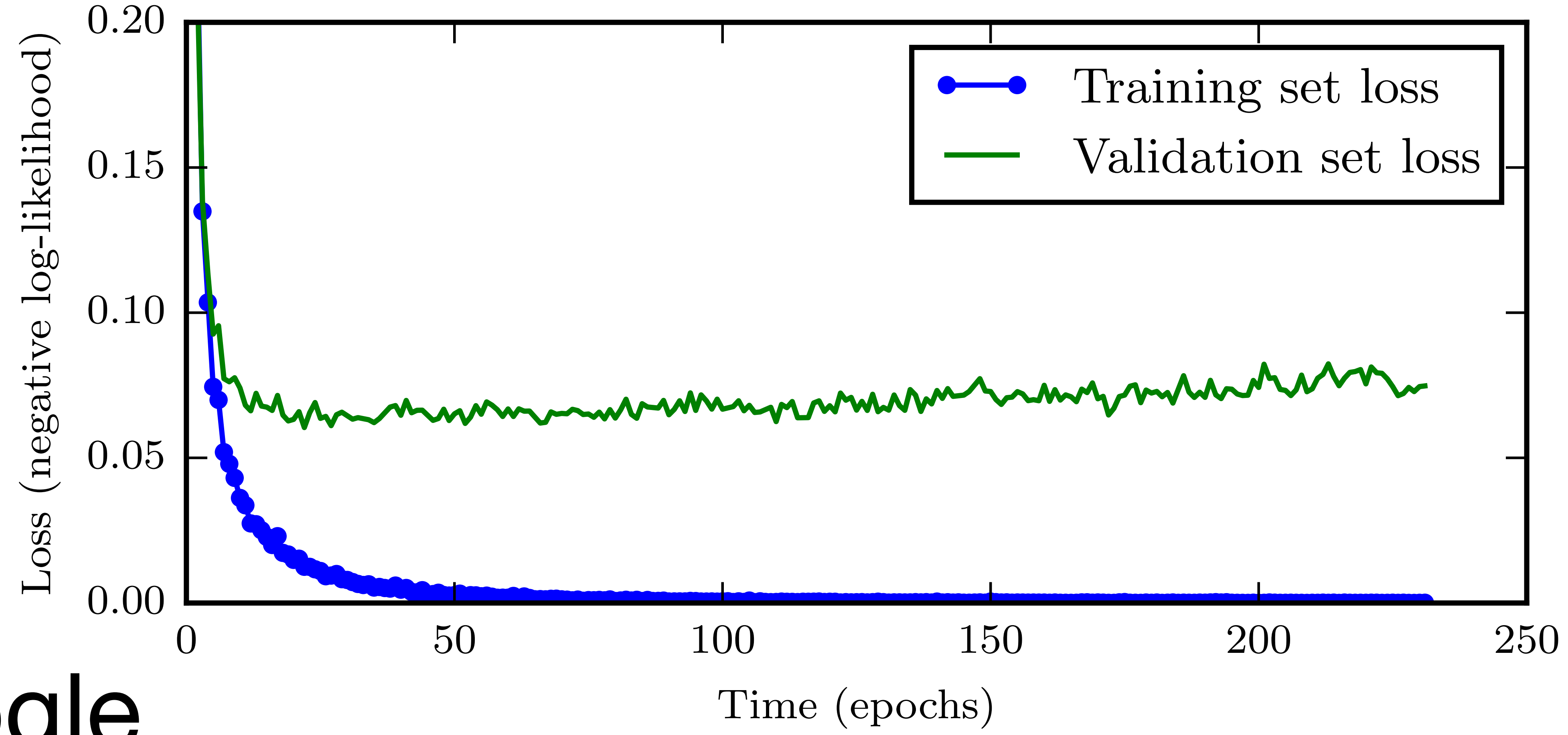
The only additional information we get from Theorem 4.12 is that the Lagrange multipliers λ_i must be positive or zero. Figures 4.15 and 4.16 illustrate the positivity requirements: the constraints $I(\boldsymbol{x}^*)$ are active, so the point $\boldsymbol{x}^*$ is in the intersection of the curves $g_i(\boldsymbol{x}) = 0$, for $i \in I(\boldsymbol{x}^*)$. We know that the feasible region is inside the set Ω, that is that $g_i(\boldsymbol{x}) \leq 0$, and also that $g_i(\boldsymbol{x})$ is increasing in the direction $\nabla g_i(\boldsymbol{x})$. Since $g_i(\boldsymbol{x}^*) = 0$, then $\nabla g_i(\boldsymbol{x}^*)$ points outside the set Ω, equivalently $-\nabla g_i(\boldsymbol{x}^*)$ points inside. Likewise, if $\boldsymbol{x}^*$ is a minimum, the objective function must increase in any direction pointing into the region. However, what the theorem says is even stronger: it says that

$$\nabla f(\boldsymbol{x}^*) = -\sum_{i \in I(\boldsymbol{x}^*)} \lambda_i \nabla g_i(\boldsymbol{x}^*),$$

[5] If $I(\boldsymbol{x}^*) = \emptyset$ then $\boldsymbol{x}^*$ is not on any boundary, and the KKT condition just reverts to the familiar condition for an unconstrained problem; that is, $\nabla f(\boldsymbol{x}^*) = 0$.

Reducing error

And regularisation

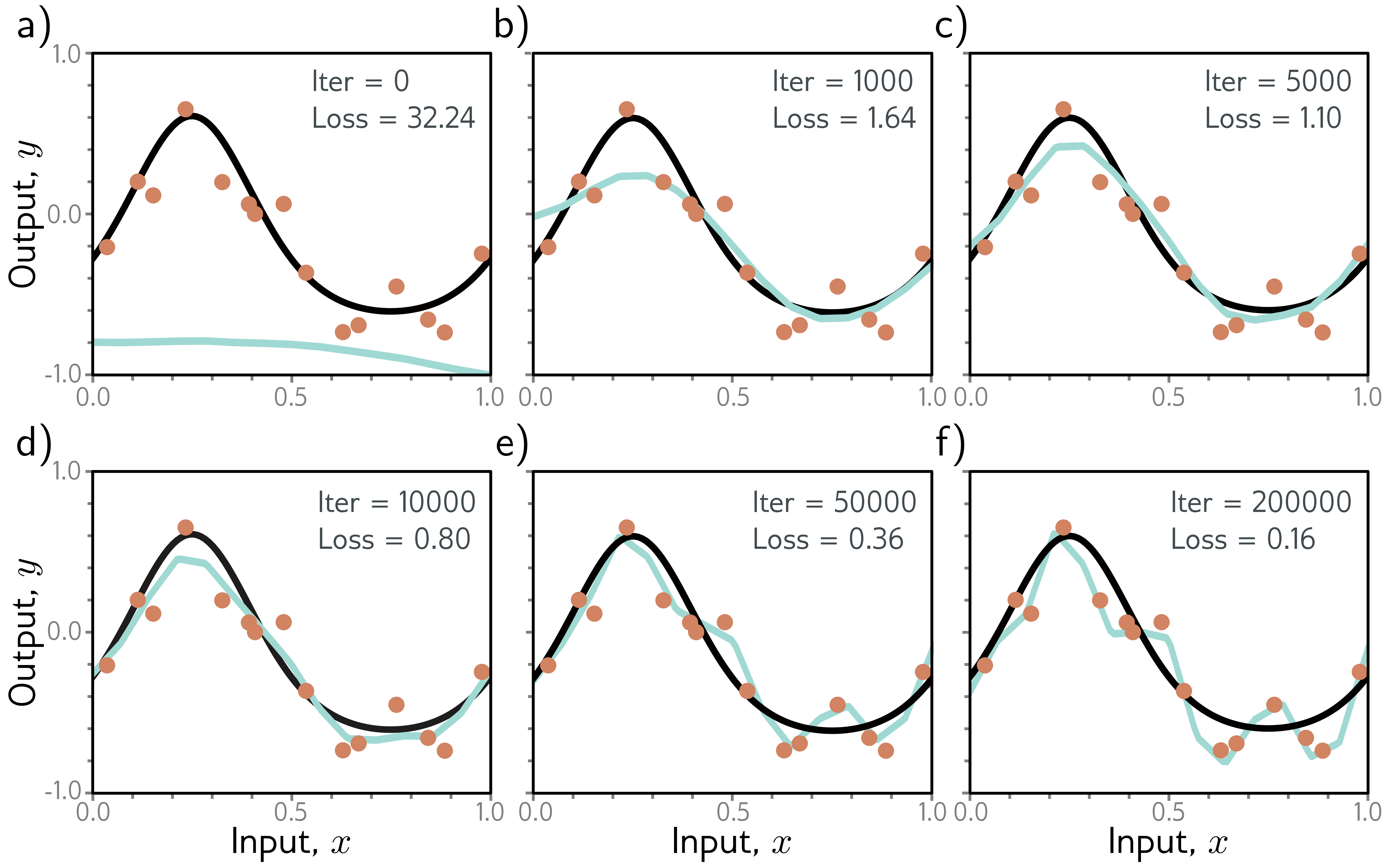


- Variance: “Just get more data” —Guy from Google
- Bias: “We have to go deeper”
- **Early stopping, i.e., “cheating”** (see Goodfellow Fig 7.4)
- **… (bagging, multi-task learning, …)**
- **Sparse representations! (cf. compressive sensing…)**
- **Dropout**

Goodfellow *et al* (2016), *Deep Learning*

Early stopping

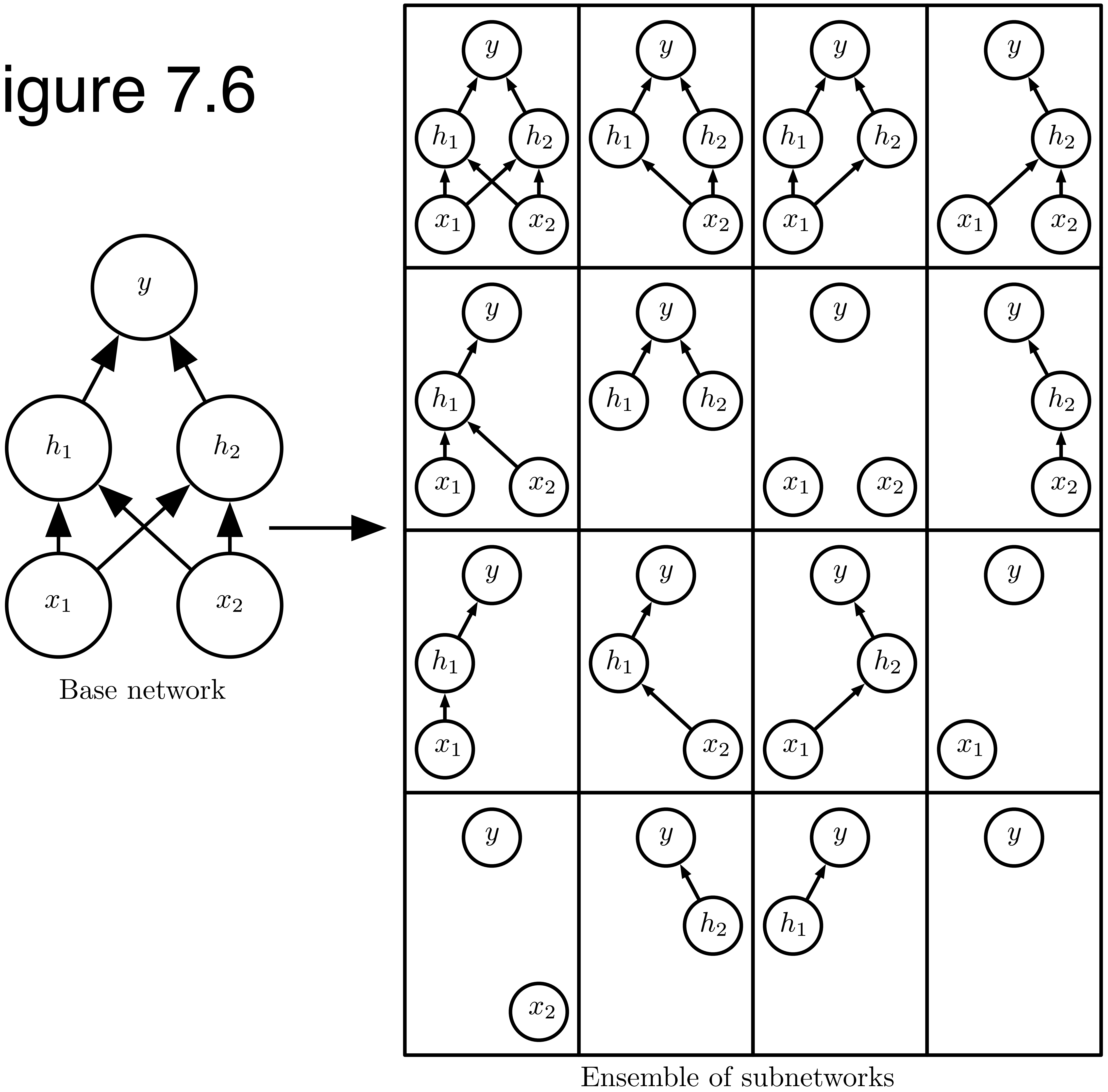
On our toy model



Prince (2023), *Understanding Deep Learning*

Dropout

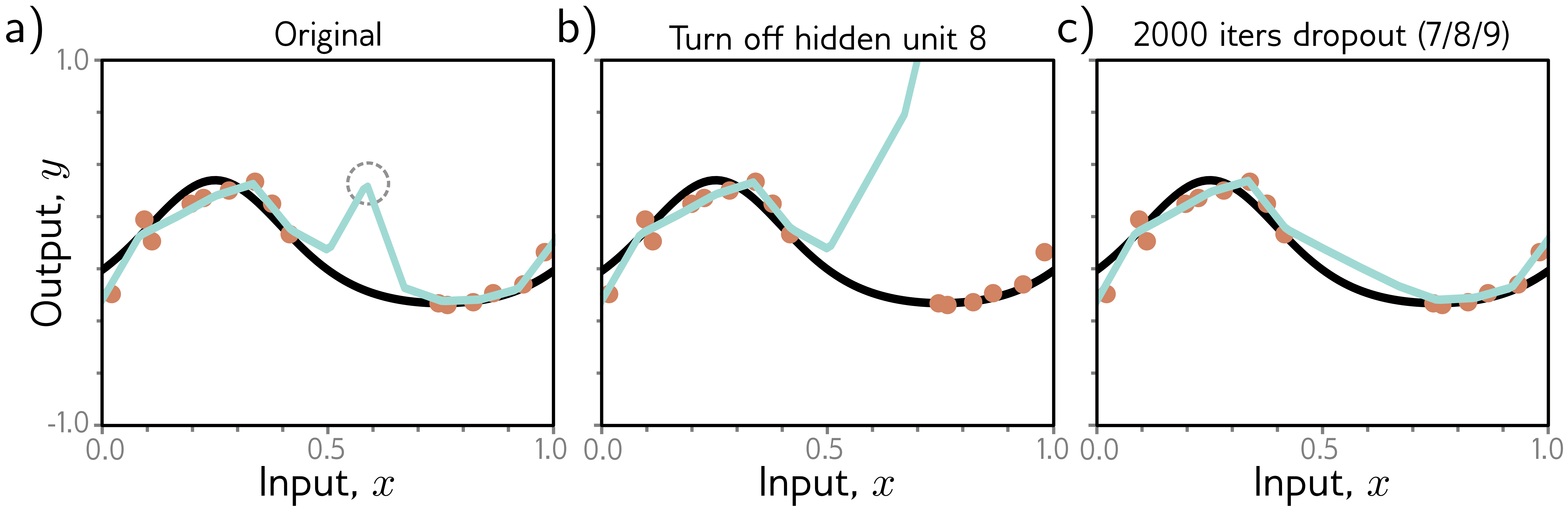
Figure 7.6



(Goodfellow 2016)

Dropout

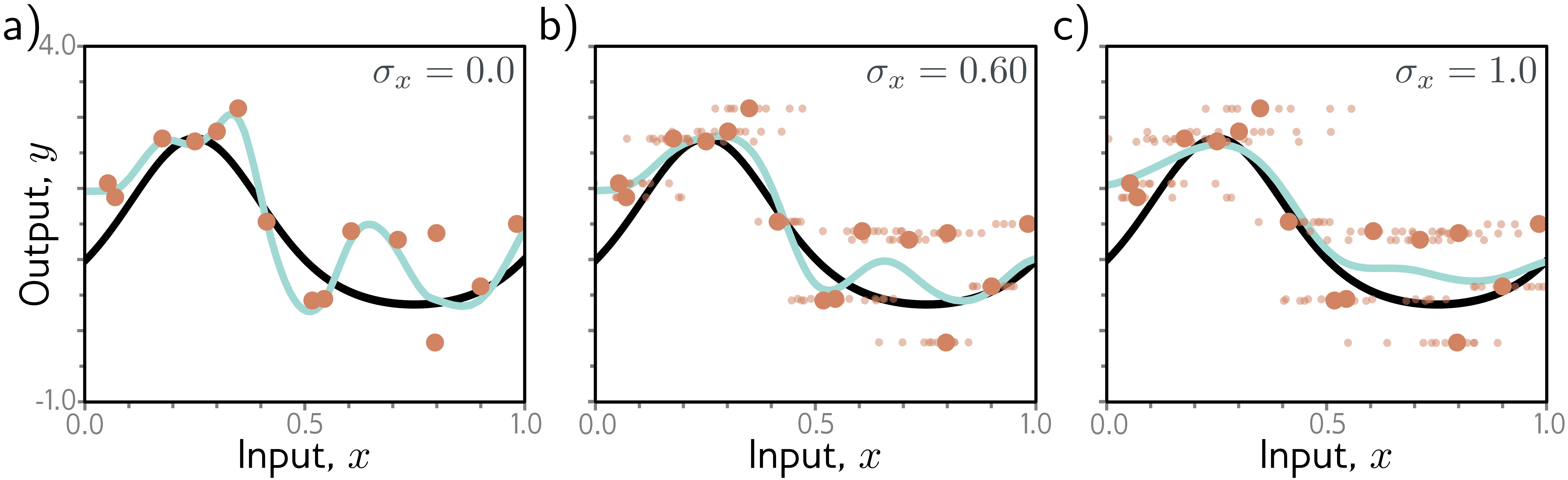
On our toy model



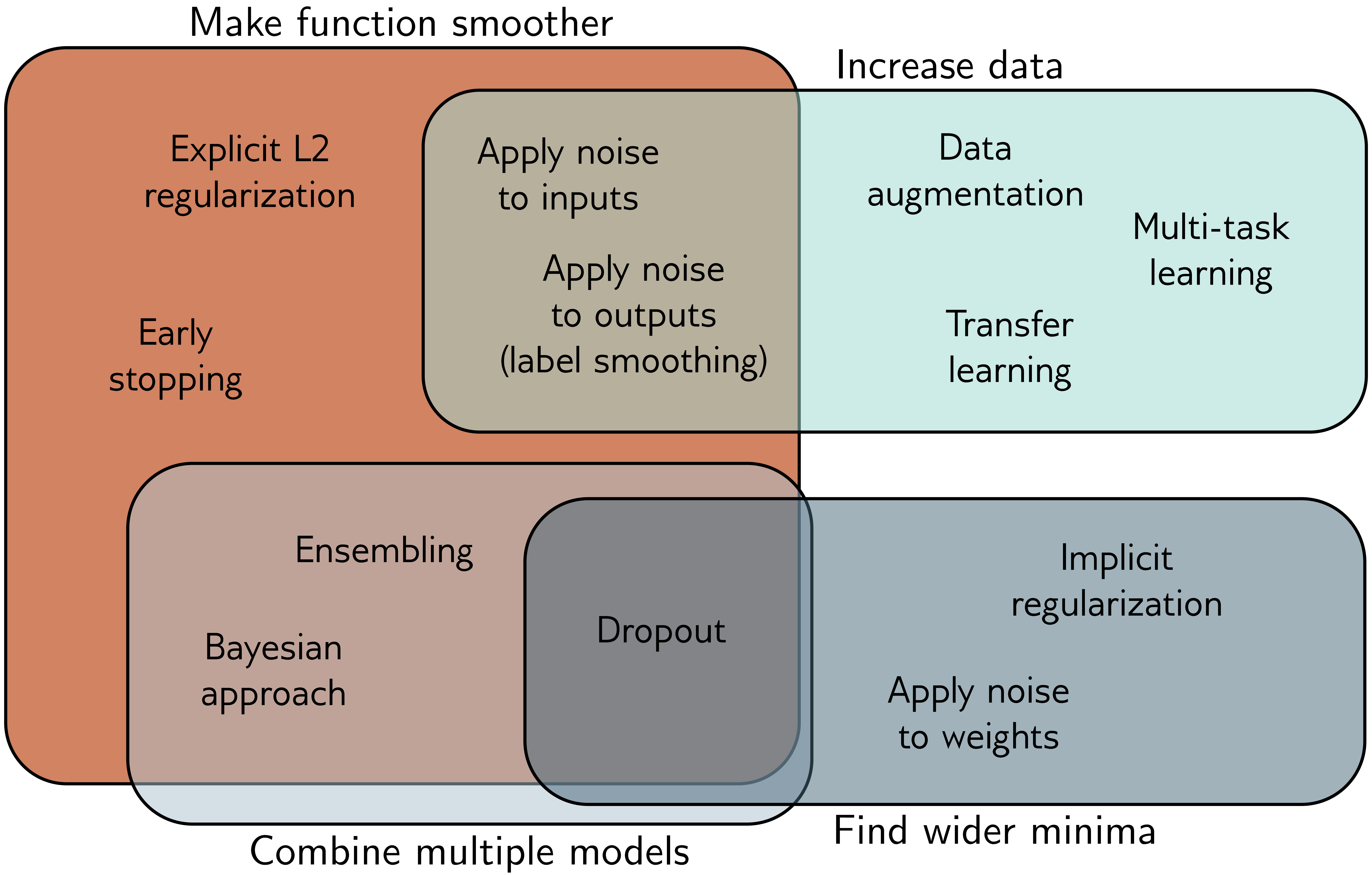
Prince (2023), *Understanding Deep Learning*

Input noise

On our toy model



Prince (2023), *Understanding Deep Learning*



Prince (2023), *Understanding Deep Learning*