Regularization

And other ways to improve test performance

DL4DS – Spring 2025

Regularization

- Why is there a generalization gap between training and test data?
  - Overfitting (model describes statistical peculiarities)
  - Model unconstrained in areas where there are no training examples
- Regularization = methods to reduce the generalization gap
- Technically means adding terms to loss function
- But colloquially means any method (hack) to reduce gap between training and test data

Regularization

- Explicit regularization
- Implicit regularization
- Early stopping
- Ensembling
- Dropout
- Adding noise
- Transfer learning, multi-task learning, self-supervised learning
- Data augmentation

Explicit regularization

- Standard loss function:

$$\begin{aligned}\hat{\boldsymbol{\phi}} &= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\big[\mathrm{L}[\boldsymbol{\phi}]\big] \\ &= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[\sum_{i=1}^{I}\ell_i[\mathbf{x}_i,\mathbf{y}_i]\right]\end{aligned}$$

Explicit regularization

- Standard loss function:

$$\hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\big[\mathrm{L}[\boldsymbol{\phi}]\big] = \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[\sum_{i=1}^{I}\ell_i[\mathbf{x}_i,\mathbf{y}_i]\right]$$

- Regularization adds an extra term

$$\hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[\sum_{i=1}^{I}\ell_i[\mathbf{x}_i,\mathbf{y}_i] + \lambda\cdot \mathrm{g}[\boldsymbol{\phi}]\right]$$

Explicit regularization

- Standard loss function:

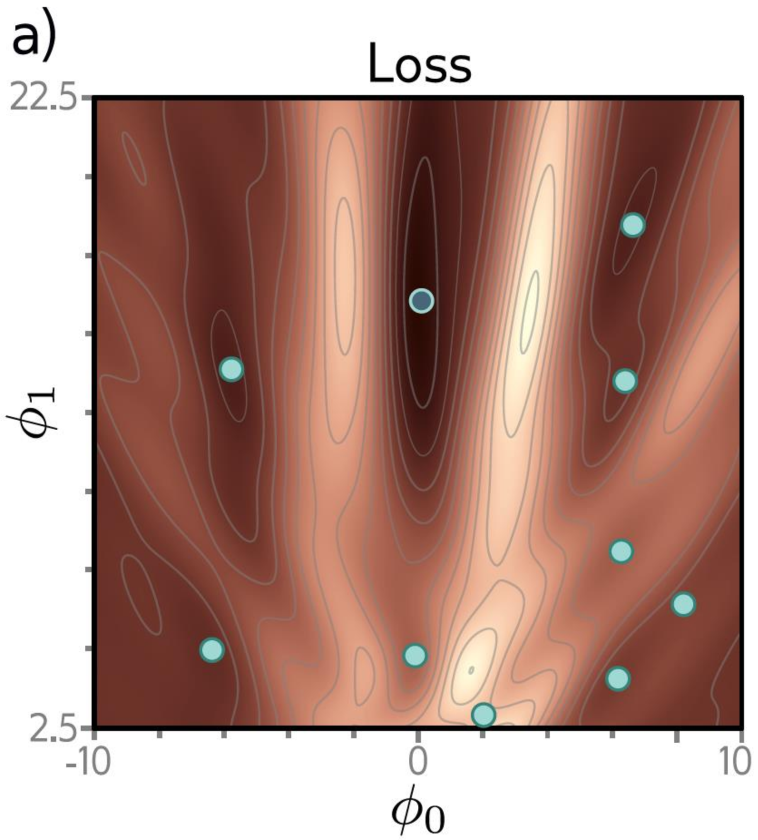
$$\hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\big[\mathrm{L}[\boldsymbol{\phi}]\big] = \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[\sum_{i=1}^{I}\ell_i[\mathbf{x}_i,\mathbf{y}_i]\right]$$

- Regularization adds an extra term

$$\hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[\sum_{i=1}^{I}\ell_i[\mathbf{x}_i,\mathbf{y}_i] + \lambda\cdot\mathrm{g}[\boldsymbol{\phi}]\right]$$

- Where $\mathrm{g}[\phi]$ is smaller for preferred parameters
- $\lambda > 0$ controls the strength of influence

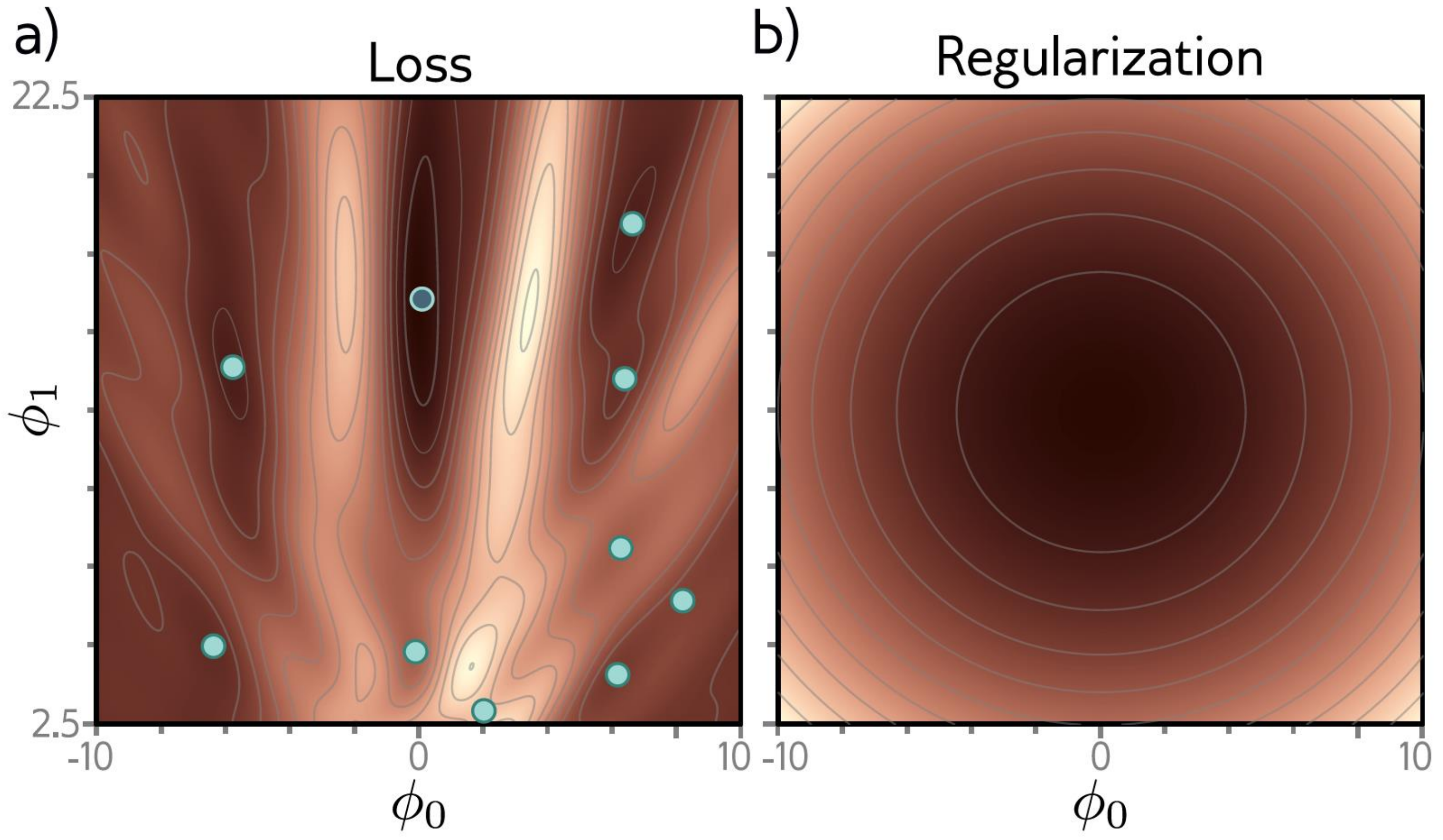
Explicit regularization



Loss function for Gabor model of Lecture 6 and Chapter 6.

● denotes local minima

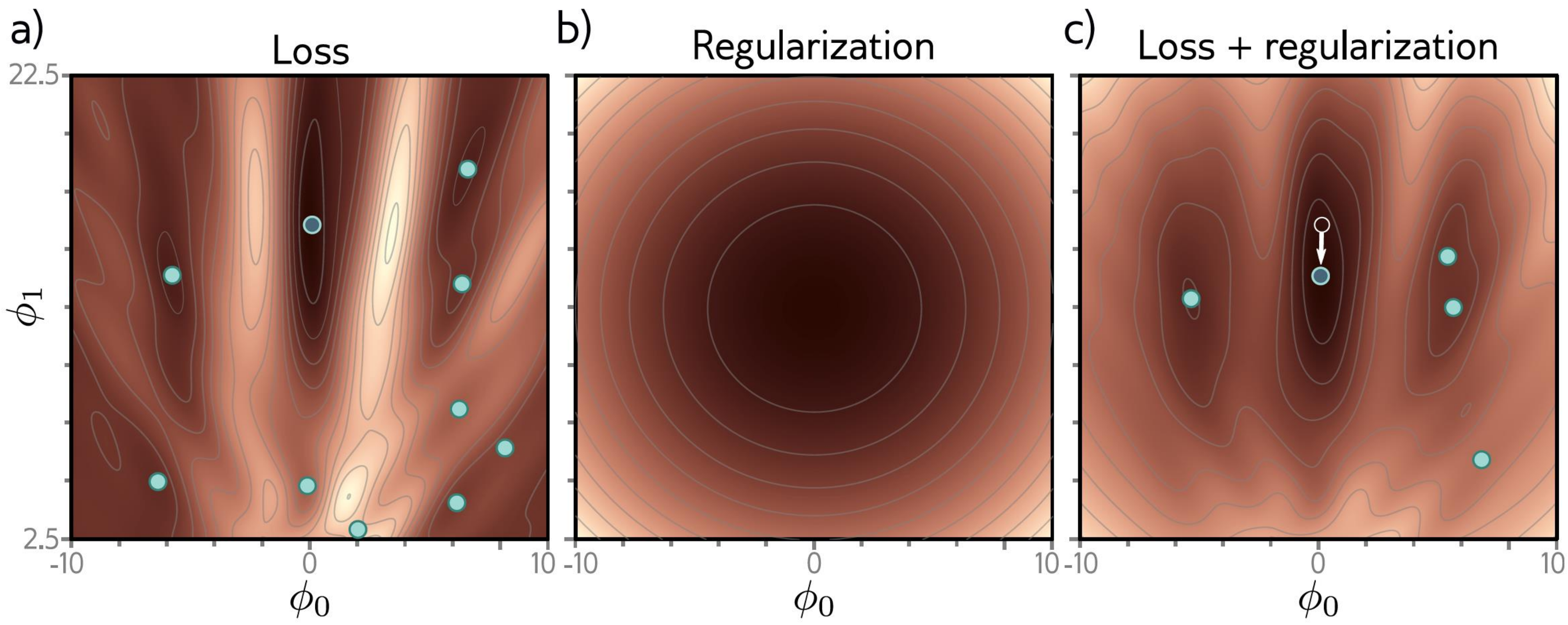
Explicit regularization



Example of a regularization function that prefers parameters close to 0.

Explicit regularization

Fewer local minima and the absolute minimum has moved.



denotes local minima

Probabilistic interpretation

- Maximum likelihood:

$$\hat{\phi} = \underset{\phi}{\operatorname{argmax}} \left[\prod_{i=1}^{I} Pr(\mathbf{y}_i|\mathbf{x}_i, \phi) \right]$$

- Regularization is equivalent to adding a prior over parameters

$$\hat{\phi} = \underset{\phi}{\operatorname{argmax}} \left[\prod_{i=1}^{I} Pr(\mathbf{y}_i|\mathbf{x}_i, \phi) Pr(\phi) \right]$$

Maximum a posteriori or MAP criterion

… what you know about parameters *before* seeing the data

Equivalence

- Explicit regularization:

$$\hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\phi}}{\operatorname{argmin}} \left[\sum_{i=1}^{I} \ell_i[\mathbf{x}_i, \mathbf{y}_i] + \lambda \cdot \mathrm{g}[\boldsymbol{\phi}] \right]$$

- Probabilistic interpretation:

$$\hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\phi}}{\operatorname{argmax}} \left[\prod_{i=1}^{I} Pr(\mathbf{y}_i | \mathbf{x}_i, \boldsymbol{\phi}) Pr(\boldsymbol{\phi}) \right]$$

- Converting to Negative Log Likelihood (e.g. $-\log(\cdot)$):

$$\lambda \cdot \mathrm{g}[\boldsymbol{\phi}] = -\log[Pr(\boldsymbol{\phi})]$$

L2 Regularization

- Most common regularizer is L2 regularization
- Favors smaller parameters (like in previous example)

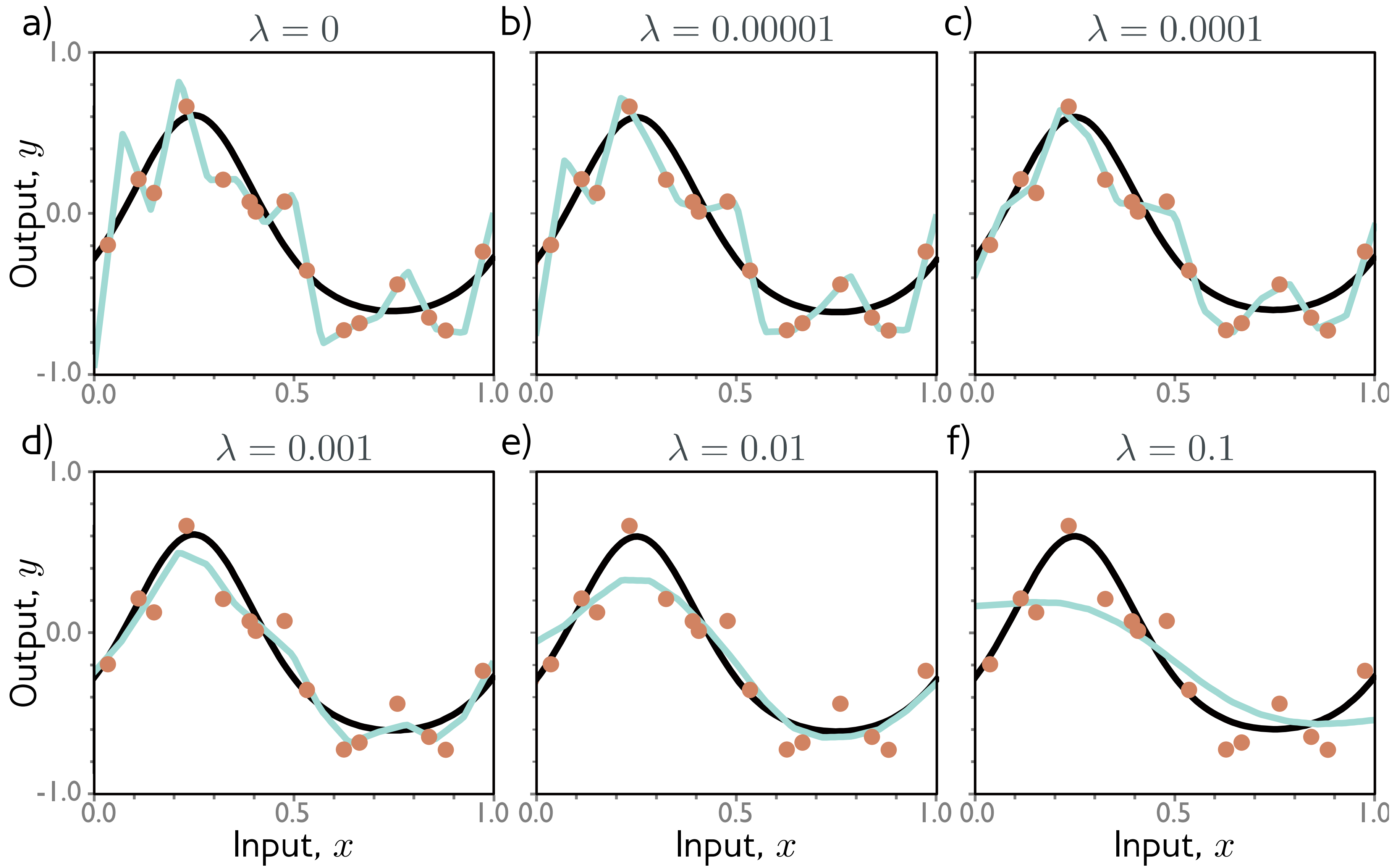
$$\hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\phi}}{\operatorname{argmin}} \left[\mathrm{L}[\boldsymbol{\phi}, \{\mathbf{x}_i, \mathbf{y}_i\}] + \lambda \sum_j \phi_j^2 \right]$$

- Also called Tikhonov regularization, ridge regression
- In neural networks, usually just for weights

Why does L2 regularization help?

- Discourages fitting excessively to the training data (overfitting)
- Encourages smoothness between datapoints

L2 regularization (simple net from last lecture)



PyTorch Explicit L2 Regularizer

SGD

CLASS torch.optim.SGD(*params, lr=0.001, momentum=0, dampening=0, weight_decay=0, nesterov=False, *, maximize=False, foreach=None, differentiable=False*) [SOURCE]

Implements stochastic gradient descent (optionally with momentum).

Parameters

- **params** (*iterable*) – iterable of parameters to optimize or dicts defining parameter groups
- **lr** (*float, optional*) – learning rate (default: 1e-3)
- **momentum** (*float, optional*) – momentum factor (default: 0)
- **weight_decay** (*float, optional*) – weight decay (L2 penalty) (default: 0)

https://pytorch.org/docs/stable/generated/torch.optim.SGD.html

ADAM

CLASS torch.optim.Adam(*params, lr=0.001, betas=(0.9, 0.999), eps=1e-08, weight_decay=0, amsgrad=False, *, foreach=None, maximize=False, capturable=False, differentiable=False, fused=None*) [SOURCE]

Implements Adam algorithm.

Parameters

- **params** (*iterable*) – iterable of parameters to optimize or dicts defining parameter groups
- **lr** (*float, Tensor, optional*) – learning rate (default: 1e-3). A tensor LR is not yet supported for all our implementations. Please use a float LR if you are not also specifying fused=True or capturable=True.
- **betas** (*Tuple[float, float], optional*) – coefficients used for computing running averages of gradient and its square (default: (0.9, 0.999))
- **eps** (*float, optional*) – term added to the denominator to improve numerical stability (default: 1e-8)
- **weight_decay** (*float, optional*) – weight decay (L2 penalty) (default: 0)

https://pytorch.org/docs/stable/generated/torch.optim.Adam.html

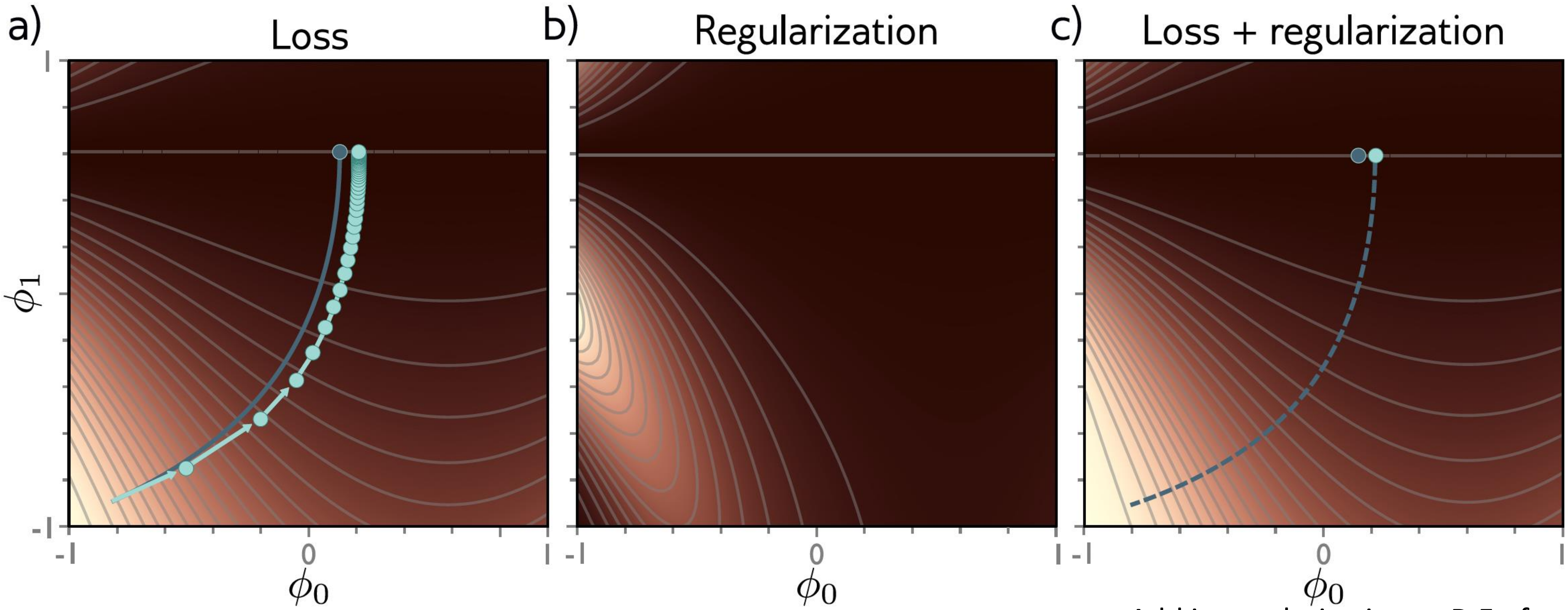
Regularization

- Explicit regularization
- Implicit regularization
- Early stopping
- Ensembling
- Dropout
- Adding noise
- Transfer learning, multi-task learning, self-supervised learning
- Data augmentation

Implicit regularization

Going to infinitesimal (continuous) step, change in ϕ governed by:

$$\frac{\partial \phi}{\partial t} = -\frac{\partial L}{\partial \phi}$$



Gradient descent approximates a differential equation (infinitesimal step size)

Approximate implicit regularization added to continuous gradient descent

Add in regularization to D.E of $\sim\left\|{}^{\partial L}/_{\partial \phi}\right\|^2$ and differential equation converges to same place

See derivation at end of UDL Ch. 9

Implicit regularization

- Gradient descent disfavors areas where gradients are steep

$$\tilde{\mathrm{L}}_{GD}[\phi] = \mathrm{L}[\phi] + \frac{\alpha}{4}\left\|\frac{\partial L}{\partial \phi}\right\|^2$$

See derivation at end of UDL Ch. 9

Implicit regularization

- Gradient descent disfavors areas where gradients are steep

$$\tilde{\mathrm{L}}_{GD}[\boldsymbol{\phi}] = \mathrm{L}[\boldsymbol{\phi}] + \frac{\alpha}{4}\left\|\frac{\partial L}{\partial \boldsymbol{\phi}}\right\|^2$$

- SGD likes all batches to have similar gradients

$$\begin{aligned}\tilde{\mathrm{L}}_{SGD}[\boldsymbol{\phi}] &= \tilde{\mathrm{L}}_{GD}[\boldsymbol{\phi}] + \frac{\alpha}{4B}\sum_{b=1}^{B}\left\|\frac{\partial L_b}{\partial \boldsymbol{\phi}} - \frac{\partial L}{\partial \boldsymbol{\phi}}\right\|^2 \\ &= \mathrm{L}[\boldsymbol{\phi}] + \frac{\alpha}{4}\left\|\frac{\partial L}{\partial \boldsymbol{\phi}}\right\|^2 + \underbrace{\frac{\alpha}{4B}\sum_{b=1}^{B}\left\|\frac{\partial L_b}{\partial \boldsymbol{\phi}} - \frac{\partial L}{\partial \boldsymbol{\phi}}\right\|^2}\end{aligned}$$

Want the batch variance to be small, rather than some batches fitting well and others not well…

Where $L = \frac{1}{I}\sum_{i=1}^{I}\ell_i[\mathbf{x}_i, y_i]$ and $L_b = \frac{1}{|\mathcal{B}|}\sum_{i\in\mathcal{B}_b}\ell_i[\mathbf{x}_i, y_i]$.

Implicit regularization

- Gradient descent disfavors areas where gradients are steep

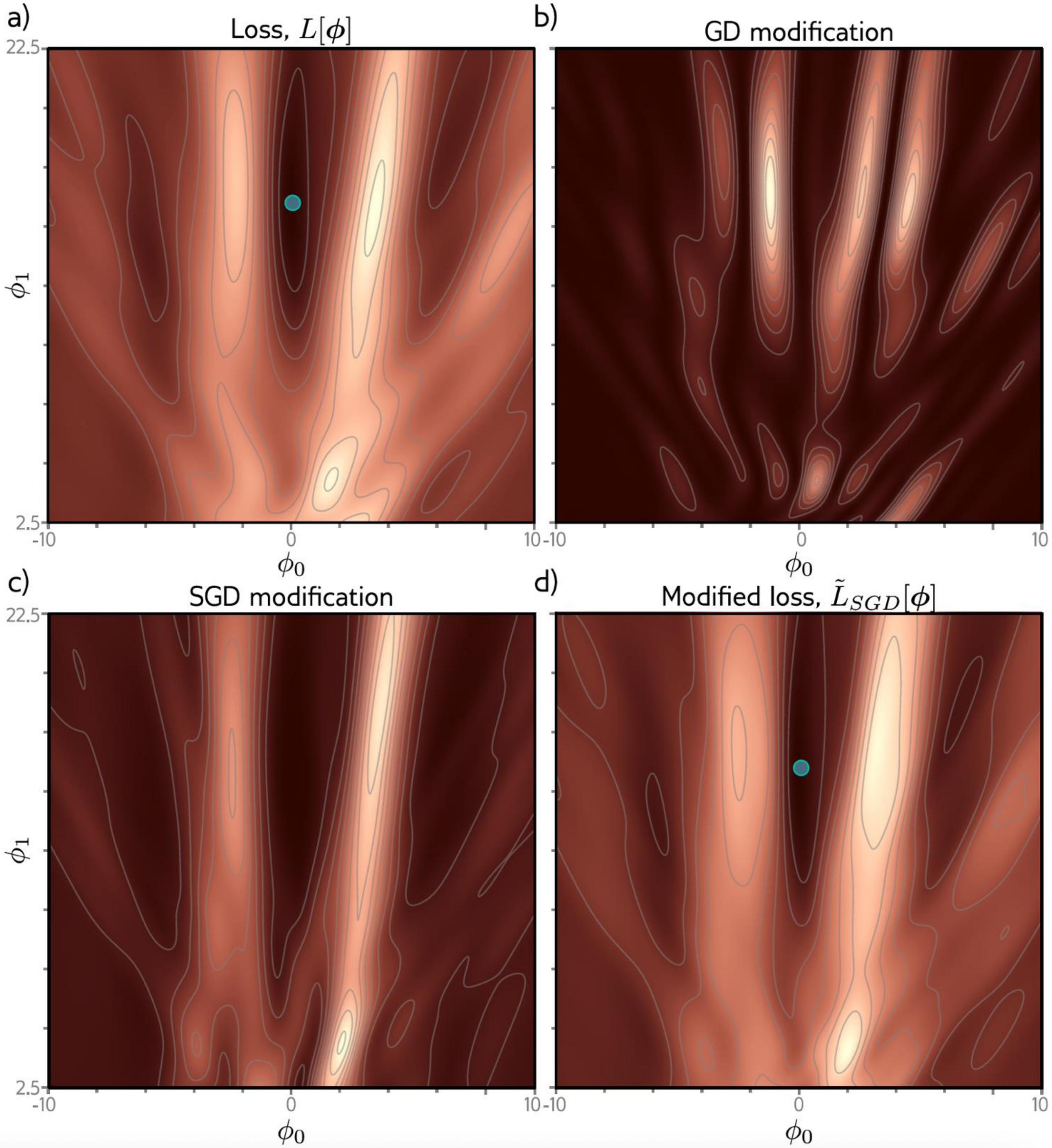
$$\tilde{\mathrm{L}}_{GD}[\boldsymbol{\phi}] = \mathrm{L}[\boldsymbol{\phi}] + \frac{\alpha}{4}\left\|\frac{\partial L}{\partial \boldsymbol{\phi}}\right\|^2$$

- SGD likes all batches to have similar gradients

$$\begin{aligned}\tilde{\mathrm{L}}_{SGD}[\boldsymbol{\phi}] &= \tilde{\mathrm{L}}_{GD}[\boldsymbol{\phi}] + \frac{\alpha}{4B}\sum_{b=1}^{B}\left\|\frac{\partial L_b}{\partial \boldsymbol{\phi}} - \frac{\partial L}{\partial \boldsymbol{\phi}}\right\|^2 \\ &= \mathrm{L}[\boldsymbol{\phi}] + \frac{\alpha}{4}\left\|\frac{\partial L}{\partial \boldsymbol{\phi}}\right\|^2 + \frac{\alpha}{4B}\sum_{b=1}^{B}\left\|\frac{\partial L_b}{\partial \boldsymbol{\phi}} - \frac{\partial L}{\partial \boldsymbol{\phi}}\right\|^2\end{aligned}$$

- Depends on learning rate – perhaps why larger learning rates generalize better.

Original Gabor Model Loss

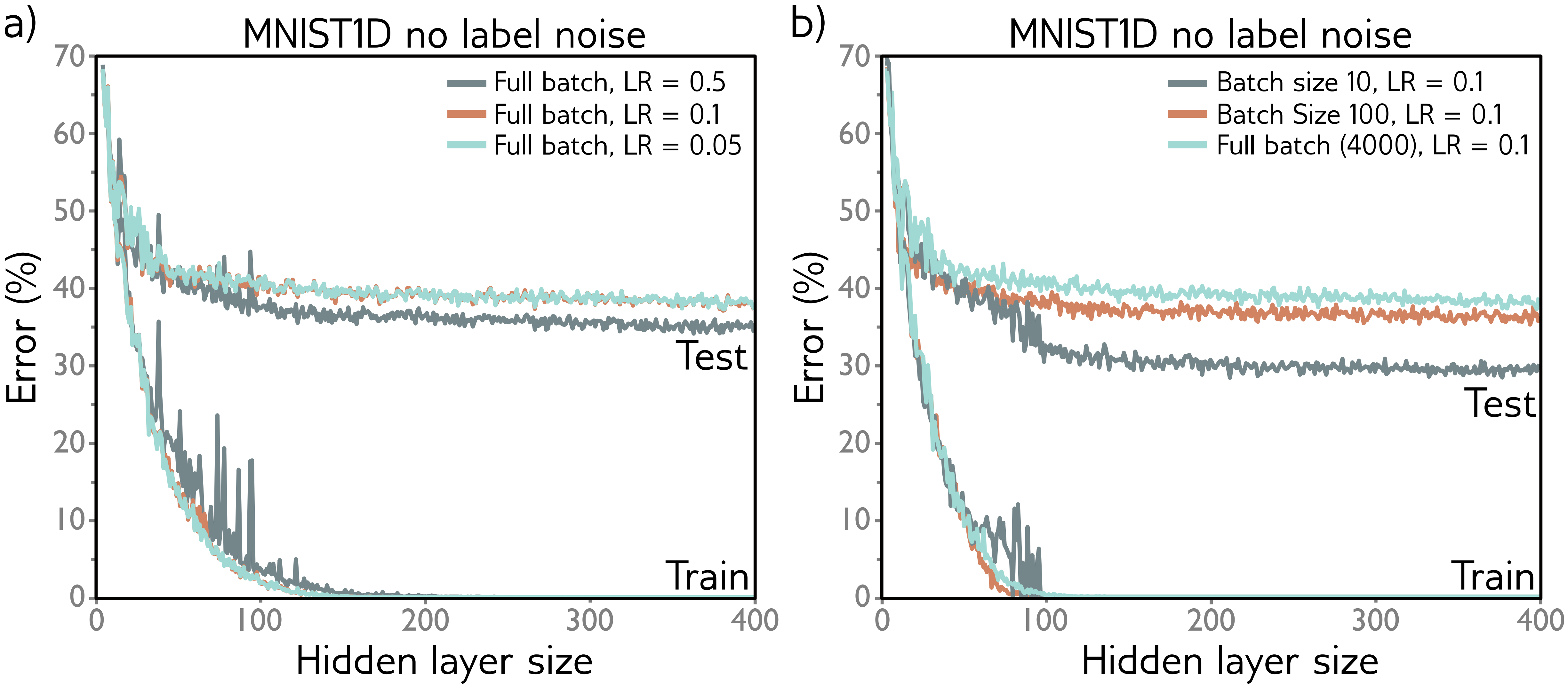


$$\frac{\alpha}{4}\left\|\frac{\partial L}{\partial \phi}\right\|^2$$

$$\frac{\alpha}{4B}\sum_{b=1}^{B}\left\|\frac{\partial L_b}{\partial \phi}-\frac{\partial L}{\partial \phi}\right\|^2$$

$$\tilde{\mathrm{L}}_{SGD}[\phi]$$

$$= \mathrm{L}[\phi] + \frac{\alpha}{4}\left\|\frac{\partial L}{\partial \phi}\right\|^2 + \frac{\alpha}{4B}\sum_{b=1}^{B}\left\|\frac{\partial L_b}{\partial \phi}-\frac{\partial L}{\partial \phi}\right\|^2$$



Generally, performance is

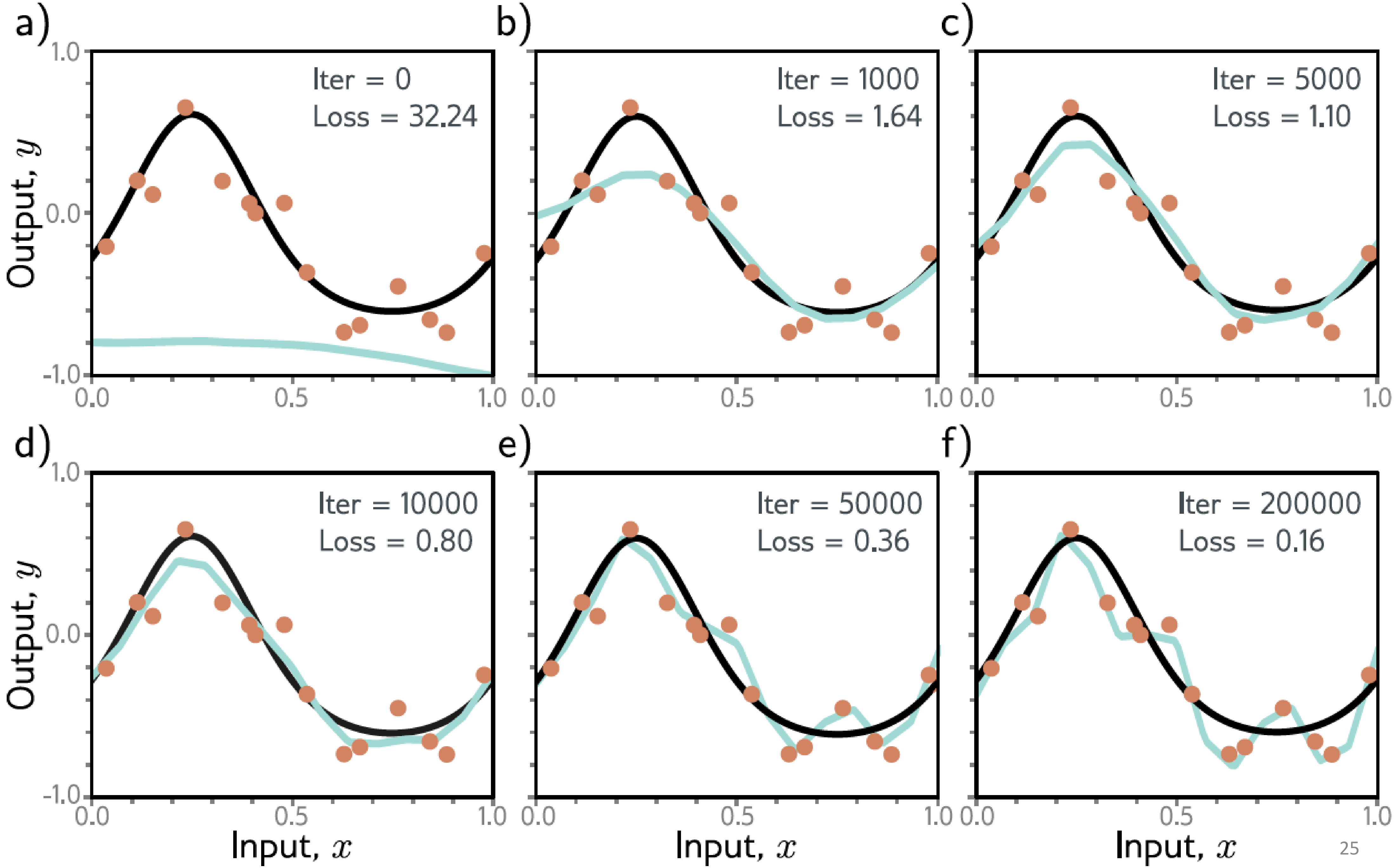
- best for larger learning rates
- best with smaller batches

Regularization

- Explicit regularization
- Implicit regularization
- Early stopping
- Ensembling
- Dropout
- Adding noise
- Transfer learning, multi-task learning, self-supervised learning
- Data augmentation

Early stopping

- If we stop training early, weights don’t have time to overfit to noise
- Weights start small, don’t have time to get large
- Reduces effective model complexity
- Known as early stopping
- Don’t have to re-train with different hyper-parameters – just ”checkpoint” regularly and pick the model with lowest validation loss

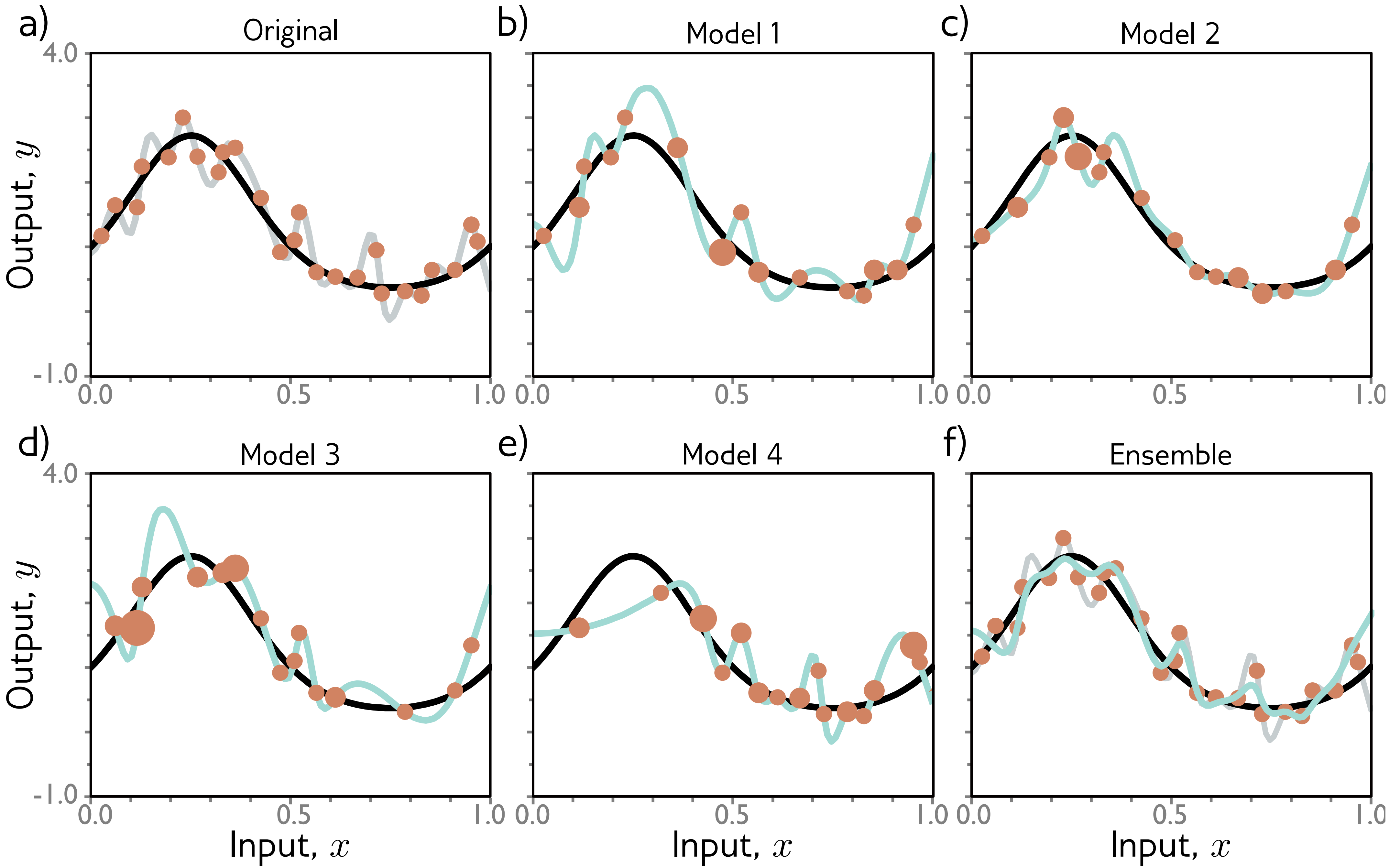

a)
Iter = 0
Loss = 32.24
b)
Iter = 1000
Loss = 1.64
c)
Iter = 5000
Loss = 1.10
d)
Iter = 10000
Loss = 0.80
e)
Iter = 50000
Loss = 0.36
f)
Iter = 200000
Loss = 0.16
Output, y
Input, x
1.0
0.0
-1.0
0.0
0.5
1.0

Regularization

- Explicit regularization
- Implicit regularization
- Early stopping
- Ensembling
- Dropout
- Adding noise
- Transfer learning, multi-task learning, self-supervised learning
- Data augmentation

Ensembling

- Average together several models – an ensemble
- Can take mean or median
  - Before softmax for classification
- Simply different initializations or even different models
- Or train with different subsets of the data resampled with replacements -- bagging

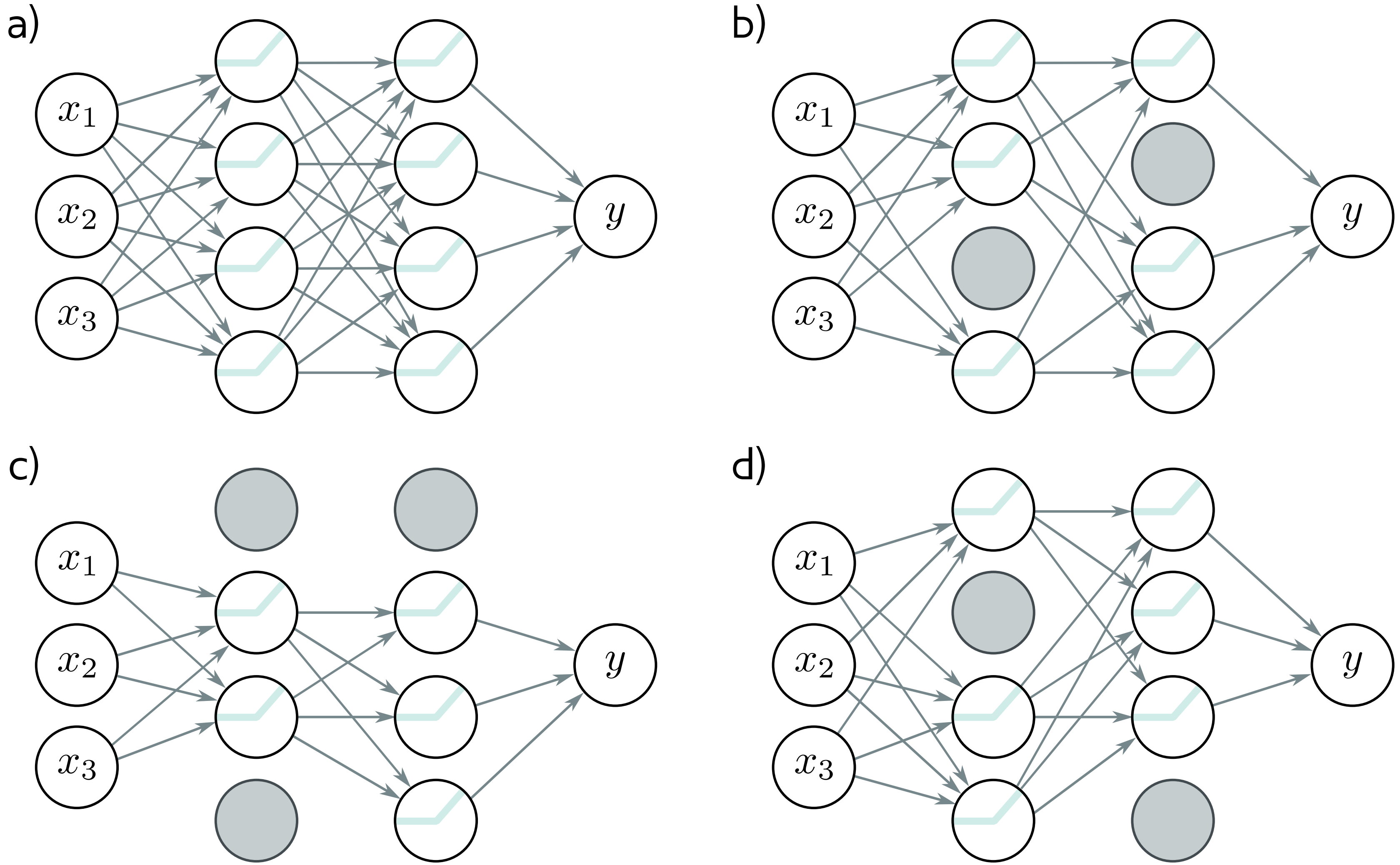

a)
Original
b)
Model 1
c)
Model 2
d)
Model 3
e)
Model 4
f)
Ensemble
4.0
-1.0
0.0
0.5
1.0
Output, y
Input, x

Regularization

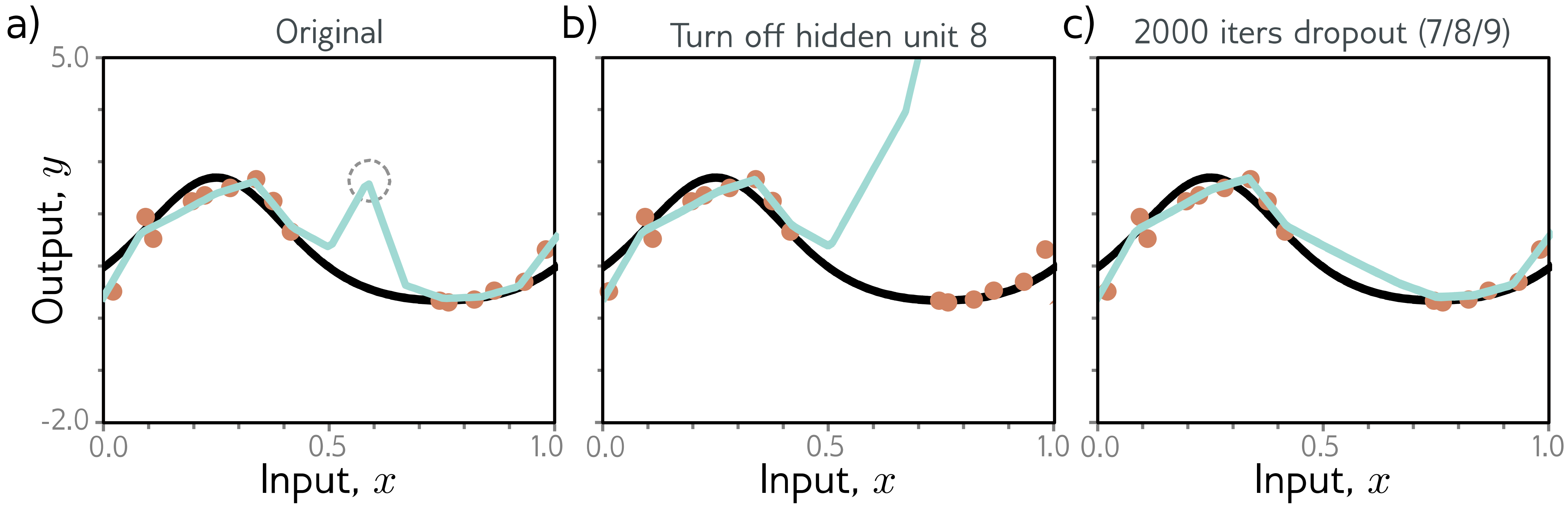
- Explicit regularization
- Implicit regularization
- Early stopping
- Ensembling
- Dropout
- Adding noise
- Transfer learning, multi-task learning, self-supervised learning
- Data augmentation

Dropout

Randomly clamp ~50% of hidden units to 0 on each iteration.



Dropout

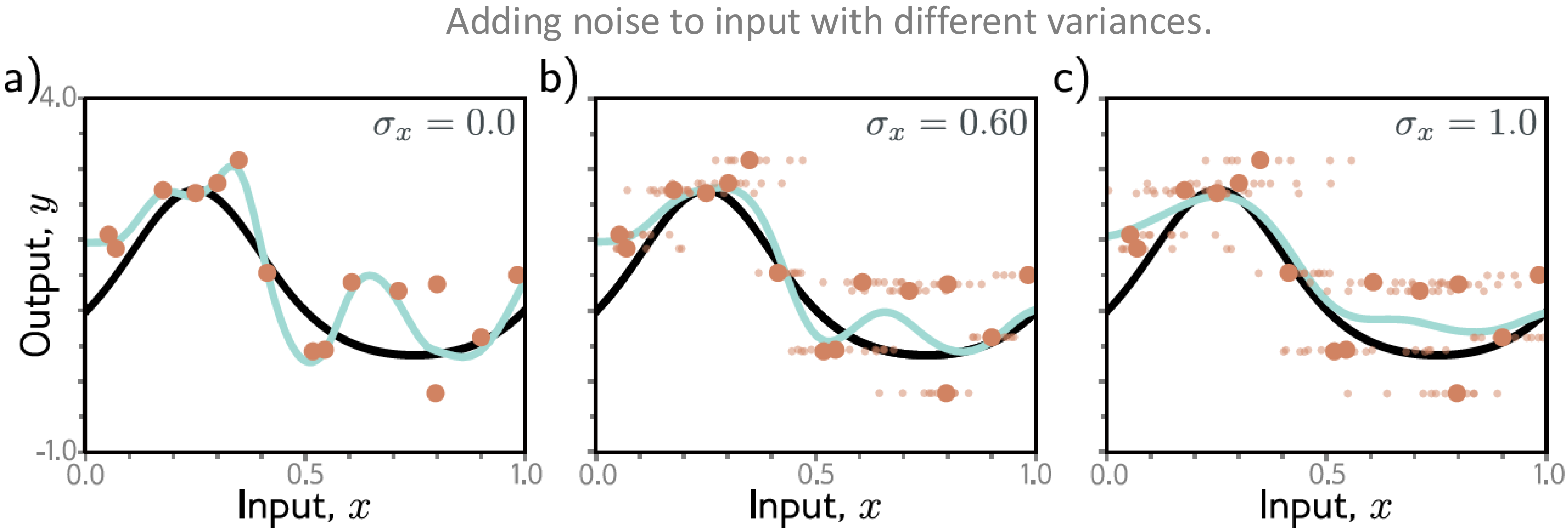


- Makes the network less dependent on any given hidden unit.
- Prevents situations where subsequent hidden units correct for excessive swings from earlier hidden units
- Can eliminate kinks in function that are far from data and don't contribute to training loss
- Must use *weight scaling inference rule* – multiple weights by (1 – dropout probability)

Regularization

- Explicit regularization
- Implicit regularization
- Early stopping
- Ensembling
- Dropout
- Adding noise
- Transfer learning, multi-task learning, self-supervised learning
- Data augmentation

Adding noise



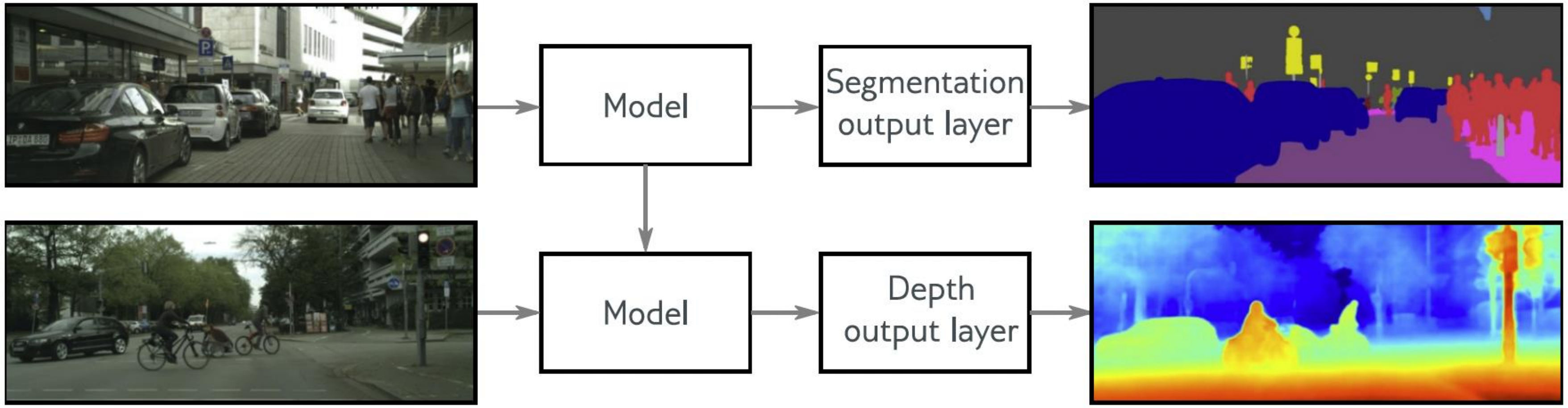
- to inputs – induces weight regularization (see Exercise 9.3 in UDL)
- to weights – makes robust to small weight perturbations
- to outputs (labels) – reduces “overconfident” probability for target class

Regularization

- Explicit regularization
- Implicit regularization
- Early stopping
- Ensembling
- Dropout
- Adding noise
- Transfer learning, multi-task learning, self-supervised learning
- Data augmentation

Transfer Learning

(1) Train the model for segmentation



Assume we have lots of segmentation training data

Assume we limited depth training data

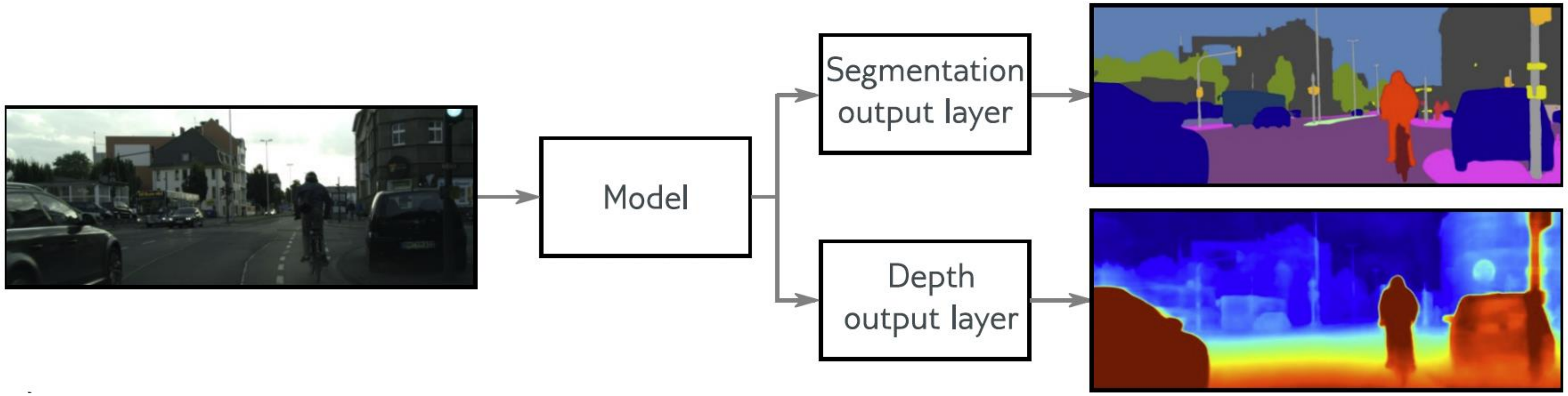
(2) Replace the final layers to match the new task and

(3) Either:

a) Freeze the rest of the layers and train the final layers

b) Fine tune the entire model

Multi-Task Learning



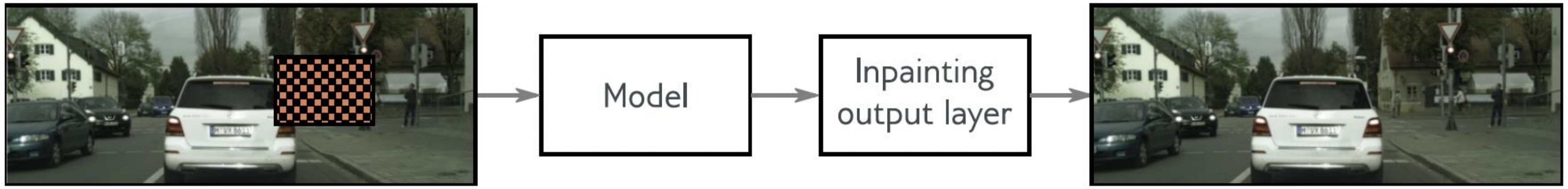
- Train the model for 2 or more tasks simultaneously
  - Weighted combo of loss fncs

$$L_{total} = \alpha \cdot L_{segmentaiton} + \beta \cdot L_{depth}$$

- Less likely to overfit to training data of one task

- Can be harder to get training to converge. Might have to vary the individual task loss weightings, α and β.

Self-Supervised Learning



The animal didn’t cross the because it was too tired.

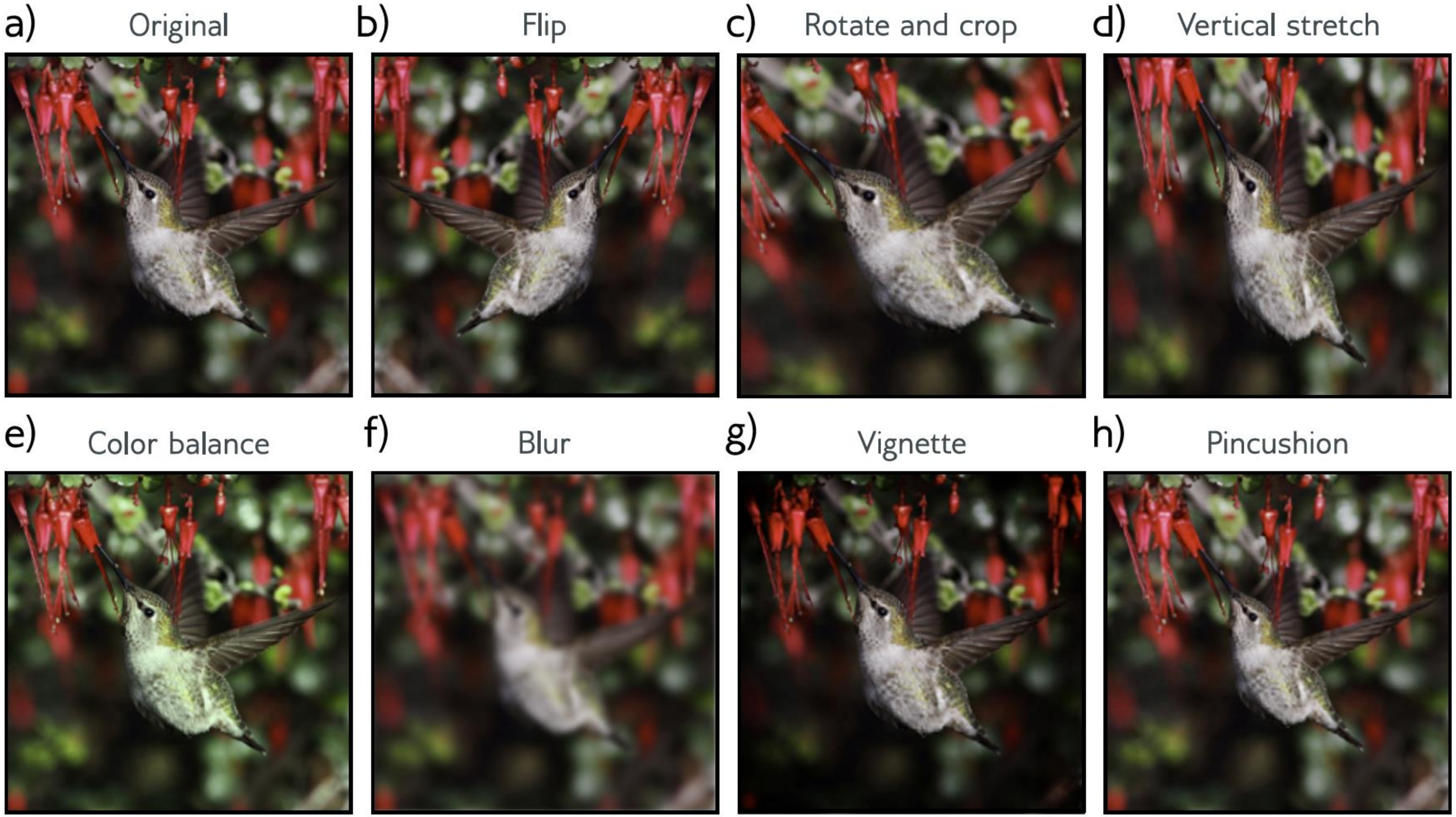
- Mask out part of the training data
- Train model to try to infer missing data
  - masked data is the target
- ➔ Model learns characteristics of the data

- Then apply transfer learning

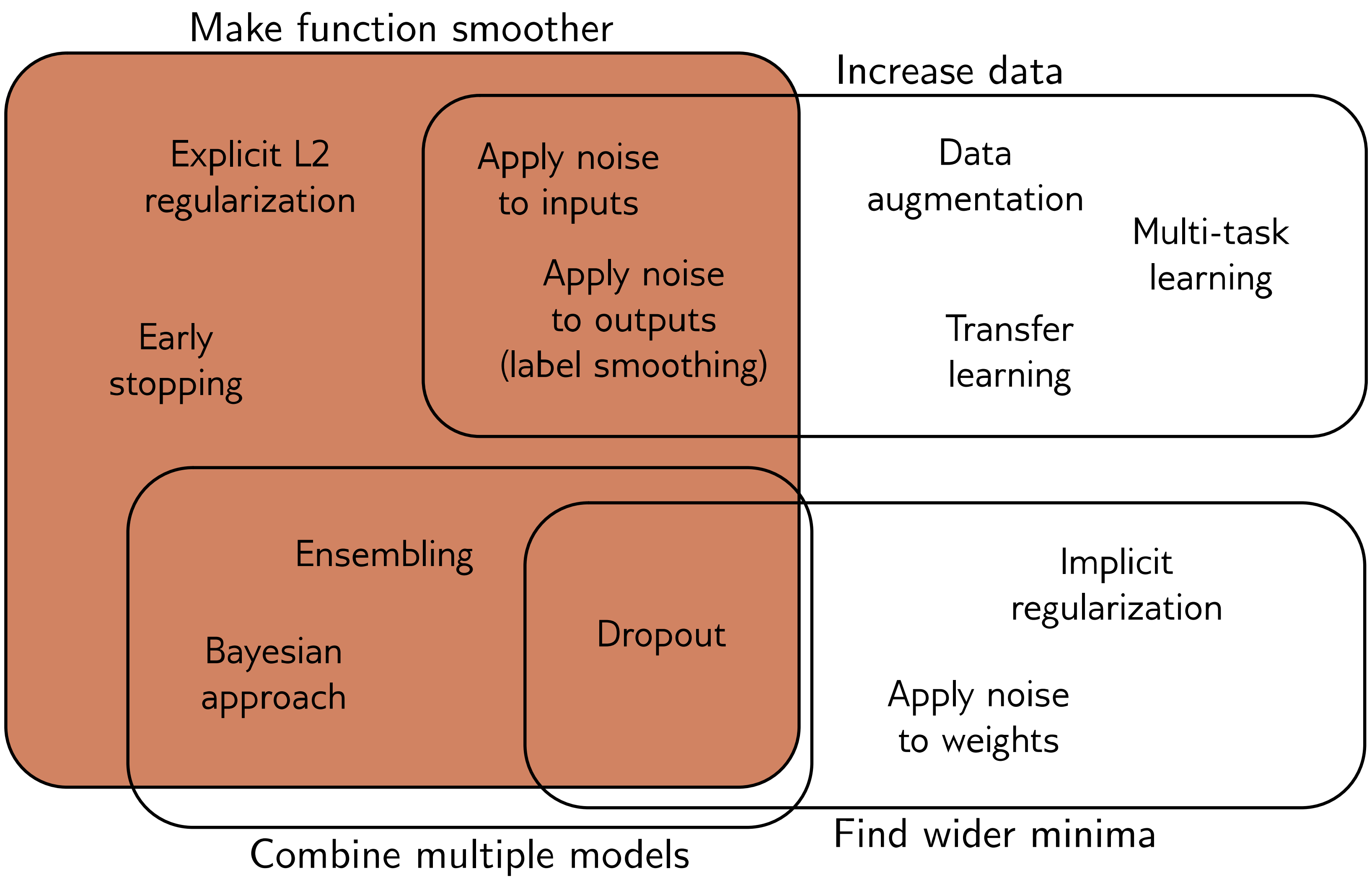
Regularization

- Explicit regularization
- Implicit regularization
- Early stopping
- Ensembling
- Dropout
- Adding noise
- Transfer learning, multi-task learning, self-supervised learning
- Data augmentation

Data augmentation



Regularization overview



Feedback?

Link