Using Deep Learning When Class Labels Have A Natural Order

Predicting Ratings And Rankings Using PyTorch Lightning

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https://lightning.ai

SciPy2022

Scientific Computing with Python

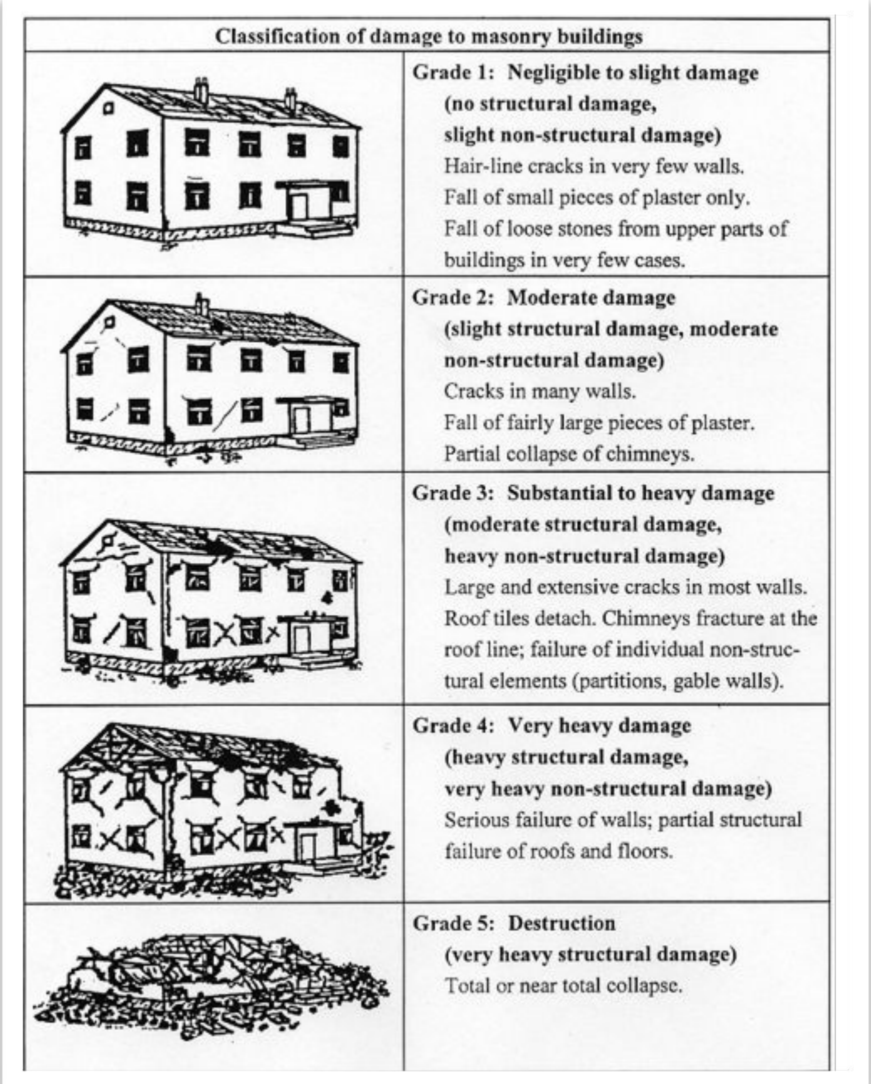
Austin, TX • July 11 - July 17

Code & slides

https://github.com/rasbt/scipy2022-talk

Many real-world predictions problems have ordered labels

Damage assessment


Classification of damage to masonry buildings

Grade 1: Negligible to slight damage
(no structural damage, slight non-structural damage)
Hair-line cracks in very few walls.
Fall of small pieces of plaster only.
Fall of loose stones from upper parts of buildings in very few cases.

Grade 2: Moderate damage
(slight structural damage, moderate non-structural damage)
Cracks in many walls.
Fall of fairly large pieces of plaster.
Partial collapse of chimneys.

Grade 3: Substantial to heavy damage
(moderate structural damage, heavy non-structural damage)
Large and extensive cracks in most walls.
Roof tiles detach. Chimneys fracture at the roof line; failure of individual non-structural elements (partitions, gable walls).

Grade 4: Very heavy damage
(heavy structural damage, very heavy non-structural damage)
Serious failure of walls; partial structural failure of roofs and floors.

Grade 5: Destruction
(very heavy structural damage)
Total or near total collapse.

https://emergency.copernicus.eu/mapping/ems/damage-assessment

Plant disease

Index	Reaction	PLRV
0	Highly Resistance	No visible symptoms.
1	Resistance	Rolling of leaves in case of primary infection and lower leaves in case of secondary infection, erect growth
2	Moderately Resistance	Rolling of leaves extending, leaves become stiff and leathery, stunting of plants and erect growth
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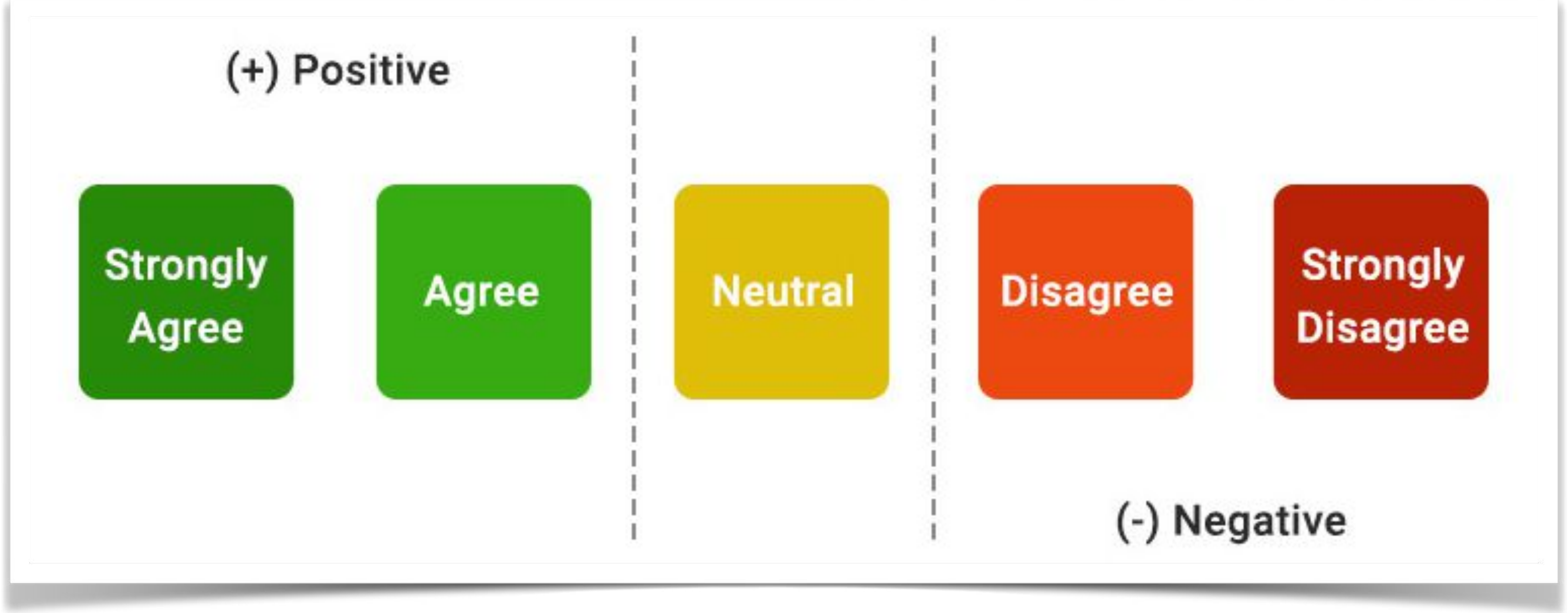
Islam, M. U., et al. "Screening of potato germplasm against RNA viruses and their identification through ELISA." J Green Physiol Genet Genom 1 (2015): 22-31.

Credit risk rating

PASS					SPECIAL MENTION	SUB-STANDARD	DOUBTFUL	LOSS
1	2	3	4	5	6	7	8	9
Largely risk free	Minimal risk	Modest risk	Bankable	Addition-al review	Criticized	Classified	Classified	Classified

https://www.abrigo.com/blog/how-to-create-a-credit-risk-rating-system/

Likert scale for customer satisfaction



https://www.questionpro.com/blog/ordinal-scale/

Ordered labels? Tell me more!

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How do ordered (ordinal) labels differ from conventional class labels

Ordered labels? Tell me more!

Classification



Setosa Versicolor Virginica

No ordering

Ordered labels? Tell me more!

Classification



1 Setosa 2 Versicolor 3 Virginica

No ordering

Ordered labels? Tell me more!

Classification

1 Setosa 2 Versicolor 3 Virginica

No ordering

Regression

1 2 3

Ordered labels? Tell me more!

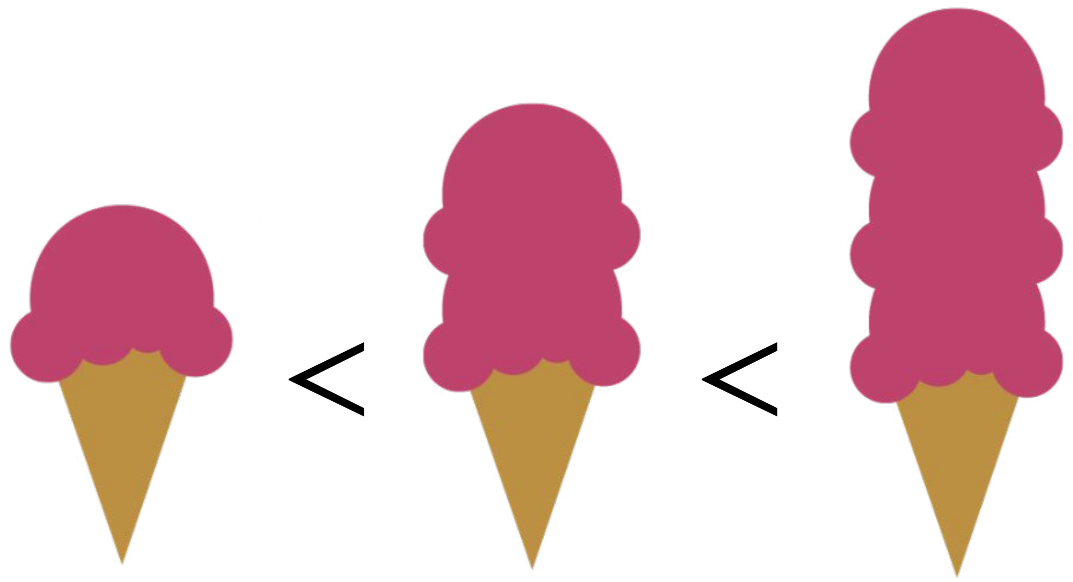
Classification



1 Setosa 2 Versicolor 3 Virginica

No ordering

Regression



1 2 3

Ordered labels? Tell me more!

Classification


1 Setosa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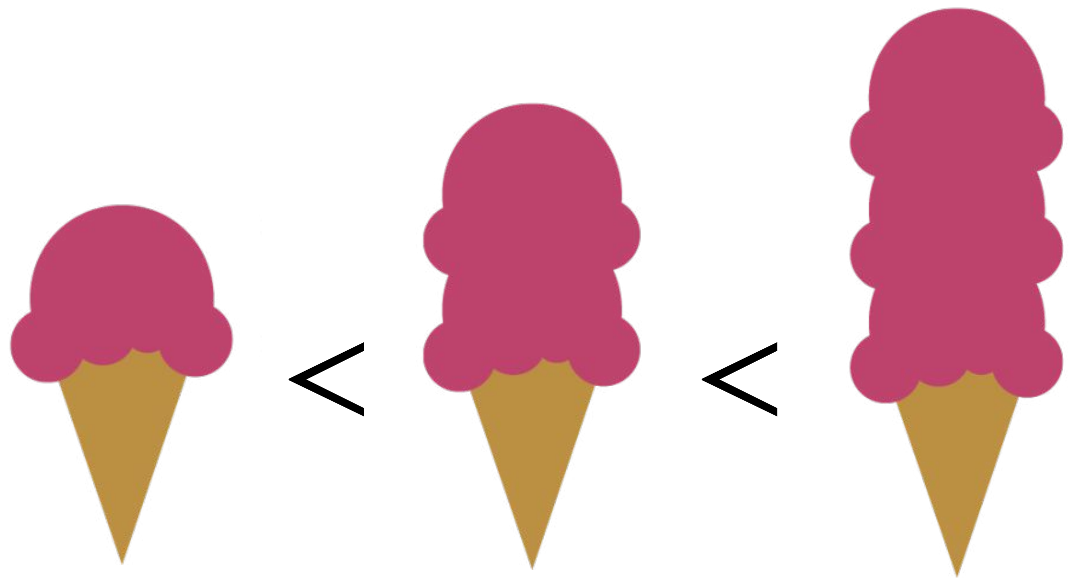
No ordering

Regression



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Identical distances

Ordered labels? Tell me more!

Classification

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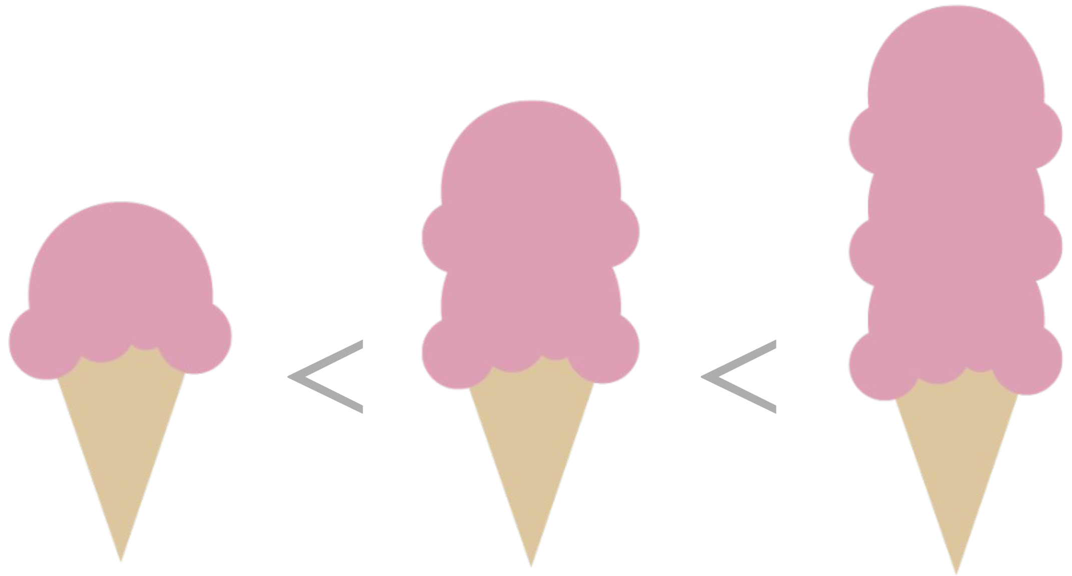
No ordering

Ordinal regression / ordinal classification

Regression



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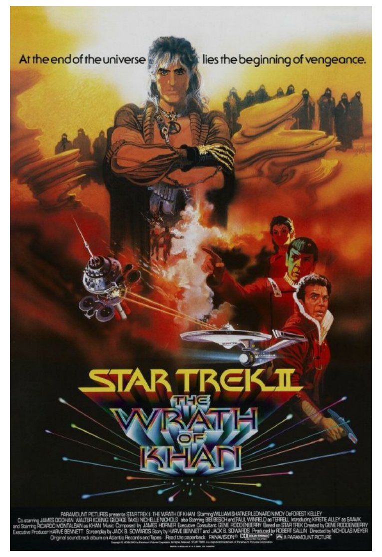
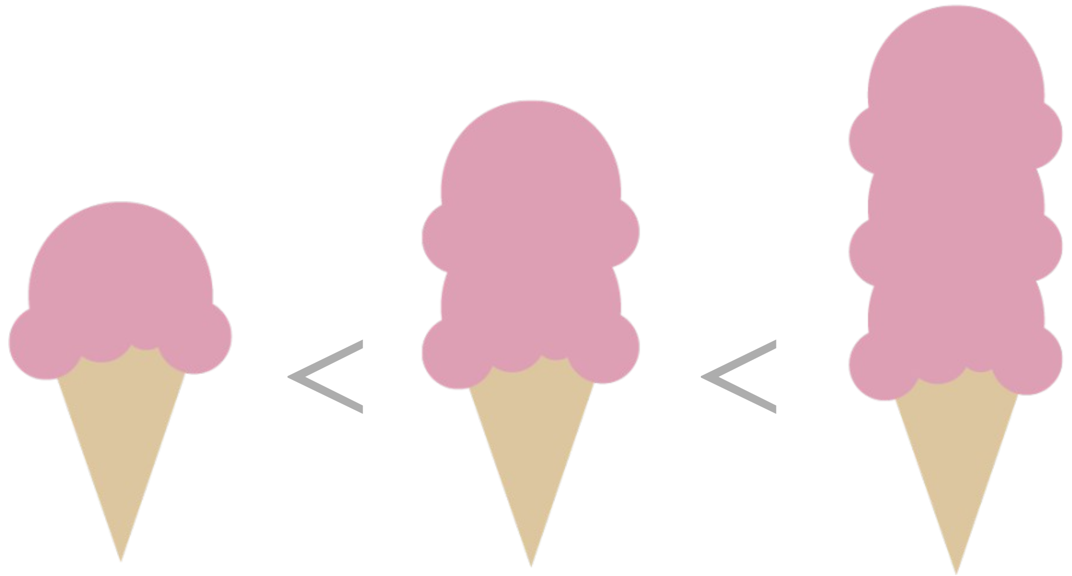


1  2  3 

Regression



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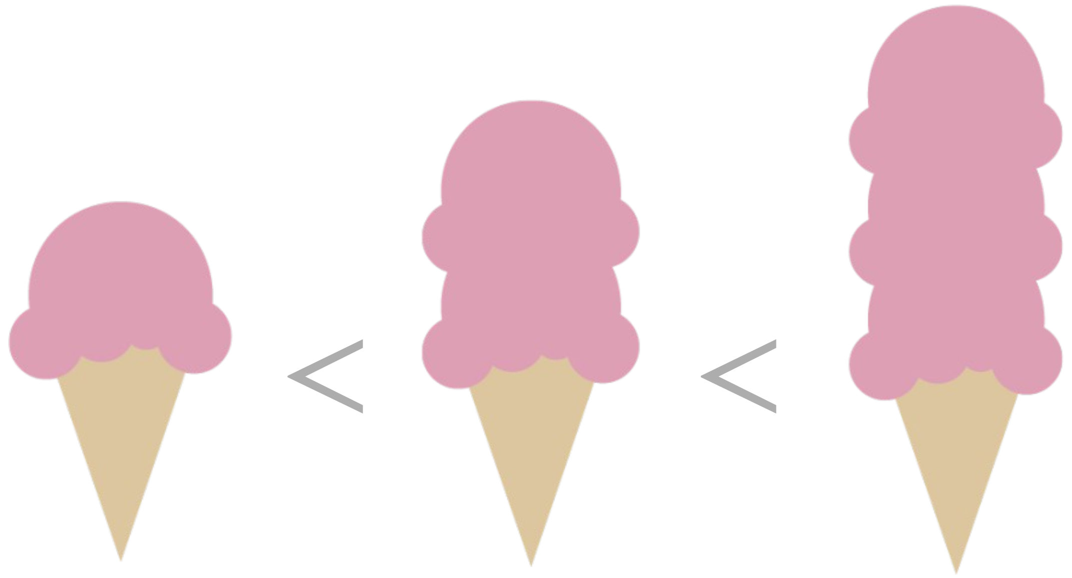

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Identical distances

Ordered labels? Tell me more!

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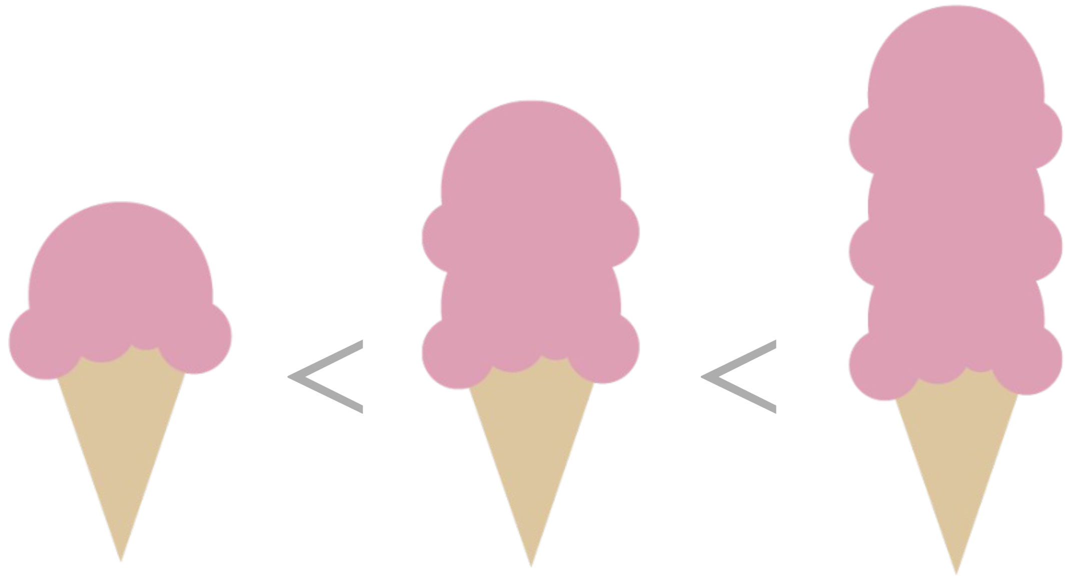
Ordinal regression / ordinal classification

$\prec$ $\prec$

1 2 3

Class labels
- but with ordering info
- and arbitrary distances

Regression



1 < 2 < 3

Identical distances

Can't we just use regular classifiers for ordered labels?

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Yes, but it is not ideal

It is not ideal because all wrong predictions look equally wrong to a classifier

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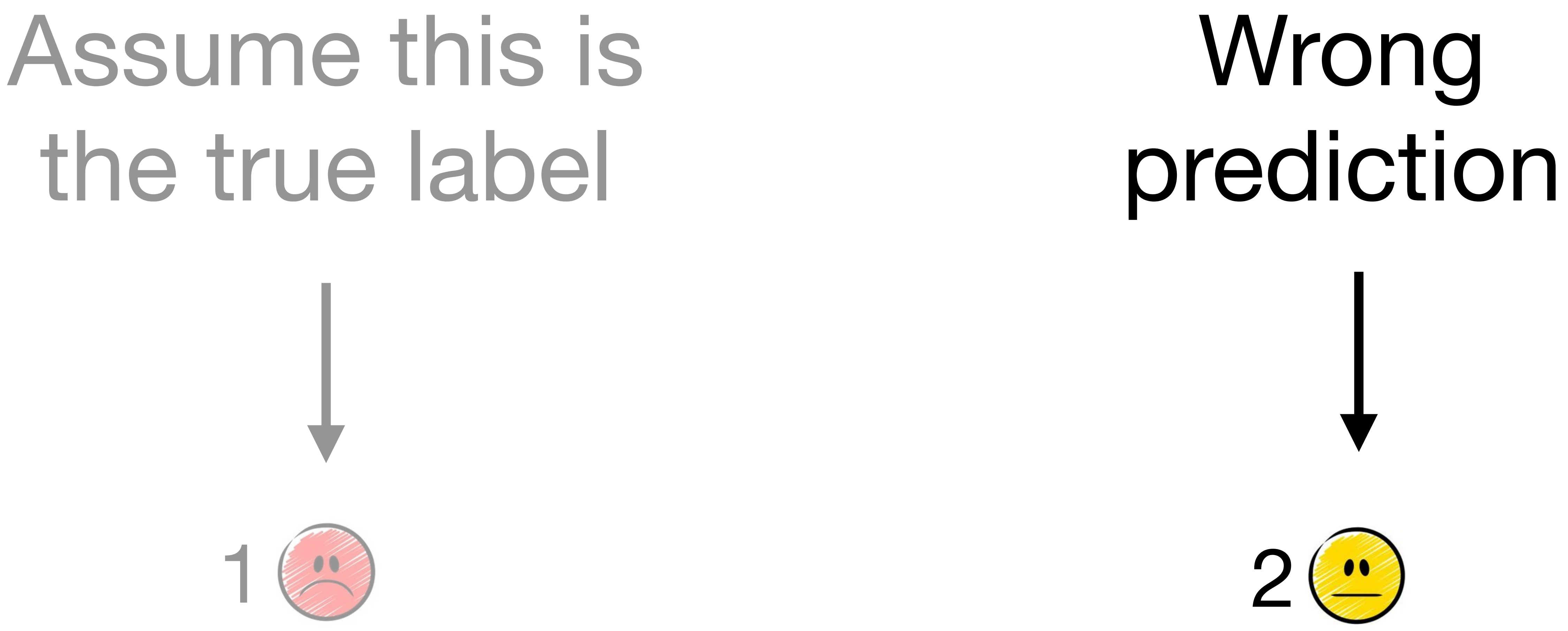
Assume this is the true label

1 

It is not ideal because all wrong predictions look equally wrong to a classifier



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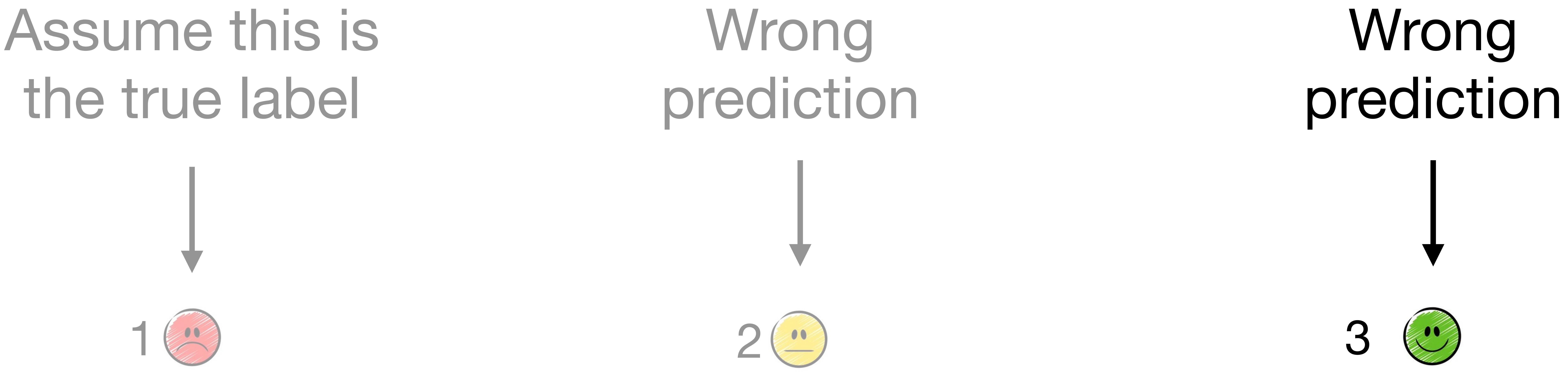

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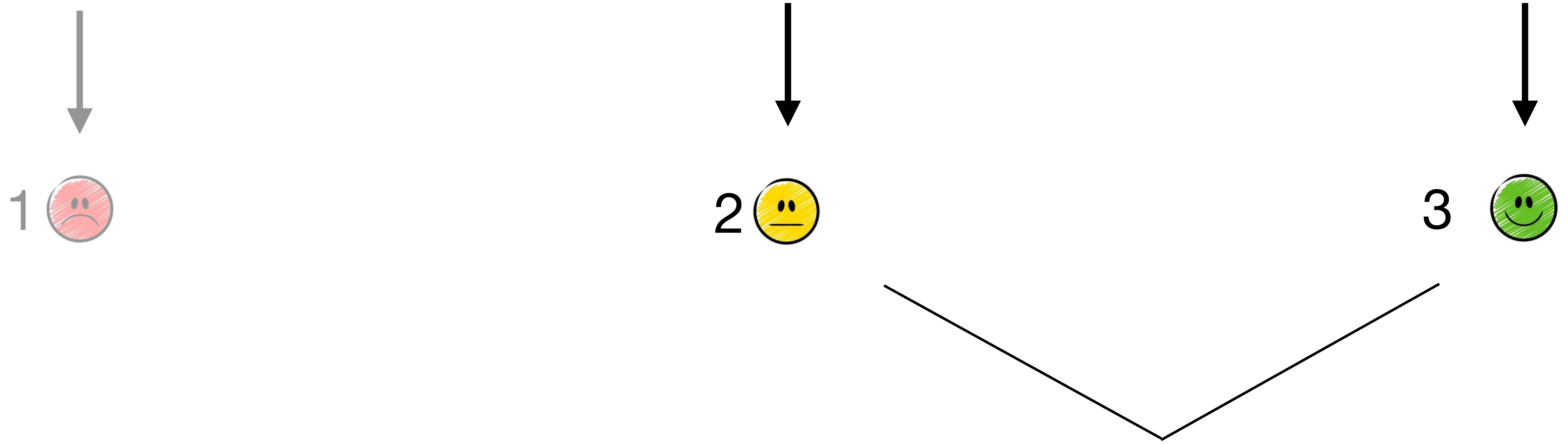
Wrong prediction

Wrong prediction



Treated equally if we compute the loss in a regular classifier

It is not ideal because all wrong predictions look equally wrong to a classifier

Assume this is the true label

1

Wrong prediction

2

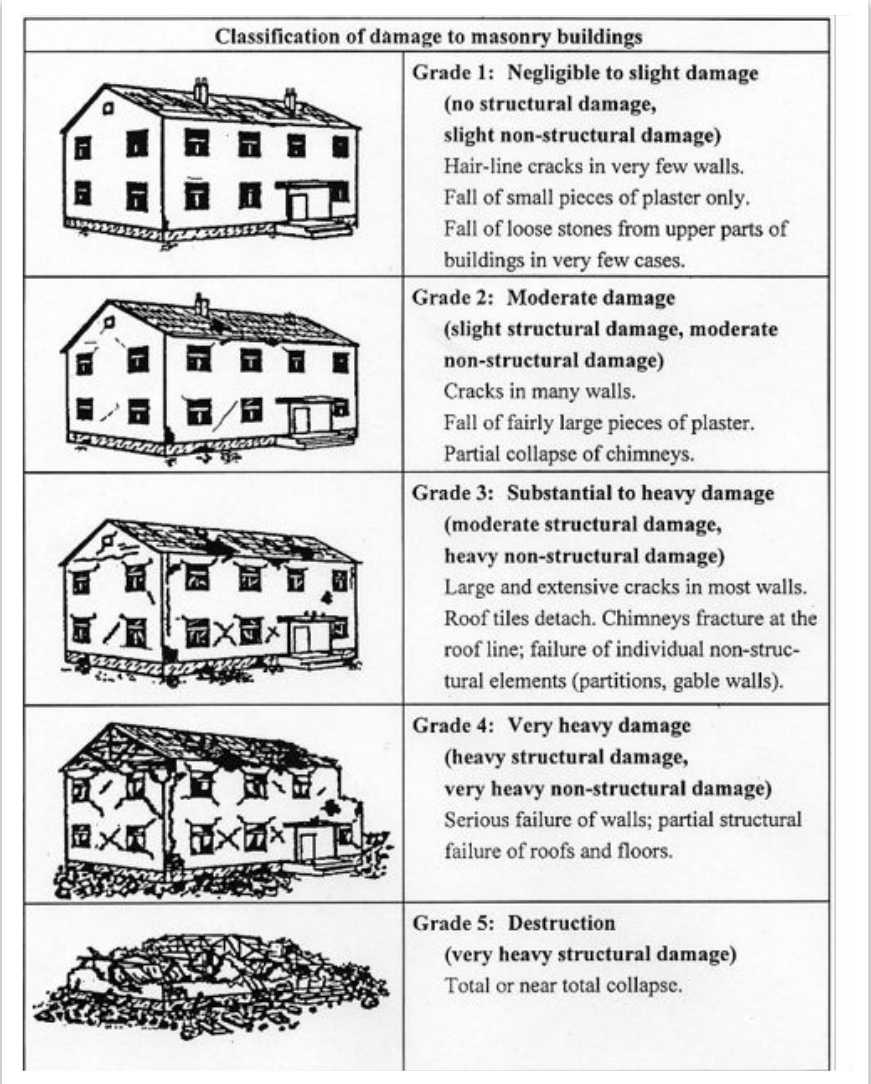
Wrong prediction

3

But this should be "more wrong"

Many real-world predictions problems have ordered labels

Damage assessment



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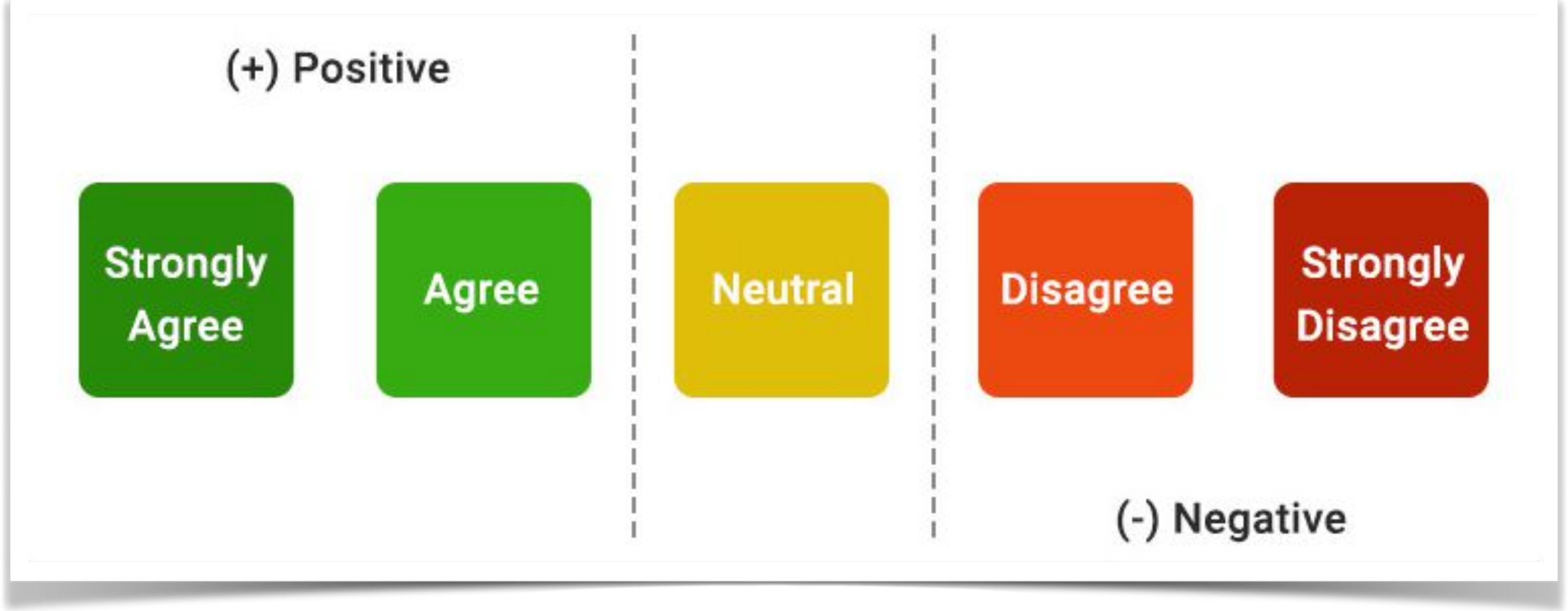

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Many real-world predictions problems have ordered labels

And we can get much better performance using ordinal regression models rather than regular classifiers

How? Let's (re)use what we already know:

An extended binary classification framework

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An extended binary classification framework

Input
(Aesthetics dataset)

Possible labels:
Rating 1, 2, 3, 4, 5

Niu Z, Zhou M, Wang L, Gao X, Hua G. Ordinal regression with multiple output CNN for age estimation. CVPR 2016

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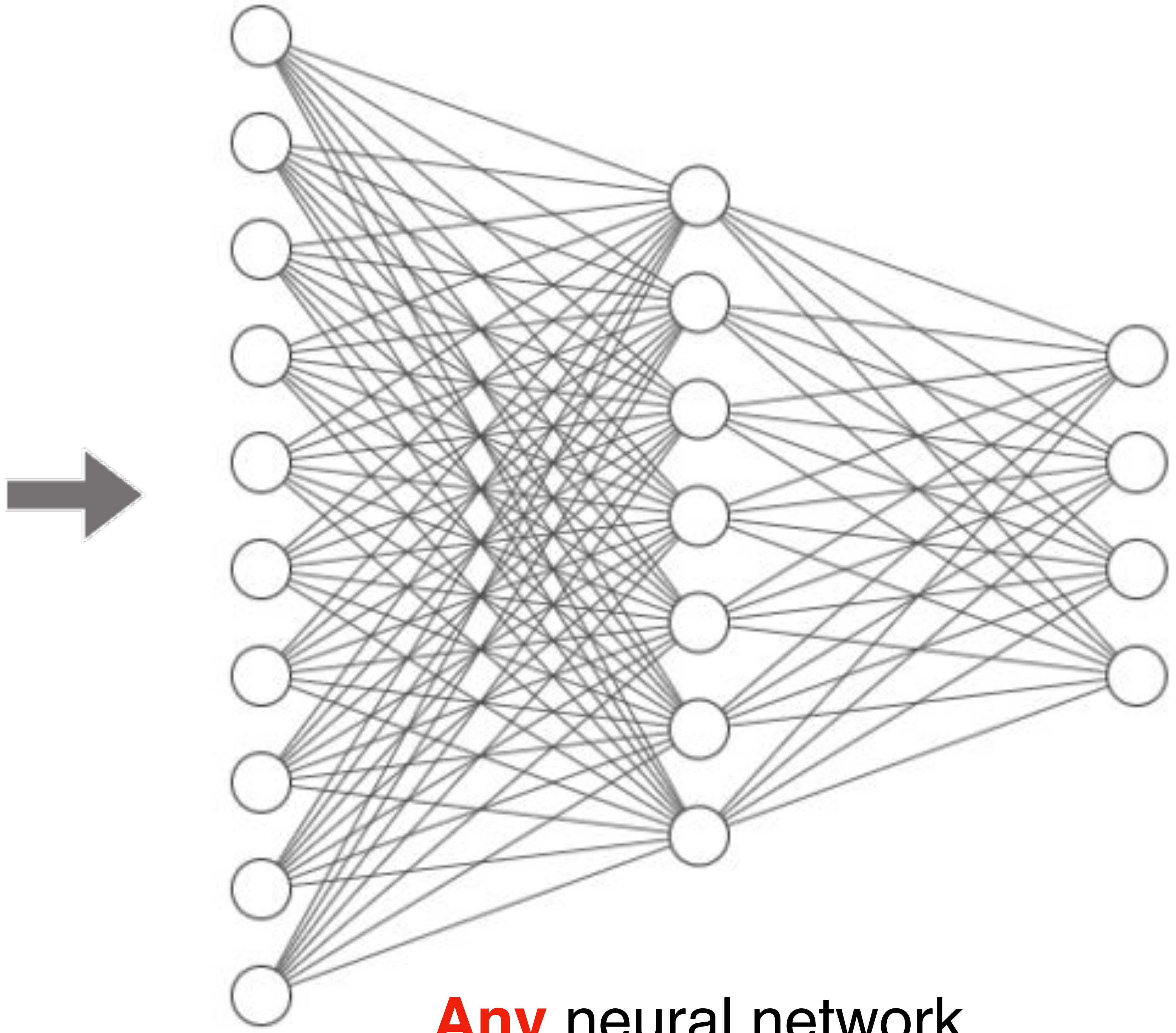

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Any neural network
(CNN, RNN, MLP, …)

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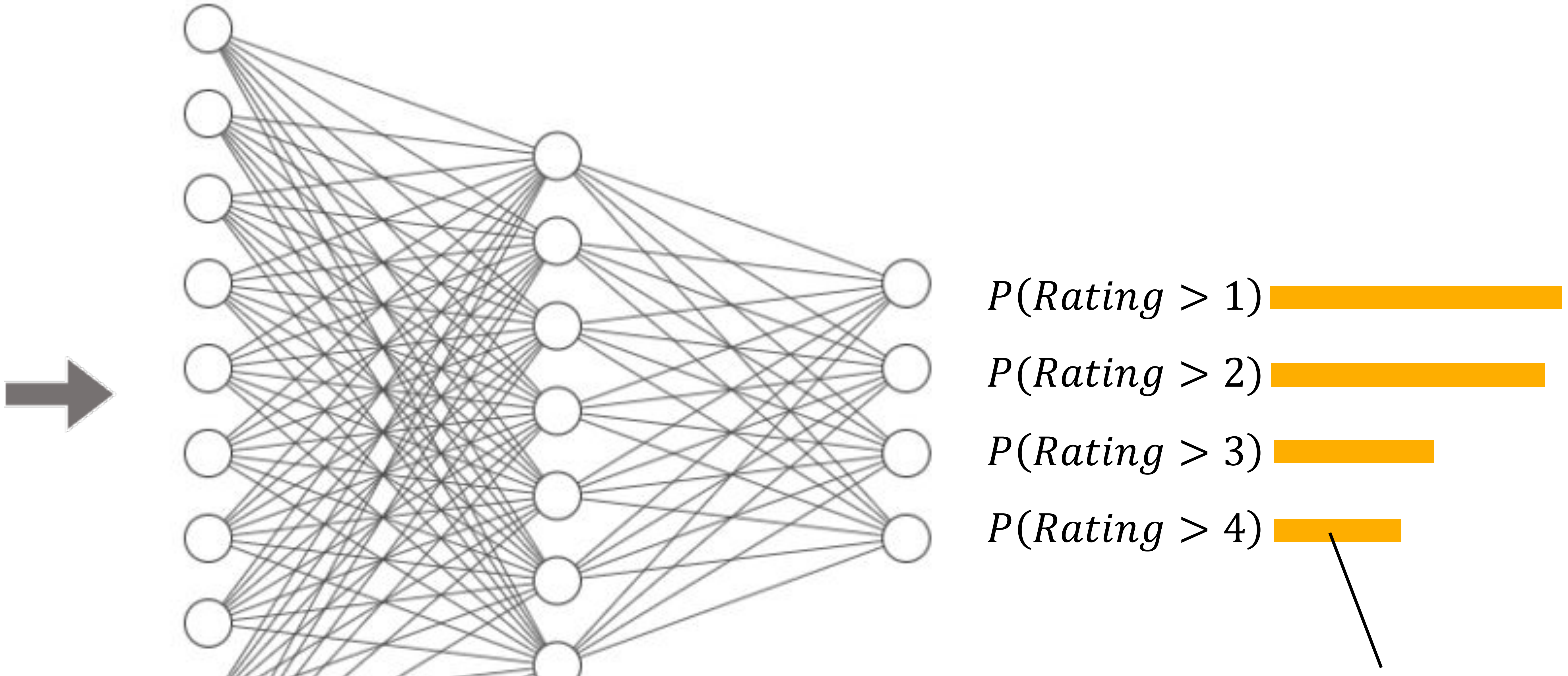

Score between 0 and 1

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(CNN, RNN, MLP, …)

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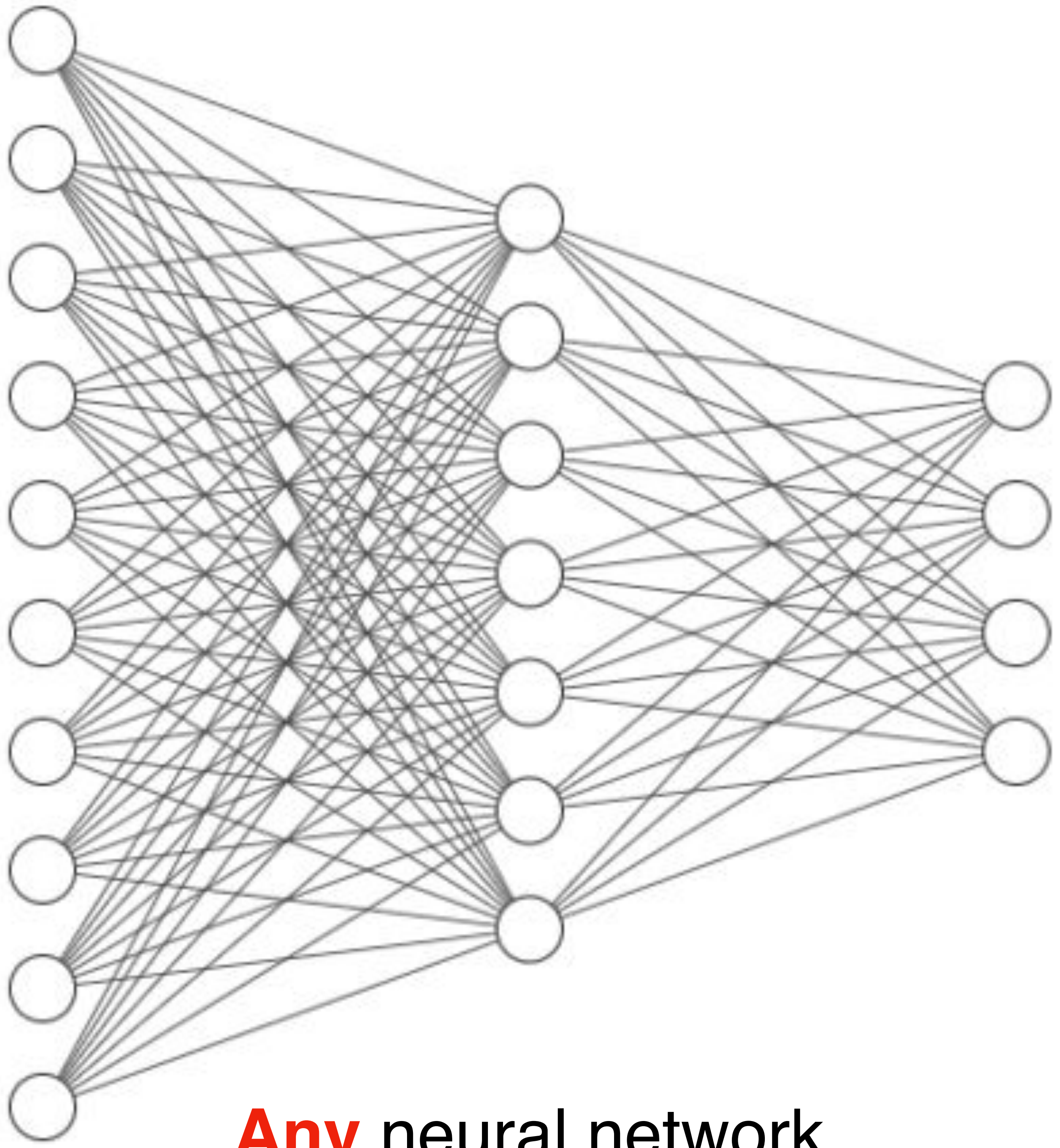
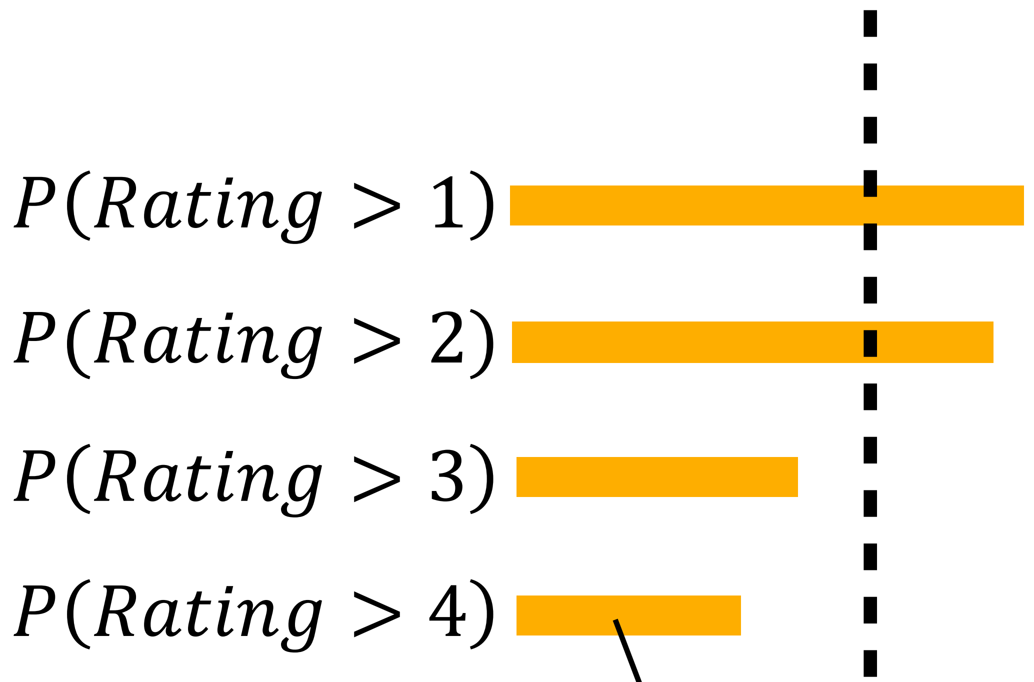


Any neural network
(CNN, RNN, MLP, …)

50% probability threshold



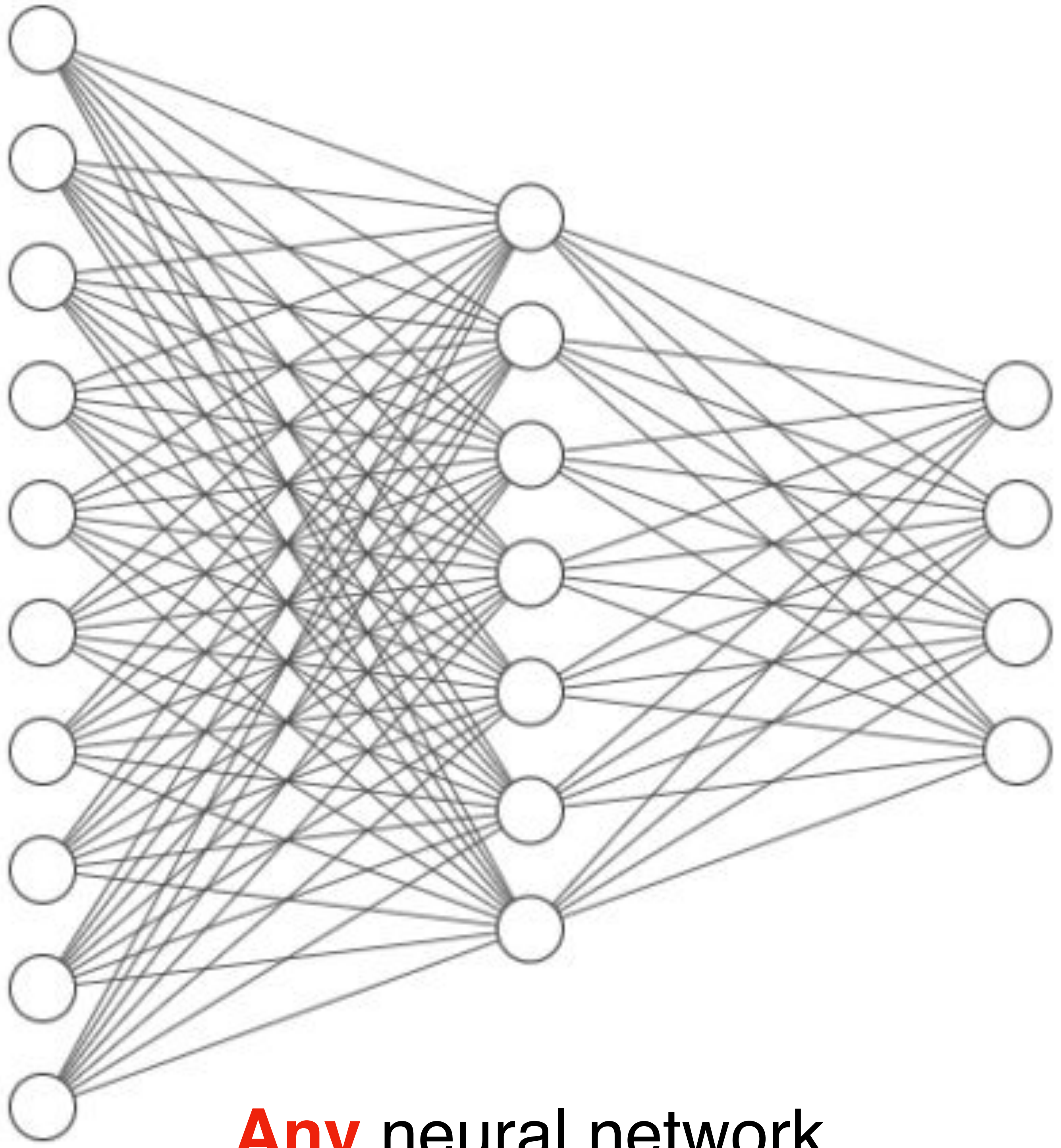
Rating > 1? → yes/no

Binary classification task

Score between 0 and 1

Input
(Aesthetics dataset)

Possible labels:
Rating 1, 2, 3, 4, 5



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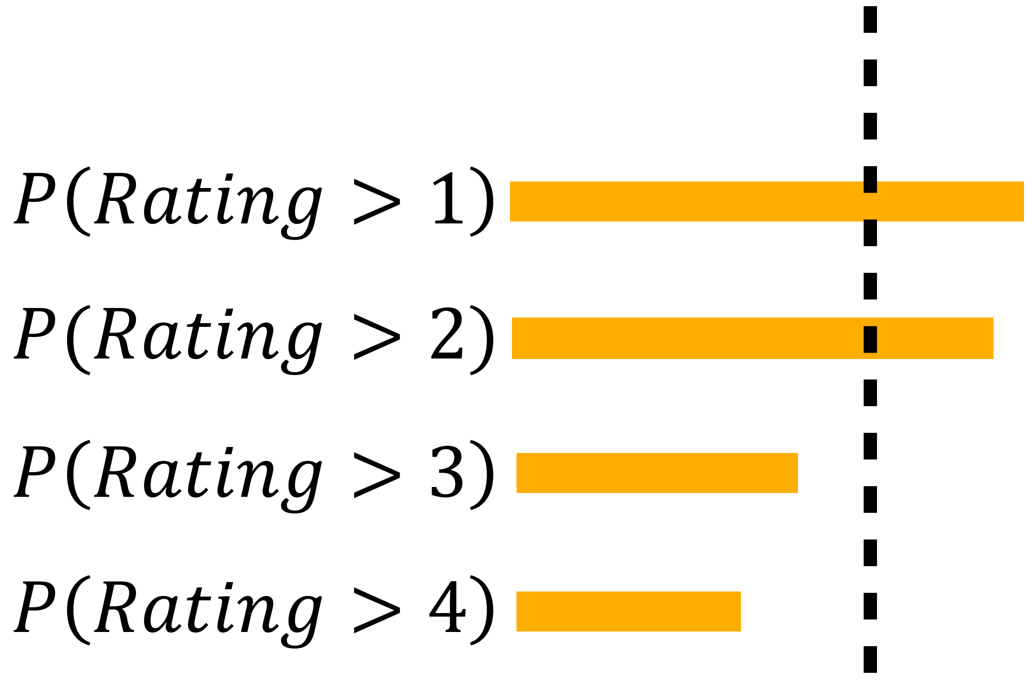


Rating > 1? → yes/no

Rating > 2? → yes/no

Rating > 3? → yes/no

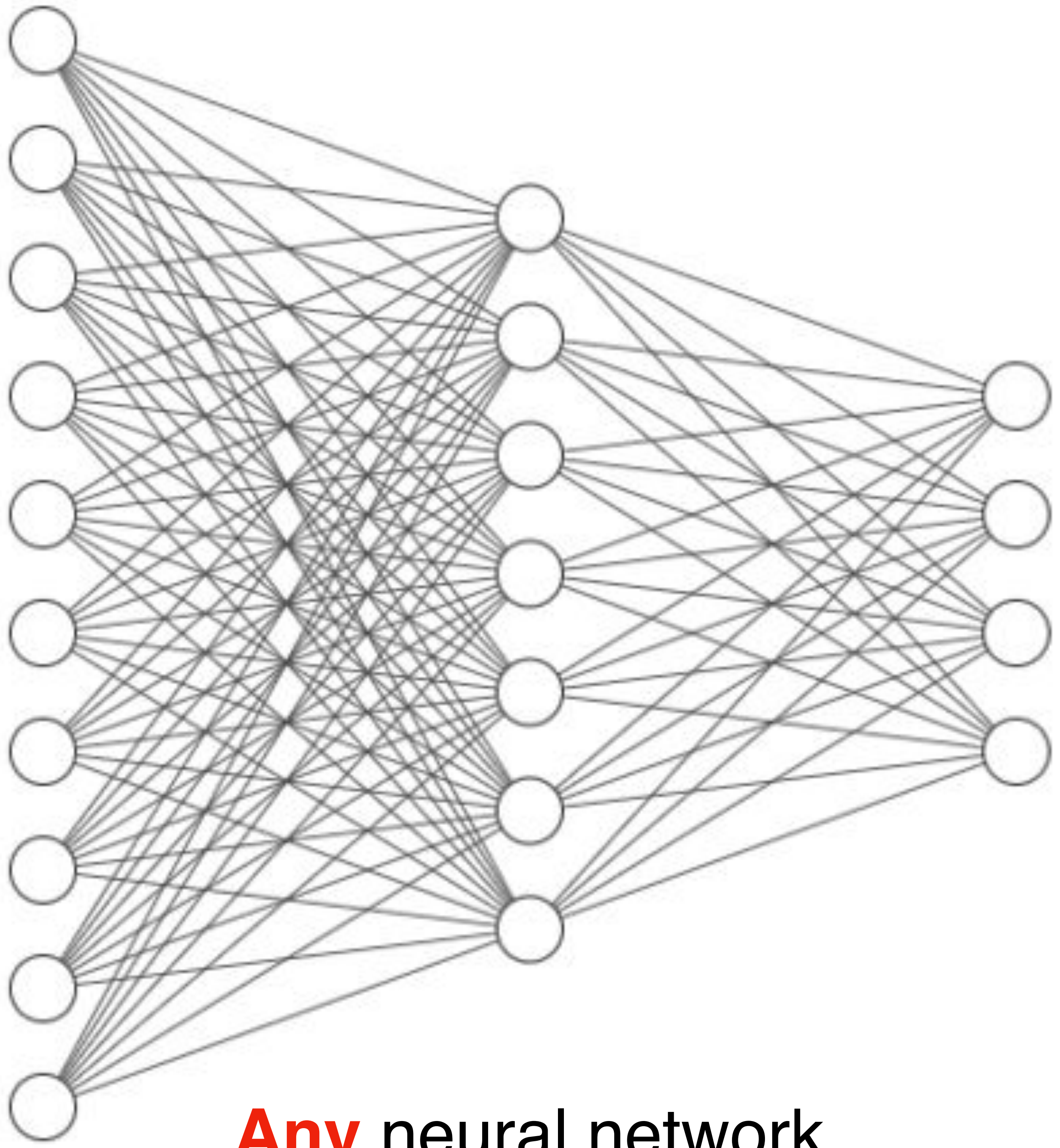
Rating > 4? → yes/no

Each output node is a binary task

Predicted ordinal label is
the sum over the **yes**es + 1

Input
(Aesthetics dataset)

Possible labels:
Rating 1, 2, 3, 4, 5



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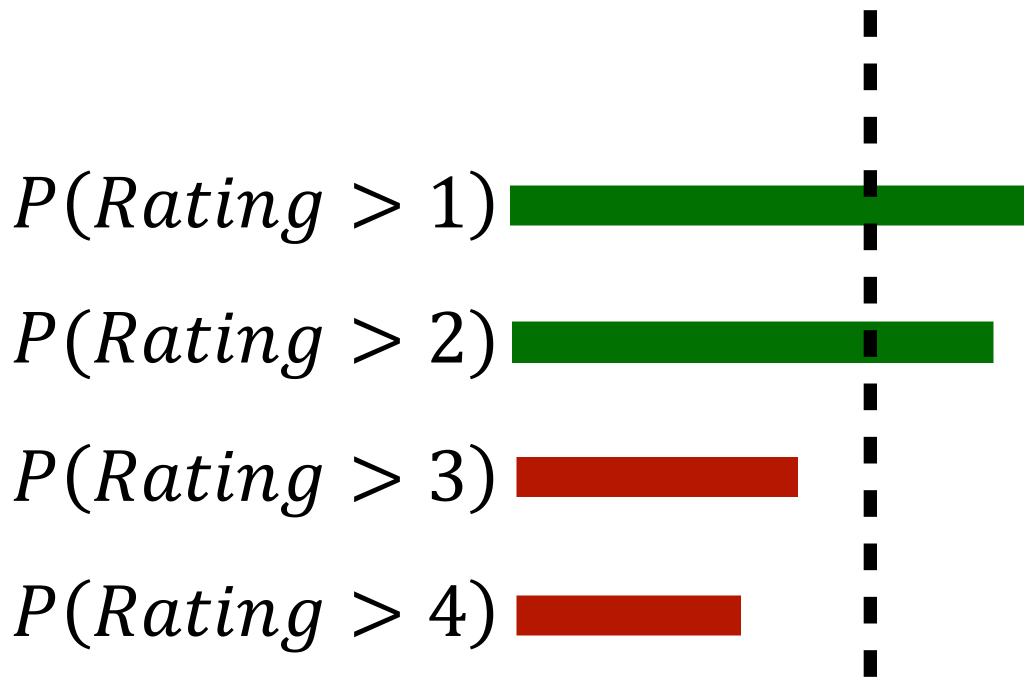


Rating > 1? → **yes**/no
Rating > 2? → **yes**/no
Rating > 3? → yes/**no**
Rating > 4? → yes/**no**

Each output node is a binary task

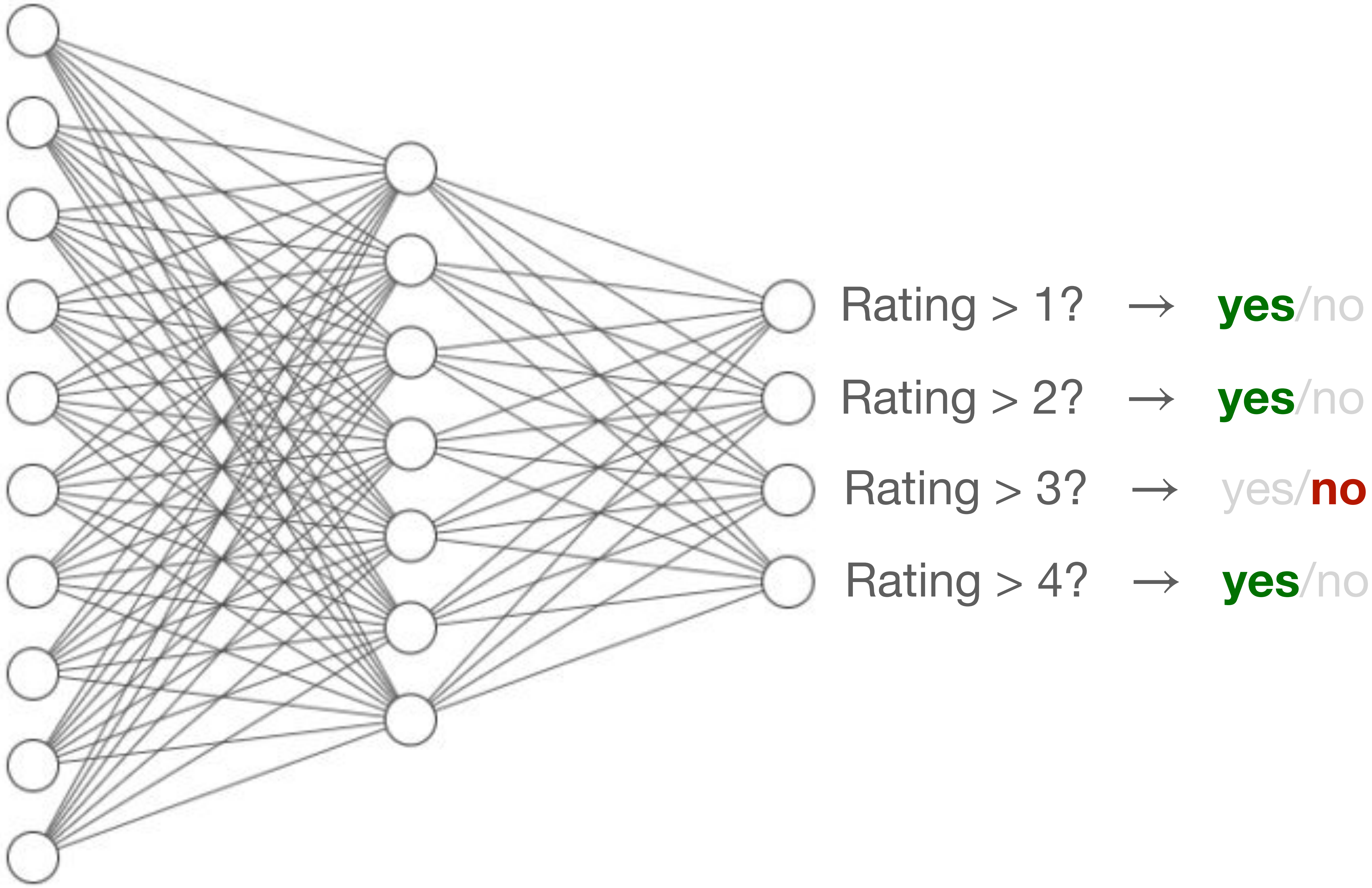
Predicted ordinal label is
the sum over the **yes**es + 1

Predicted label:

3

Problem: rank inconsistency

Problem: rank inconsistency



Predicted label:

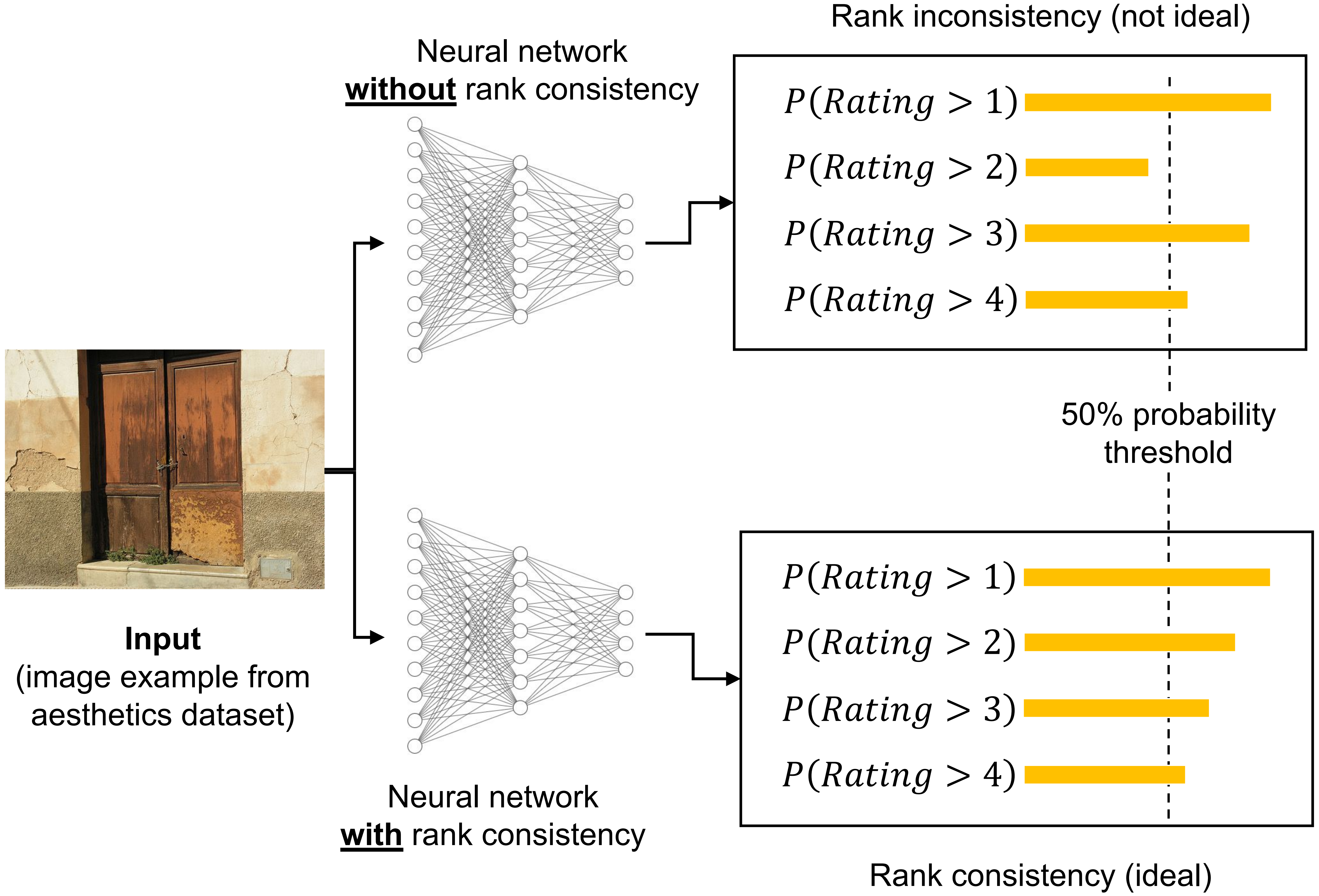
3

Greater than 4,
but not greater than 3?
That's paradoxical.

Niu Z, Zhou M, Wang L, Gao X, Hua G. Ordinal regression with multiple output CNN for age estimation. CVPR 2016

Addressing the rank inconsistency issue leads to better predictive performance

Cao, Mirjalili, Raschka (2020)
Rank Consistent Ordinal Regression for Neural Networks with Application to Age Estimation
Pattern Recognition Letters. 140, 325-331, https://www.sciencedirect.com/science/article/pii/S016786552030413X



Prev. ordinal regression network

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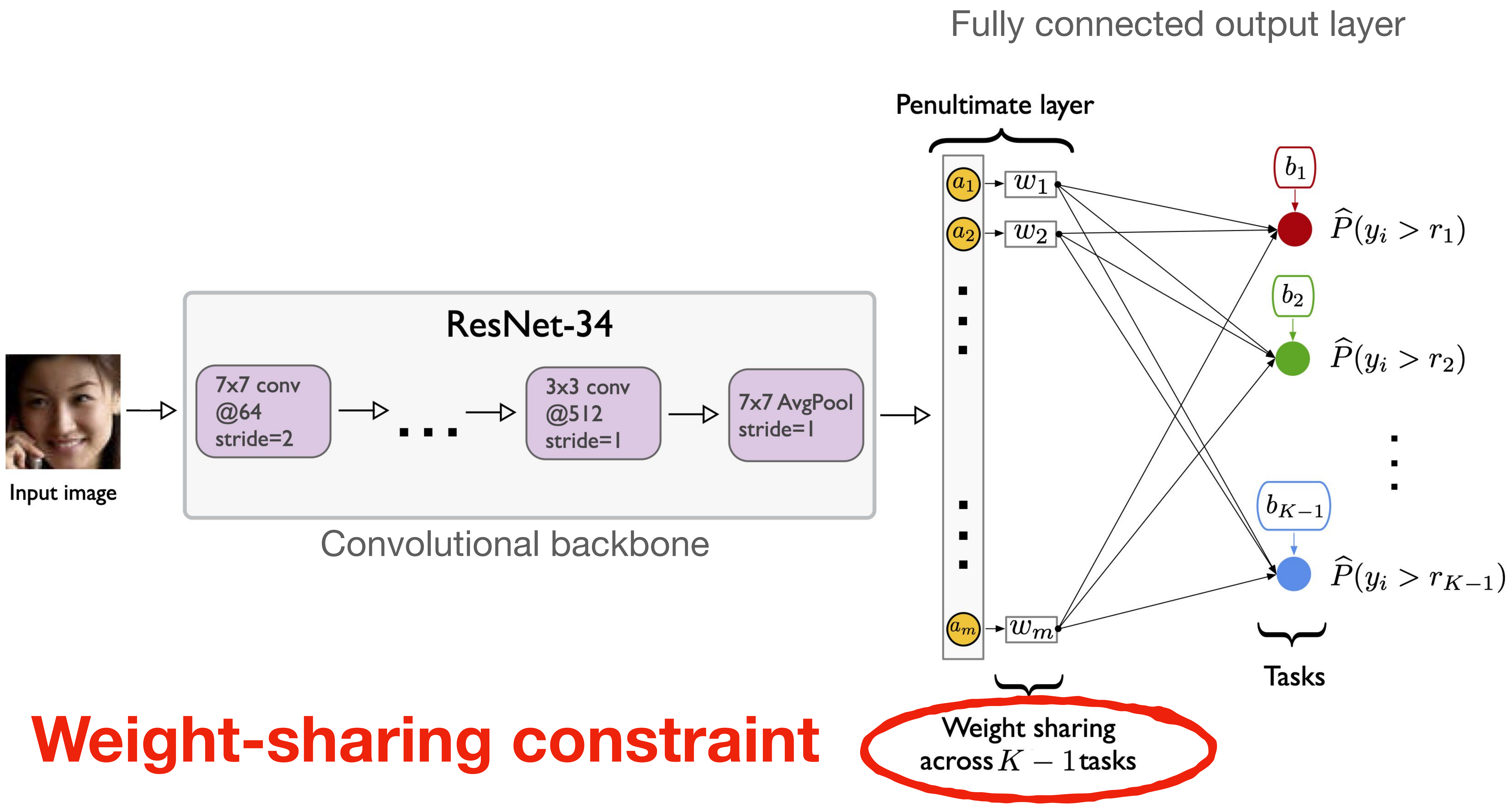
Fixing rank inconsistency introduced a limitation:
weight-sharing constraint restricts the network's capacity

Coral



Weight-sharing constraint

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Removing the weight-sharing constraint

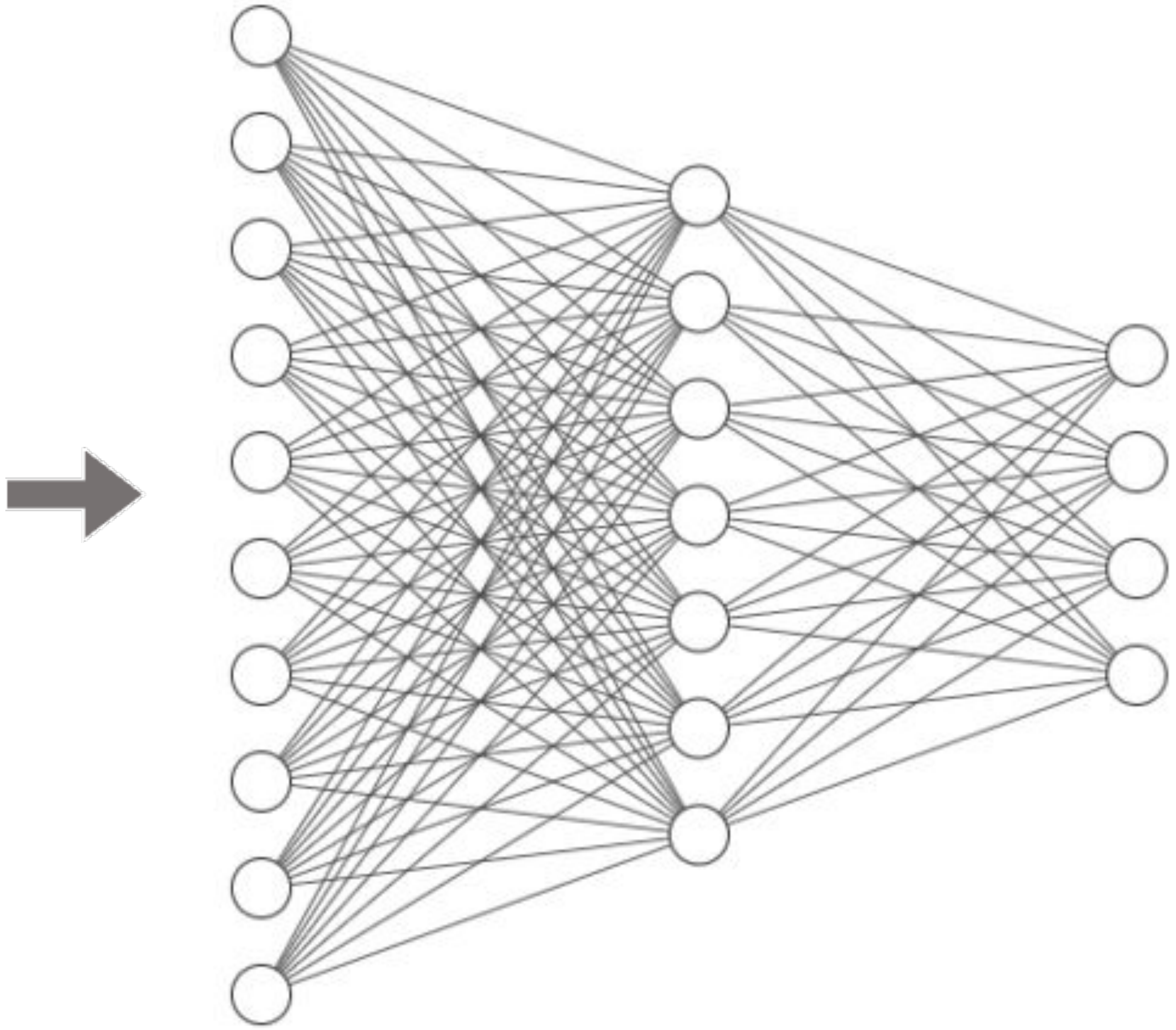
(while maintaining rank consistency)

leads to even better performance

Shi, Cao, Raschka
Deep Neural Networks for Rank-Consistent Ordinal Regression Based On Conditional Probabilities.
Arxiv preprint, https://arxiv.org/abs/2111.08851

CORN

CORN in a nutshell: chain rule for probabilities



Any neural network
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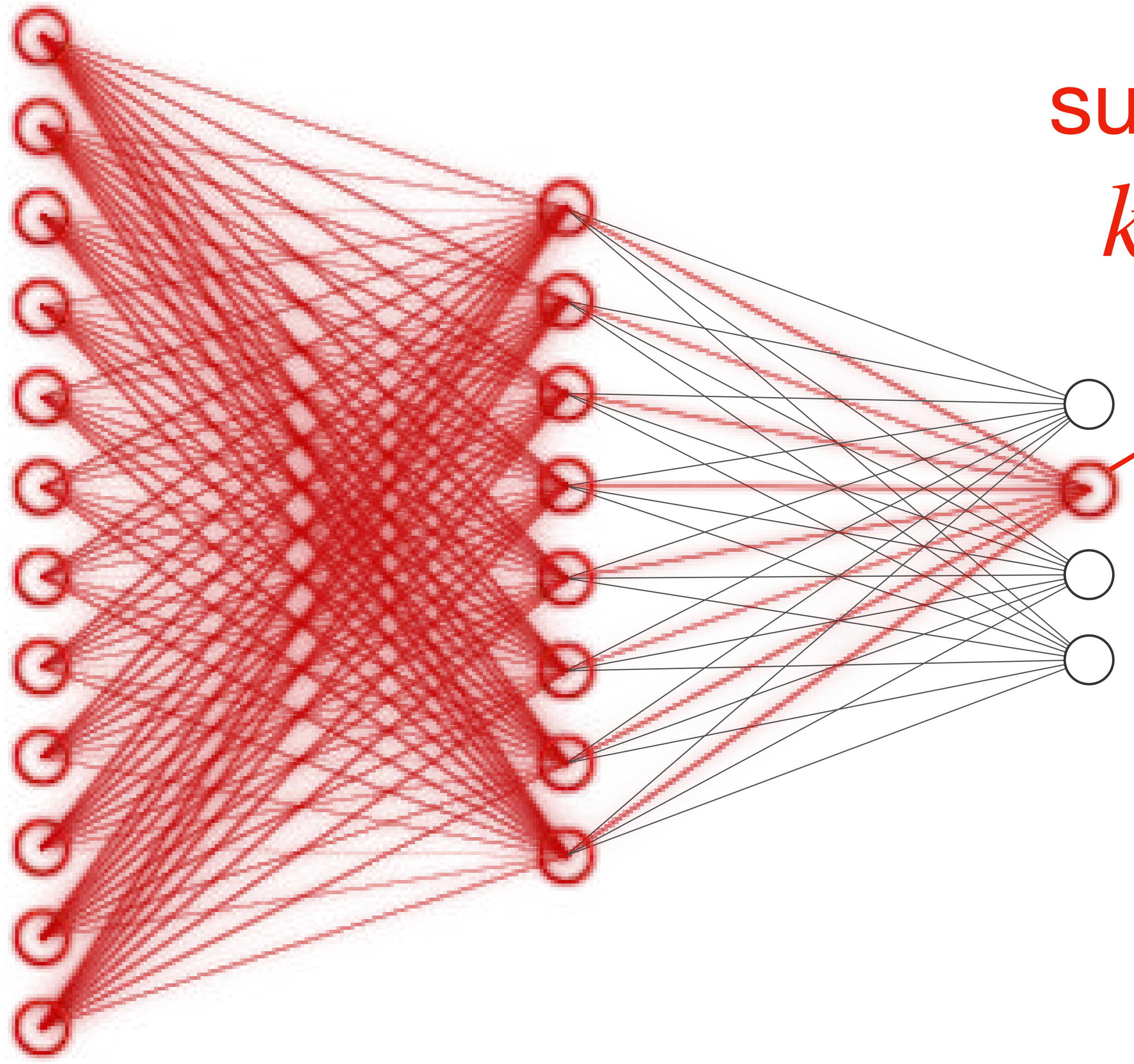


suppose
$k = 2$

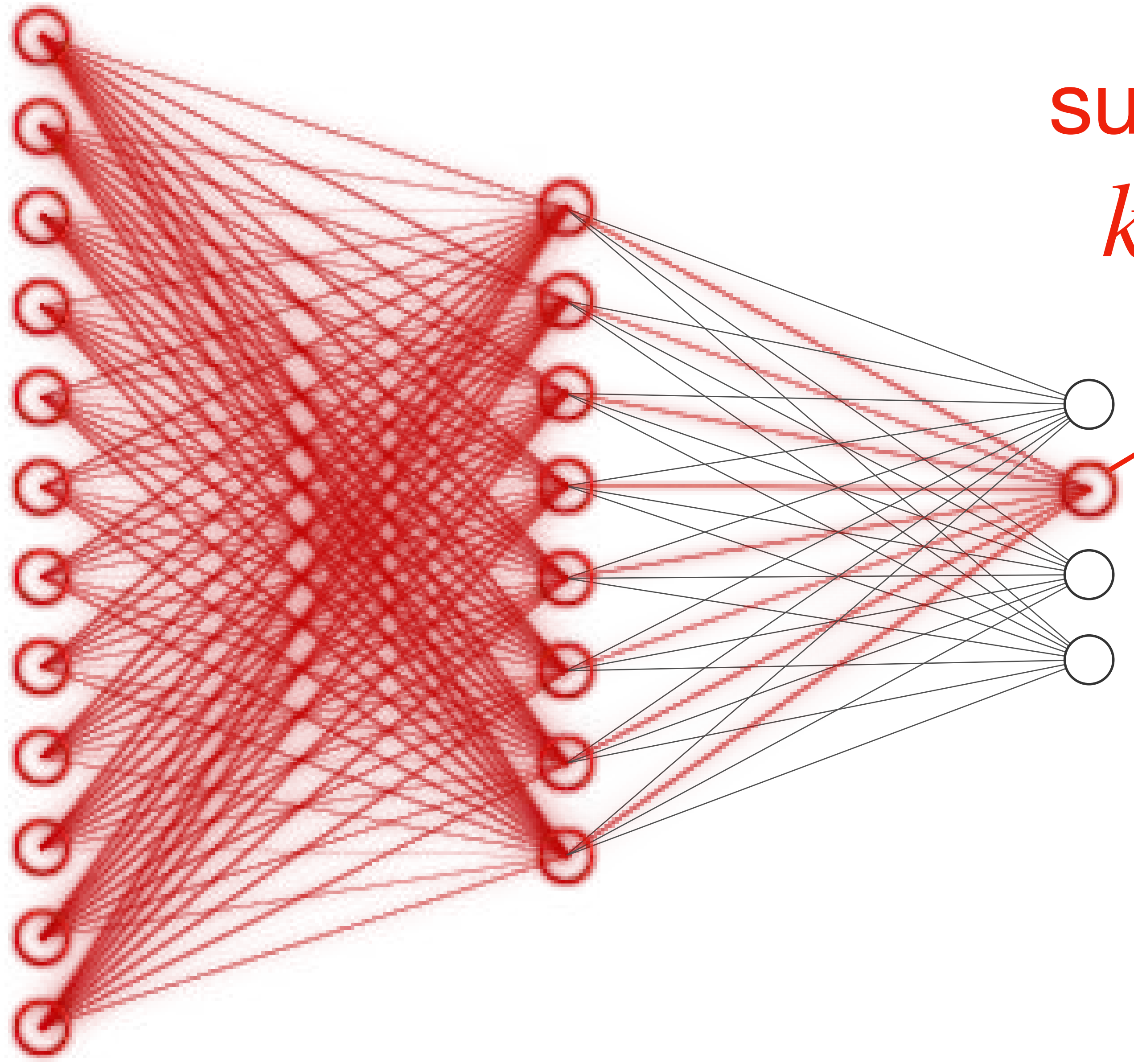
Conditional probability:

$$f_k\left(\mathbf{x}^{[i]}\right) = \hat{P}\left(y^{[i]} > r_k \mid y^{[i]} > r_{k-1}\right)$$

Input data   Label   Rank *k*

"Predicted probability that the label exceeds rank *k* given that it exceed rank *k-1*"

CORN in a nutshell: chain rule for probabilities



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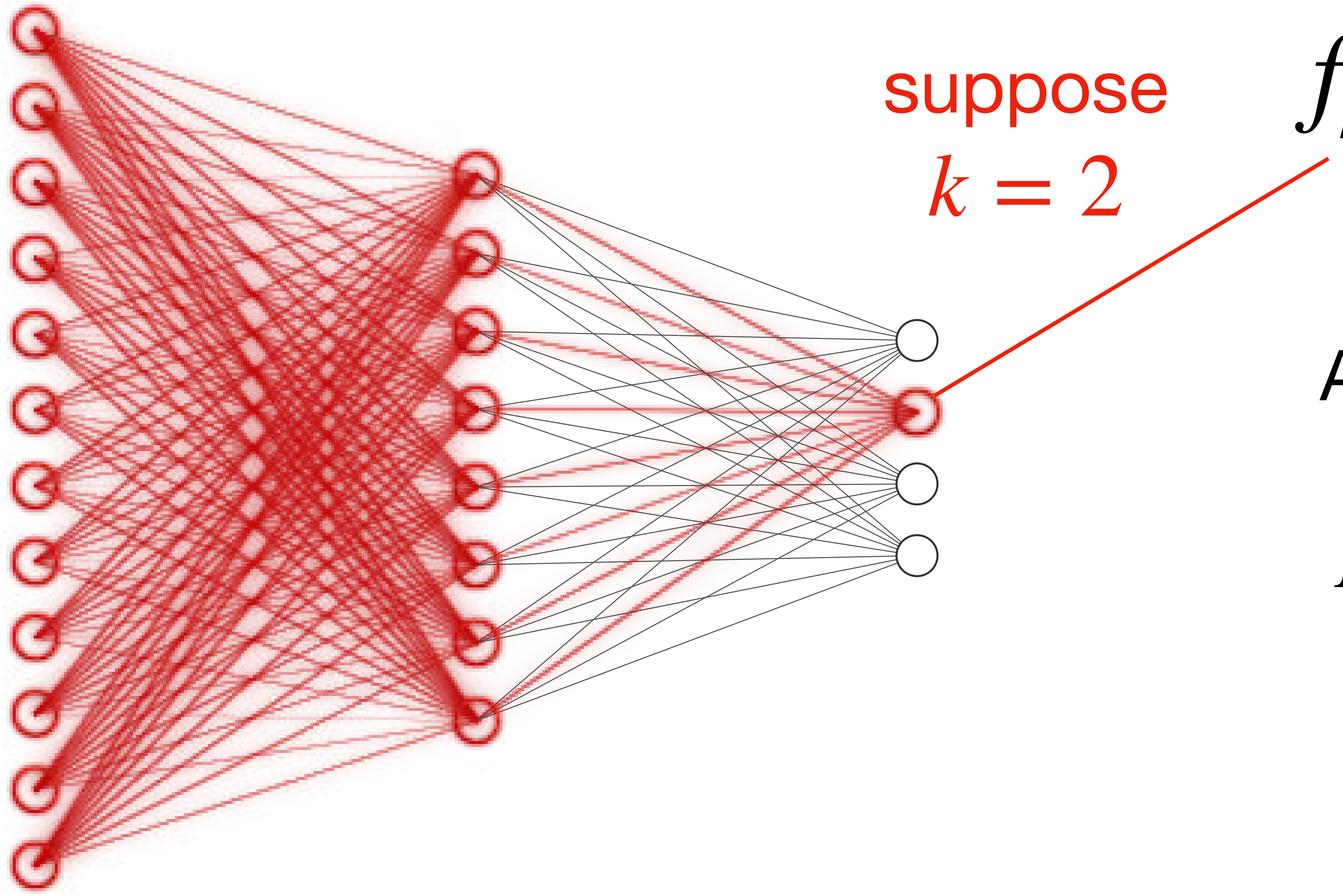
(Learned via conditional training subsets;
more details in paper)

CORN in a nutshell: chain rule for probabilities



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Apply chain rule for probabilities to obtain unconditional probability:

$$\hat{P}\left(y^{[i]} > r_k\right) = \prod_{j=1}^{k} f_j\left(\mathbf{x}^{[i]}\right)$$

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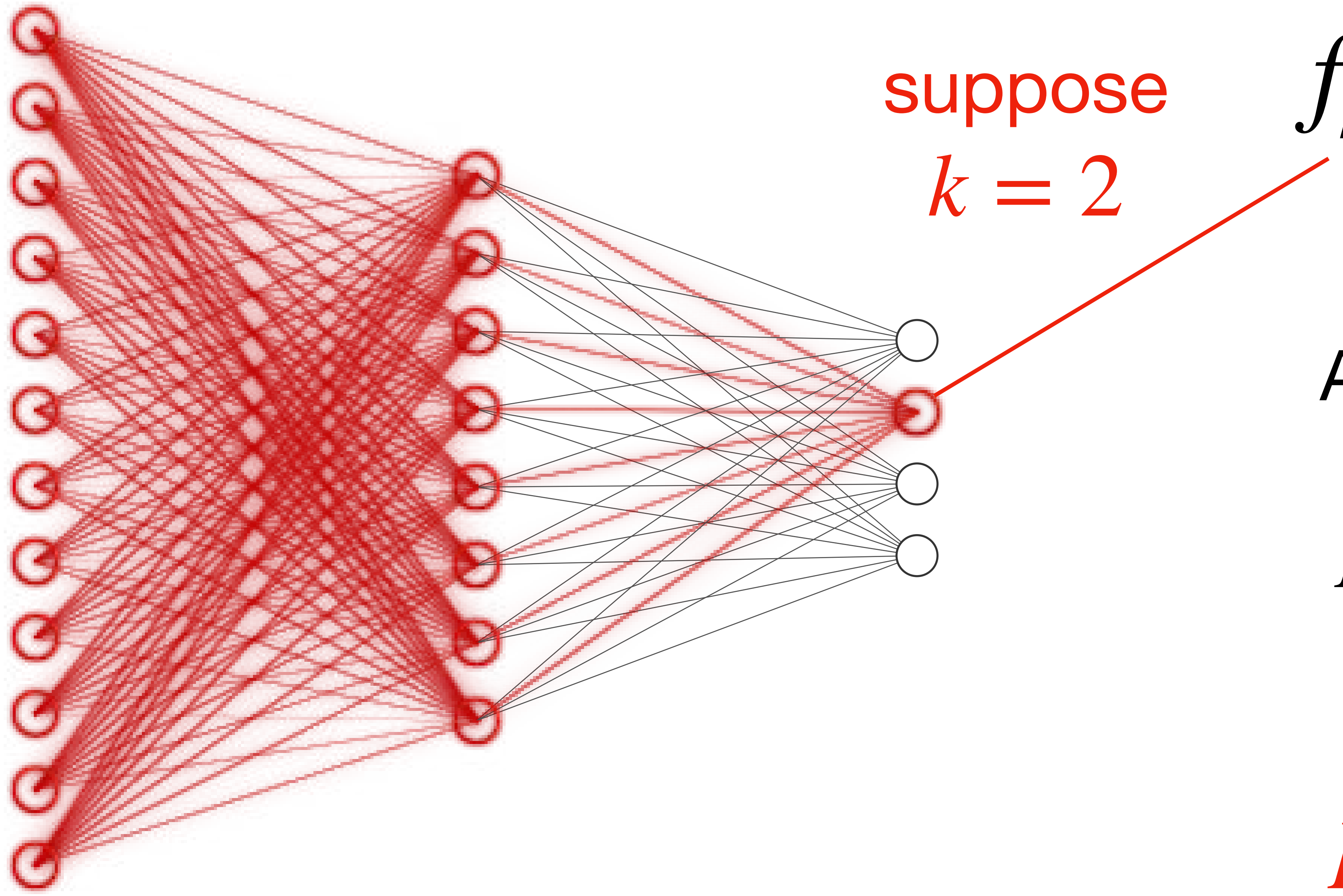

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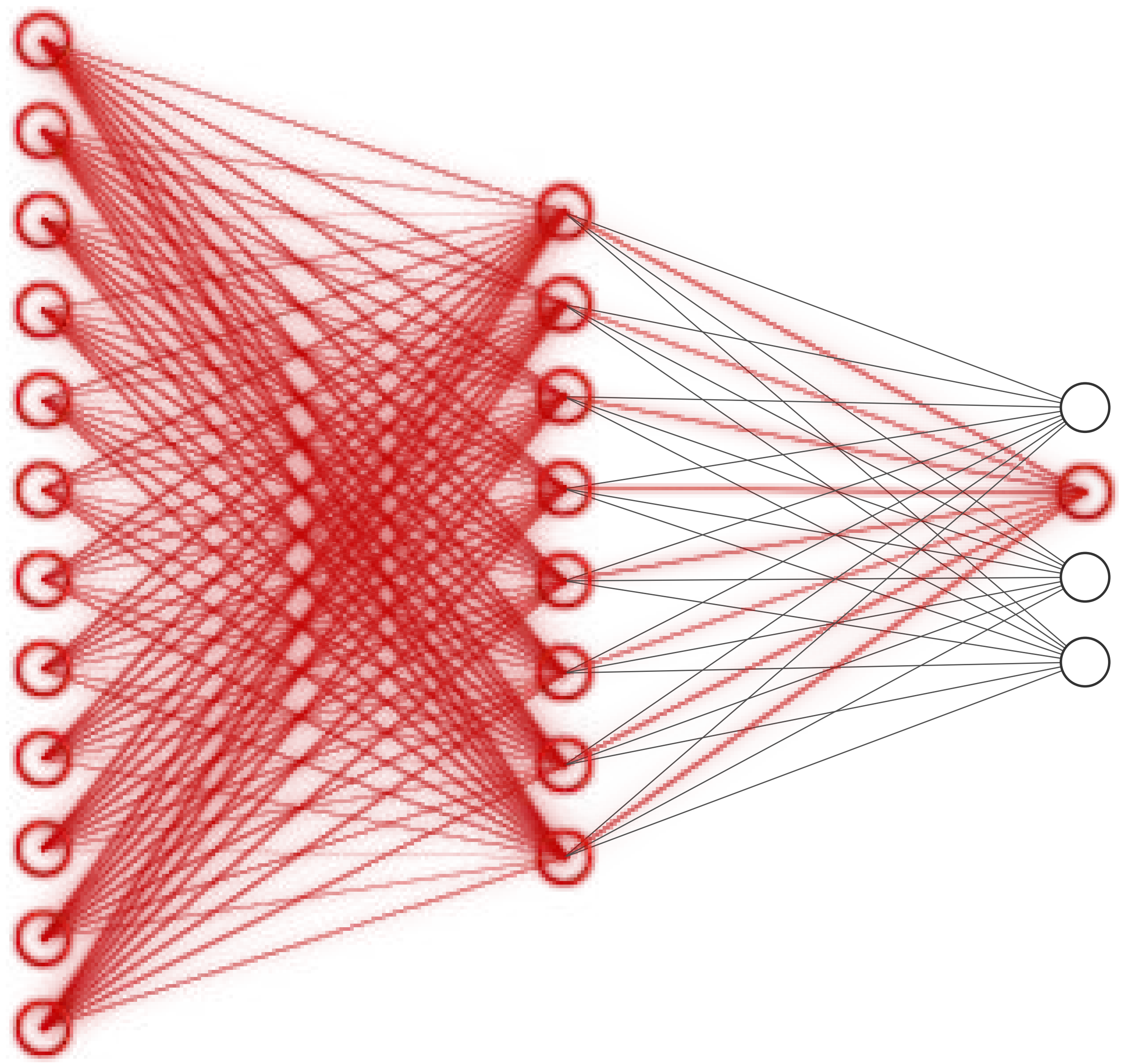
$$\hat{P}\left(y^{[i]} > r_2\right) = \hat{P}\left(y^{[i]} > r_2 \mid y^{[i]} > r_1\right) \cdot \hat{P}\left(y^{[i]} > r_1\right)$$

CORN in a nutshell: chain rule for probabilities



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≤ 1 ≤ 1

Left side guaranteed to be equal or less than right side

(Rank consistency: Rank probabilities are decreasing)

Coral

COnsistent RAnk Logits

Cao, Mirjalili, Raschka (2020)
Rank Consistent Ordinal Regression for Neural Networks with Application to Age Estimation
Pattern Recognition Letters. 140, 325-331, https://www.sciencedirect.com/science/article/pii/S016786552030413X

CORN

Conditional Ordinal Regression for Neural Networks

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Arxiv preprint, https://arxiv.org/abs/2111.08851

How do these methods compare?

How?

Coral

Weight-sharing in output layer
(mathematical proof in paper)

How?

Coral

Weight-sharing in output layer
(mathematical proof in paper)

CORN

Chain rule for probabilities
& conditional training sets

	How?	Advantages
Coral	Weight-sharing in output layer (mathematical proof in paper)	• Easy to implement • Reduced overfitting • Fast
CORN	Chain rule for probabilities & conditional training sets	

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Coral	Weight-sharing in output layer (mathematical proof in paper)	• Easy to implement • Reduced overfitting • Fast
CORN	Chain rule for probabilities & conditional training sets	• Easy to implement • Higher capacity • Better predictive performance

Skipping over further mathematical details ...
How do we use this in practice?

Converting a classifier into a CORN model in 3 lines of code

PyTorch Lightning

Full examples:
https://raschka-research-group.github.io/coral-pytorch/

Converting a classifier into a CORN model
in 3 lines of code

More code examples for tabular, text, and image data

PyTorch Lightning

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Converting a classifier into a CORN model in 3 lines of code

```
class NeuralNetwork(torch.nn.Module):
    def __init__(self, input_size, hidden_units, num_classes):
        super().__init__()

        # ... define hidden layers ...

        output_layer = torch.nn.Linear(hidden_units[-1],
                                       num_classes)

        all_layers.append(output_layer)
        self.model = torch.nn.Sequential(*all_layers)

    def forward(self, x):
        x = self.model(x)
        return x
```

Any neural network (CNN, RNN, MLP, …)

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① `num_classes-1)`

Update the number of classes

PyTorch Lightning

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① `num_classes-1)`

Why -1

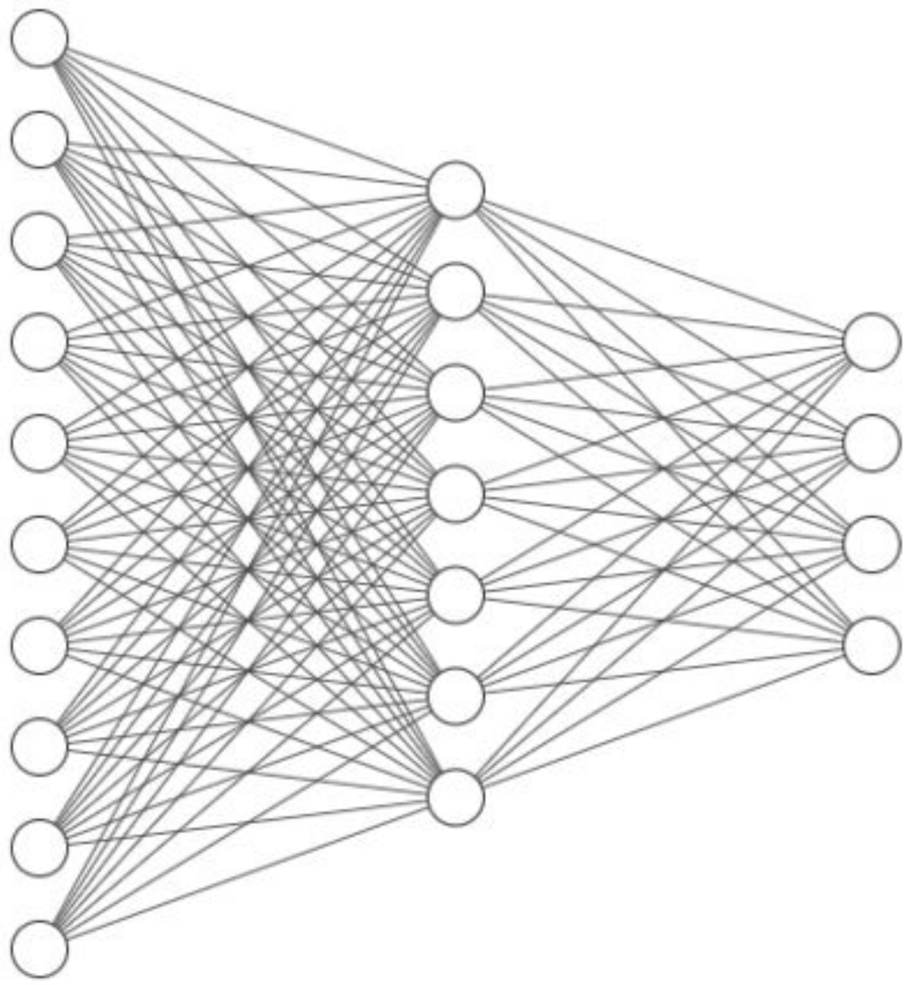
PyTorch Lightning

Full examples:
https://raschka-research-group.github.io/coral-pytorch/

Converting a classifier into a CORN model
in 3 lines of code

```python
class NeuralNetwork(torch.nn.Module):
    def __init__(self, input_size, hidden_units, num_classes):
        super().__init__()

        # ... define hidden layers ...

        output_layer = torch.nn.Linear(hidden_units[-1],
                                       num_classes)

        all_layers.append(output_layer)
        self.model = torch.nn.Sequential(*all_layers)

    def forward(self, x):
        x = self.model(x)
        return x
```

① `num_classes-1)`



Rating > 1? → yes/no
Rating > 2? → yes/no
Rating > 3? → yes/no
Rating > 4? → yes/no

"Rating > 4? Yes" implies Rating = 5

PyTorch Lightning

Full examples:
https://raschka-research-group.github.io/coral-pytorch/

Converting a classifier into a CORN model in 3 lines of code

```
import pytorch_lightning as pl


class LightningMLP(pl.LightningModule):
    def __init__(self, model):
        super().__init__()

    def _shared_forward_step(self, batch, batch_idx):
        features, true_labels = batch

        logits = self(features)

        loss = torch.nn.functional.cross_entropy(logits, true_labels)

        predicted_labels = torch.argmax(logits, dim=1)

        return loss, predicted_labels
```

② Replace the standard cross entropy loss

PyTorch Lightning

Full examples:
https://raschka-research-group.github.io/coral-pytorch/

Converting a Classifier into a CORN Model

in 3 Lines of Code

```python
import pytorch_lightning as pl


class LightningMLP(pl.LightningModule):
    def __init__(self, model):
        super().__init__()

    def _shared_forward_step(self, batch, batch_idx):
        features, true_labels = batch

        logits = self(features)

        loss = torch.nn.functional.cross_entropy(logits, true_labels)

        predicted_labels = torch.argmax(logits, dim=1)

        return loss, predicted_labels
```

```python
from coral_pytorch.losses import corn_loss
```

2

```python
loss = corn_loss(logits, true_labels,
                 num_classes=self.model.num_classes)
```

PyTorch Lightning

Full examples:
https://raschka-research-group.github.io/coral-pytorch/

Converting a classifier into a CORN model in 3 lines of code

```
import pytorch_lightning as pl


class LightningMLP(pl.LightningModule):
    def __init__(self, model):
        super().__init__()

    def _shared_forward_step(self, batch, batch_idx):
        features, true_labels = batch

        logits = self(features)

        loss = torch.nn.functional.cross_entropy(logits, true_labels)

        predicted_labels = torch.argmax(logits, dim=1)

        return loss, predicted_labels
```

3 Convert logits to classes

PyTorch Lightning

Full examples:
https://raschka-research-group.github.io/coral-pytorch/

Converting a Classifier into a CORN Model
in 3 Lines of Code

```
import pytorch_lightning as pl


class LightningMLP(pl.LightningModule):
    def __init__(self, model):
        super().__init__()

    def _shared_forward_step(self, batch, batch_idx):
        features, true_labels = batch

        logits = self(features)

        loss = torch.nn.functional.cross_entropy(logits, true_labels)

        predicted_labels = torch.argmax(logits, dim=1)

        return loss, predicted_labels
```

```
from coral_pytorch.dataset import corn_label_from_logits
```

3

```
predicted_labels = corn_label_from_logits(logits)
```

PyTorch Lightning

Full examples:
https://raschka-research-group.github.io/coral-pytorch/

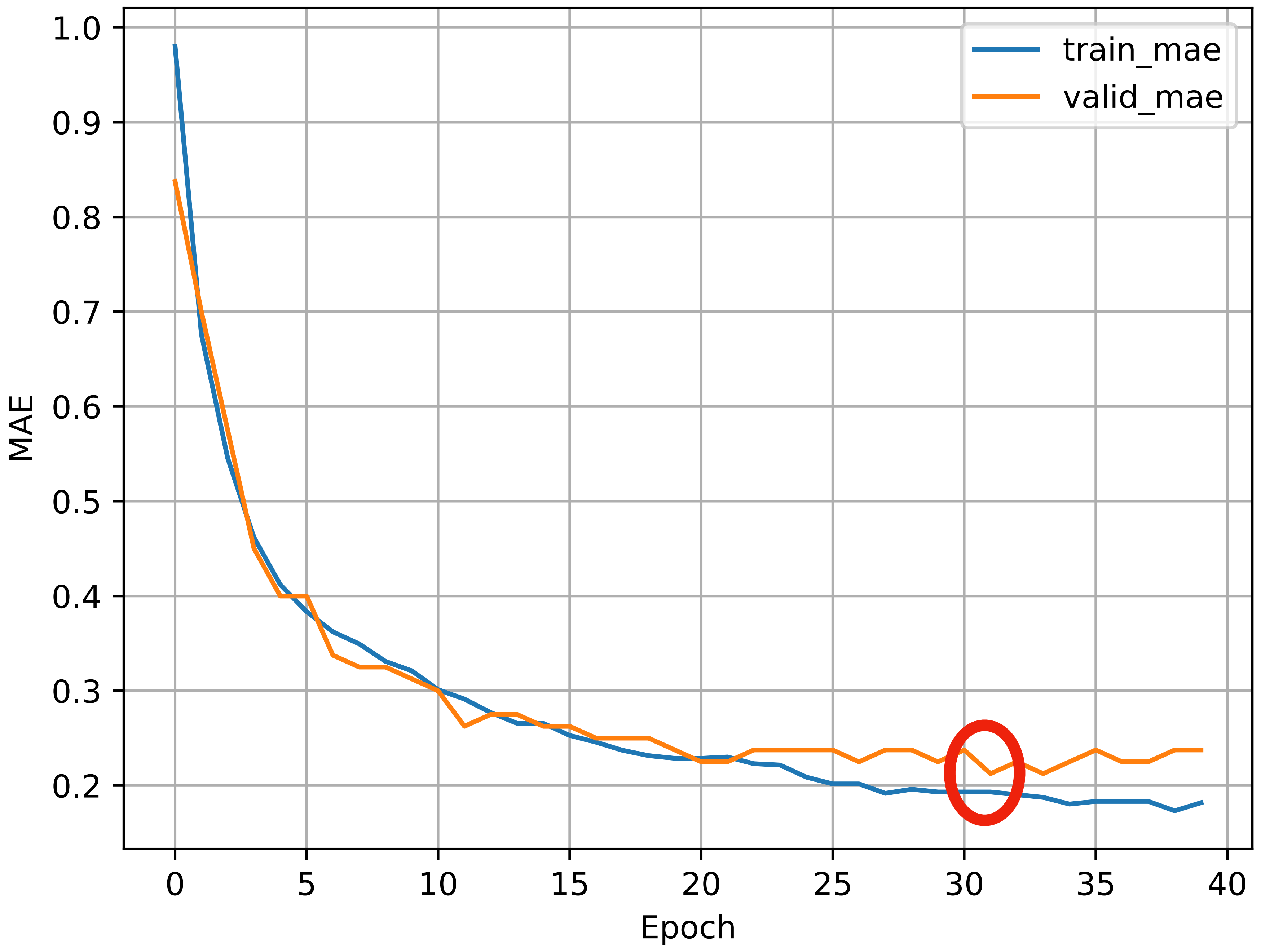
Code

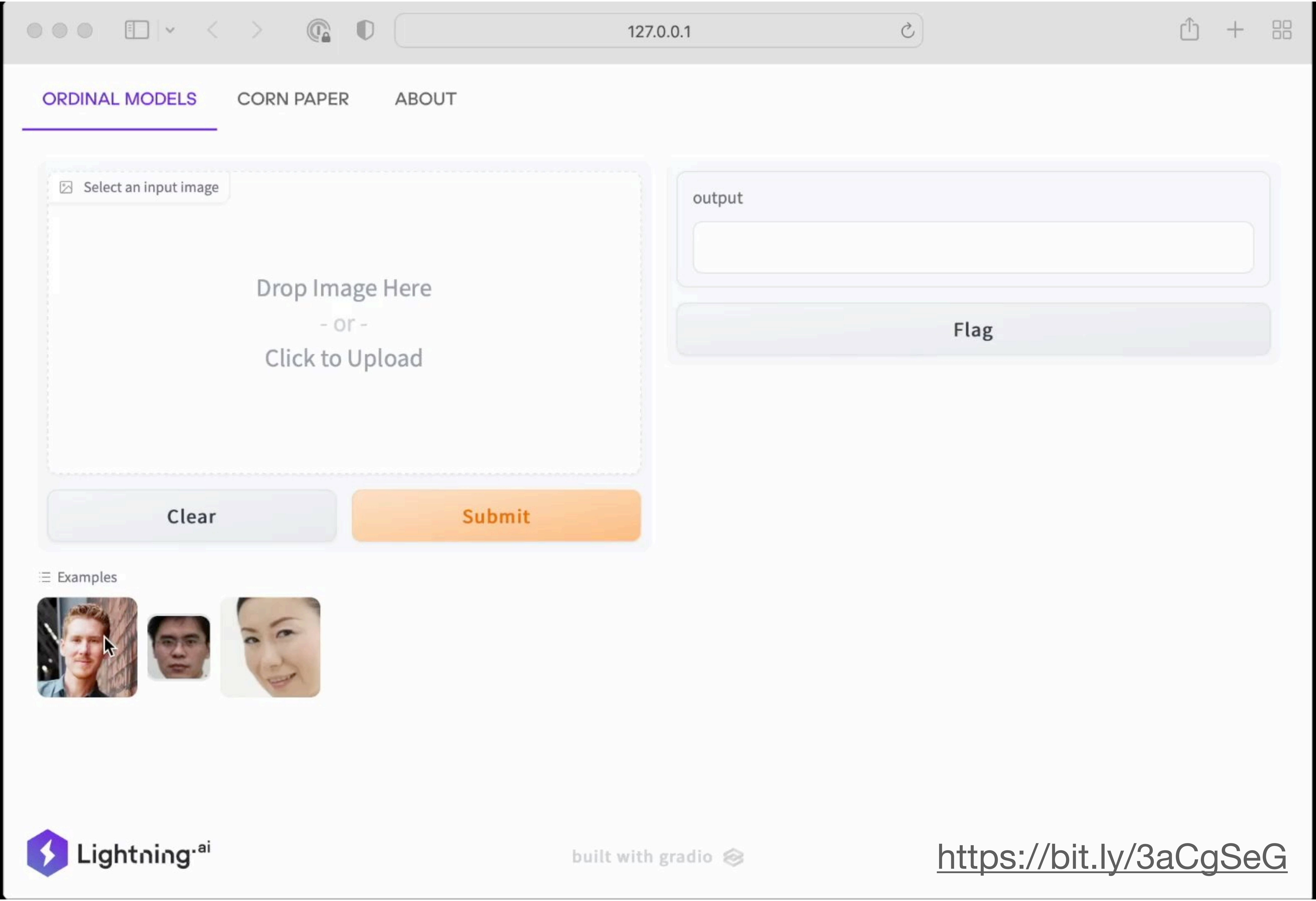
🎮 https://github.com/rasbt/scipy2022-talk

Desktop — grid session ssh scipy2022-talk — grid — ssh ◂ python3.9 ~/miniforge3/bin/grid session ssh scipy2022-talk — 99×28

```
(coral-pytorch) gridai@session:~/scipy2022-talk/src → python main_mlp.py \
> --batch_size 16 \
> --data_path ../datasets/ \
> --learning_rate 0.005 \
> --mixed_precision true \
> --num_epochs 40 \
> --num_workers 3 \
> --output_path ./cement_strength \
> --loss_mode crossentropy
```

```
python main_mlp.py \
--batch_size 16 \
--data_path ../datasets/ \
--learning_rate 0.005 \
--mixed_precision true \
--num_epochs 40 \
--num_workers 3 \
--output_path ./cement_strength \
--loss_mode corn
```

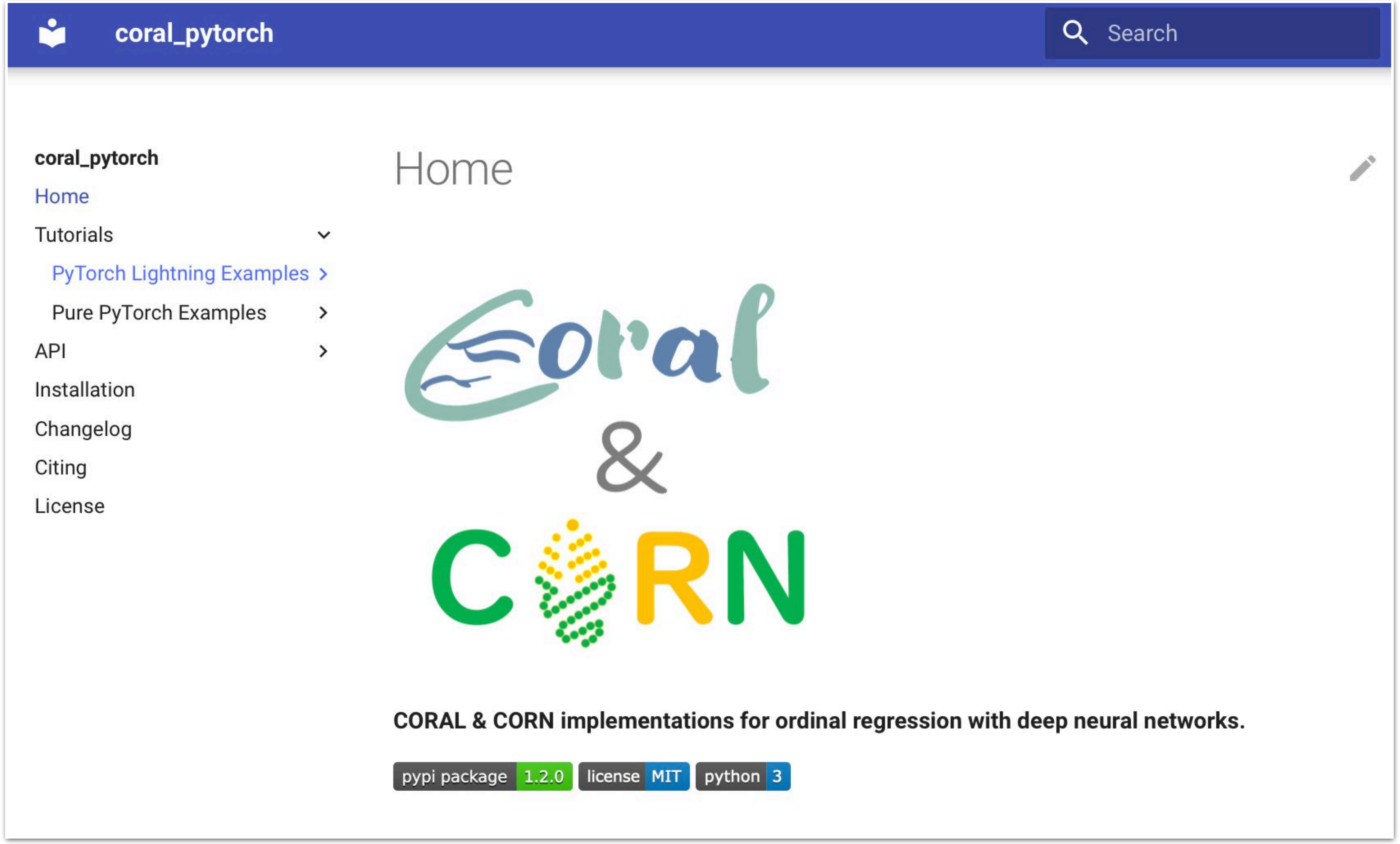




https://bit.ly/3aCgSeG

Code

🎮 https://github.com/rasbt/scipy2022-talk



More examples (CNN, RNN, MLP):

https://raschka-research-group.github.io/coral-pytorch/

Acknowledgements

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Feb 25

https://sebastianraschka.com/books/

https://github.com/rasbt/machine-learning-book

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https://sebastianraschka.com

Code & slides

https://github.com/rasbt/scipy2022-talk

Additional Slides for Q&A

Converting a Classifier into a CORAL Model

in 4 Lines of Code

PyTorch Lightning

Full examples:
https://raschka-research-group.github.io/coral-pytorch/

Converting a Classifier into a CORAL Model

in 4 Lines of Code

```
class NeuralNetwork(torch.nn.Module):
    def __init__(self, input_size, hidden_units, num_classes):
        super().__init__()

        # ... define hidden layers ...

        output_layer = torch.nn.Linear(hidden_units[-1],
                                       num_classes)

        all_layers.append(output_layer)
        self.model = torch.nn.Sequential(*all_layers)

    def forward(self, x):
        x = self.model(x)
        return x
```

PyTorch Lightning

Full examples:
https://raschka-research-group.github.io/coral-pytorch/

Converting a Classifier into a CORAL Model in 4 Lines of Code

```
class NeuralNetwork(torch.nn.Module):
    def __init__(self, input_size, hidden_units, num_classes):
        super().__init__()

        # ... define hidden layers ...

        output_layer = torch.nn.Linear(hidden_units[-1],
                                       num_classes)

        all_layers.append(output_layer)
        self.model = torch.nn.Sequential(*all_layers)

    def forward(self, x):
        x = self.model(x)
        return x
```

PyTorch Lightning

Full examples:
https://raschka-research-group.github.io/coral-pytorch/

Converting a Classifier into a CORAL Model in 4 Lines of Code

```python
class NeuralNetwork(torch.nn.Module):
    def __init__(self, input_size, hidden_units, num_classes):
        super().__init__()

        # ... define hidden layers ...

        output_layer = torch.nn.Linear(hidden_units[-1],
                                       num_classes)

        all_layers.append(output_layer)
        self.model = torch.nn.Sequential(*all_layers)

    def forward(self, x):
        x = self.model(x)
        return x
```

```python
from coral_pytorch.layers import CoralLayer
```

```python
output_layer = CoralLayer(size_in=hidden_units[-1],
                          num_classes=num_classes)
```

1

PyTorch Lightning

Full examples:
https://raschka-research-group.github.io/coral-pytorch/

Converting a Classifier into a CORAL Model in 4 Lines of Code

```python
import pytorch_lightning as pl


class LightningMLP(pl.LightningModule):
    def __init__(self, model):
        super().__init__()

    def _shared_forward_step(self, batch, batch_idx):
        features, true_labels = batch

        logits = self(features)

        loss = torch.nn.functional.cross_entropy(logits, true_labels)

        predicted_labels = torch.argmax(logits, dim=1)

        return loss, predicted_labels
```

```python
from coral_pytorch.losses import coral_loss
from coral_pytorch.dataset import levels_from_labelbatch
from coral_pytorch.dataset import proba_to_label
```

2 3

```python
levels = levels_from_labelbatch(
    true_labels, num_classes=self.model.num_classes)
loss = coral_loss(logits, levels)
```

PyTorch Lightning

Full examples:
https://raschka-research-group.github.io/coral-pytorch/

Converting a Classifier into a CORAL Model in 4 Lines of Code

```python
import pytorch_lightning as pl


class LightningMLP(pl.LightningModule):
    def __init__(self, model):
        super().__init__()

    def _shared_forward_step(self, batch, batch_idx):
        features, true_labels = batch

        logits = self(features)

        loss = torch.nn.functional.cross_entropy(logits, true_labels)

        predicted_labels = torch.argmax(logits, dim=1)

        return loss, predicted_labels
```

```python
from coral_pytorch.losses import coral_loss
from coral_pytorch.dataset import levels_from_labelbatch
from coral_pytorch.dataset import proba_to_label
```

2, 3

```python
levels = levels_from_labelbatch(
    true_labels, num_classes=self.model.num_classes)
loss = coral_loss(logits, levels)
```

4

```python
predicted_labels = proba_to_label(torch.sigmoid(logits))
```

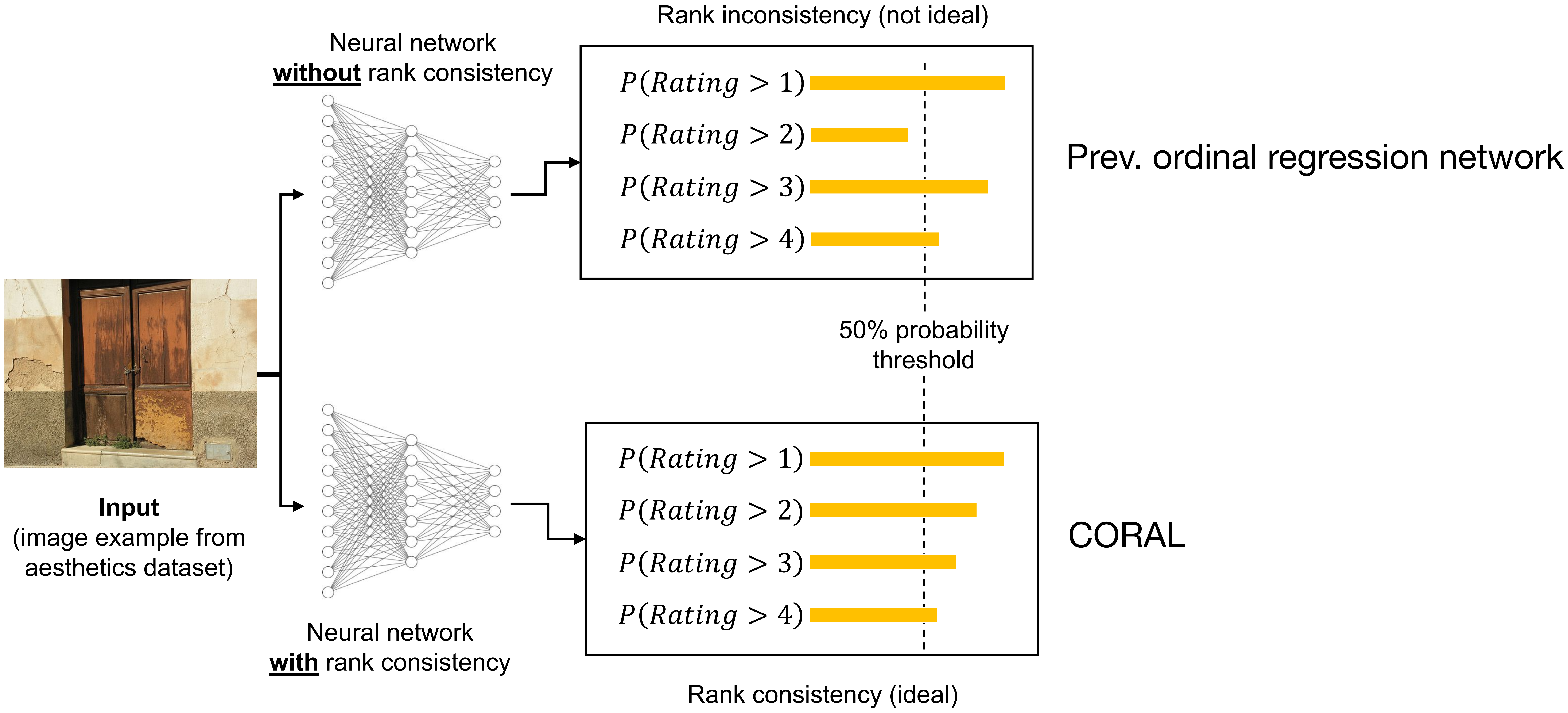
PyTorch Lightning

Full examples:
https://raschka-research-group.github.io/coral-pytorch/

CORAL Performance

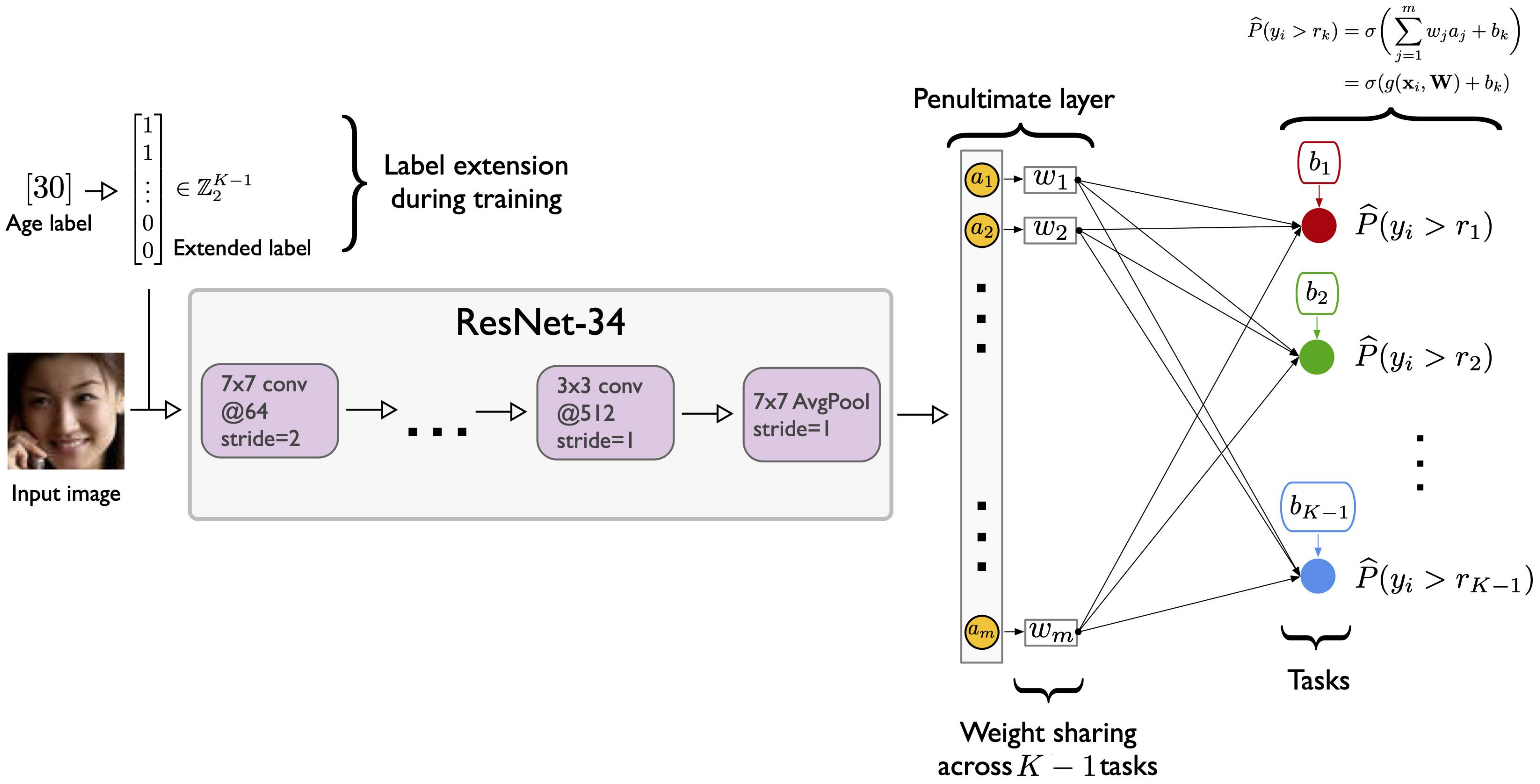
Table 1. Age prediction errors on the test sets. All models are based on the ResNet-34 architecture.

Method	Random Seed	MORPH-2		AFAD		CACD	
		MAE	RMSE	MAE	RMSE	MAE	RMSE
CE-CNN	0	3.26	4.62	3.58	5.01	5.74	8.20
	1	3.36	4.77	3.58	5.01	5.68	8.09
	2	3.39	4.84	3.62	5.06	5.53	7.92
	AVG ± SD	3.34 ± 0.07	4.74 ± 0.11	3.60 ± 0.02	5.03 ± 0.03	5.65 ± 0.11	8.07 ± 0.14
OR-CNN (Niu et al., 2016)	0	2.87	4.08	3.56	4.80	5.36	7.61
	1	2.81	3.97	3.48	4.68	5.40	7.78
	2	2.82	3.87	3.50	4.78	5.37	7.70
	AVG ± SD	2.83 ± 0.03	3.97 ± 0.11	3.51 ± 0.04	4.75 ± 0.06	5.38 ± 0.02	7.70 ± 0.09
CORAL-CNN (ours)	0	2.66	3.69	3.42	4.65	5.25	7.41
	1	2.64	3.64	3.51	4.76	5.25	7.50
	2	2.62	3.62	3.48	4.73	5.24	7.52
	AVG ± SD	**2.64 ± 0.02**	**3.65 ± 0.04**	**3.47 ± 0.05**	**4.71 ± 0.06**	**5.25 ± 0.01**	**7.48 ± 0.06**



Cao, Mirjalili, Raschka (2020)
Rank Consistent Ordinal Regression for Neural Networks with Application to Age Estimation
Pattern Recognition Letters. 140, 325-331, https://www.sciencedirect.com/science/article/pii/S016786552030413X

CORAL Architecture



CORAL Theorem

Theorem 1 (Ordered bias units). *By minimizing the loss function defined in Eq. 4, the optimal solution* $(\mathbf{W}^*, \mathbf{b}^*)$ *satisfies* $b_1^* \geq b_2^* \geq \ldots \geq b_{K-1}^*$.

Proof. Suppose $(\mathbf{W}, b)$ is an optimal solution and $b_k < b_{k+1}$ for some k. Claim: replacing b_k with b_{k+1} , or replacing b_{k+1} with b_k, decreases the objective value L. Let

$$A_1 = \{n : y_n^{(k)} = y_n^{(k+1)} = 1\},$$
$$A_2 = \{n : y_n^{(k)} = y_n^{(k+1)} = 0\},$$
$$A_3 = \{n : y_n^{(k)} = 1, \, y_n^{(k+1)} = 0\}.$$

By the ordering relationship, we have

$$A_1 \cup A_2 \cup A_3 = \{1, 2, \ldots, N\}.$$

Denote $p_n(b_k) = \sigma(g(\mathbf{x}_n, \mathbf{W}) + b_k)$ and

$$\delta_n = \log(p_n(b_{k+1})) - \log(p_n(b_k)),$$
$$\delta'_n = \log(1 - p_n(b_k)) - \log(1 - p_n(b_{k+1})).$$

Since $p_n(b_k)$ is increasing in b_k, we have $\delta_n > 0$ and $\delta'_n > 0$. If we replace b_k with b_{k+1}, the loss terms related to the k-th task are updated. The change of loss L (Eq. 4) is given as

$$\Delta_1 L = \lambda^{(k)} \Big[-\sum_{n \in A_1} \delta_n + \sum_{n \in A_2} \delta'_n - \sum_{n \in A_3} \delta_n \Big].$$

Accordingly, if we replace b_{k+1} with b_k, the change of L is given as

$$\Delta_2 L = \lambda^{(k+1)} \Big[\sum_{n \in A_1} \delta_n - \sum_{n \in A_2} \delta'_n - \sum_{n \in A_3} \delta'_n \Big].$$

By adding $\frac{1}{\lambda^{(k)}} \Delta_1 L$ and $\frac{1}{\lambda^{(k+1)}} \Delta_2 L$, we have

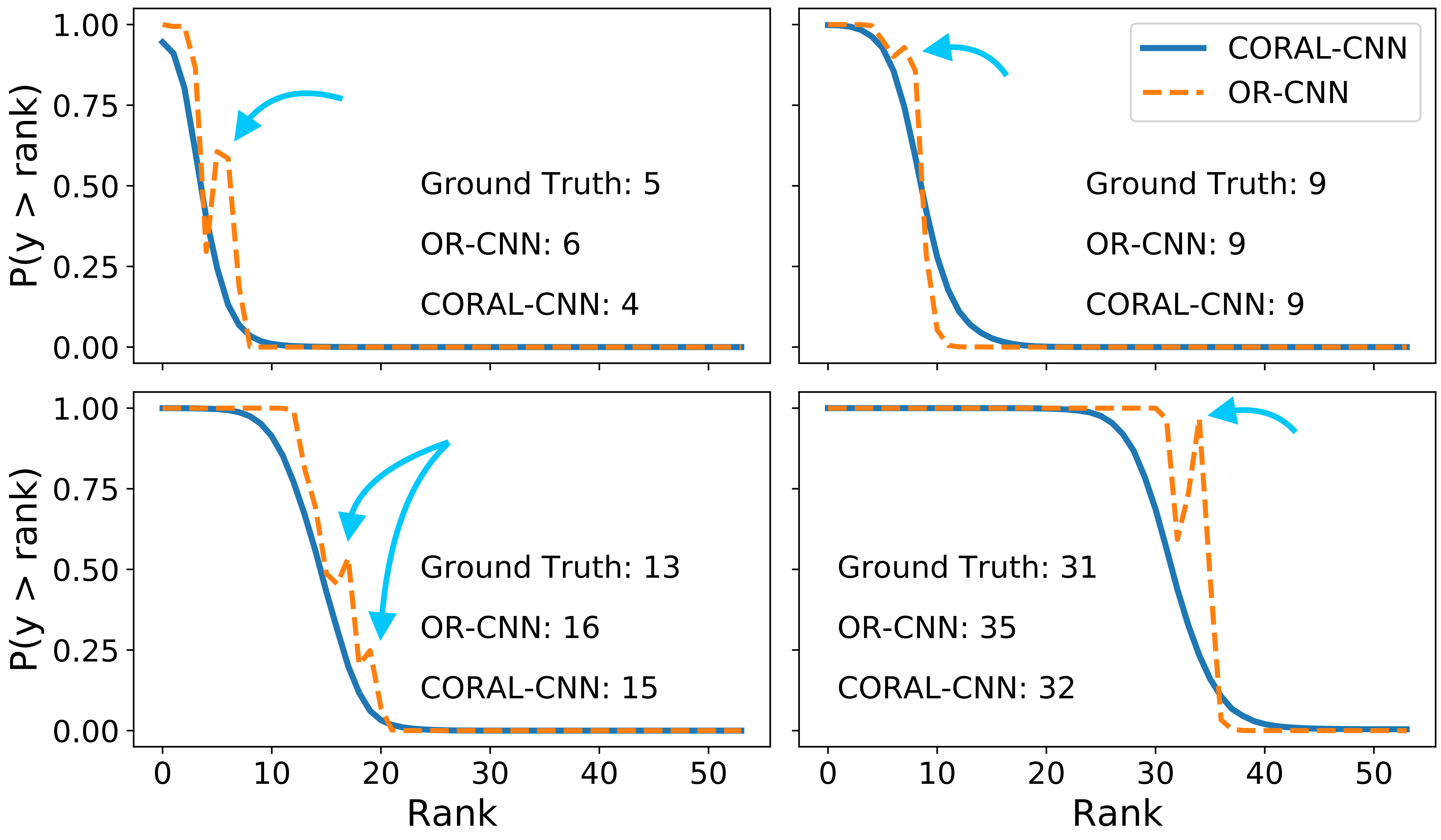
$$\frac{1}{\lambda^{(k)}} \Delta_1 L + \frac{1}{\lambda^{(k+1)}} \Delta_2 L = -\sum_{n \in A_3} (\delta_n + \delta'_n) < 0,$$

and know that either $\Delta_1 L < 0$ or $\Delta_2 L < 0$. Thus, our claim is justified. We conclude that any optimal solution $(\mathbf{W}^*, b^*)$ that minimizes L satisfies

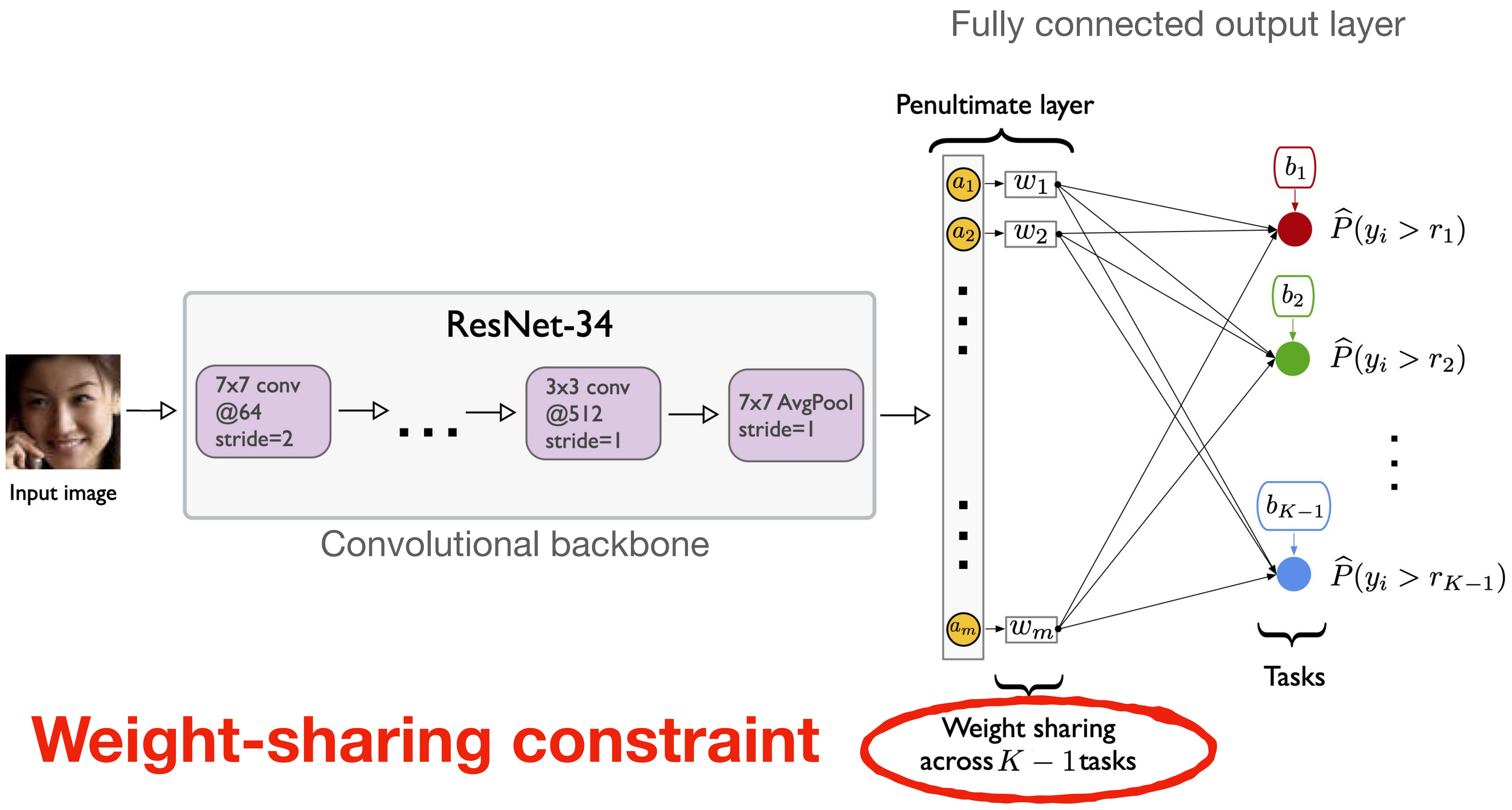
$$b_1^* \geq b_2^* \geq \ldots \geq b_{K-1}^*.$$

□

CORAL Rank Consistency



Fixing rank inconsistency introduced a limitation:
weight-sharing constraint restricts the network's capacity



Weight-sharing constraint

Cao, Mirjalili, Raschka (2020)
Rank Consistent Ordinal Regression for Neural Networks with Application to Age Estimation
Pattern Recognition Letters. 140, 325-331, https://www.sciencedirect.com/science/article/pii/S016786552030413X

Removing the weight-sharing constraint

(while maintaining rank consistency)

leads to even better performance

Shi, Cao, Raschka (2021)
Deep Neural Networks for Rank-Consistent Ordinal Regression Based On Conditional Probabilities.
Arxiv preprint, https://arxiv.org/abs/2111.08851

CORN Method 1/3

3.3. Rank-consistent Ordinal Regression based on Conditional Probabilities

Given a training set $D = \left\{\mathbf{x}^{[i]}, y^{[i]}\right\}_{i=1}^{N}$, CORN applies a label extension to the rank labels $y^{[i]}$ similar to CORAL, such that the resulting binary label $y_k^{[i]} \in \{0, 1\}$ indicates whether $y^{[i]}$ exceeds rank r_k. Similar to CORAL, CORN also uses $K - 1$ learning tasks associated with ranks $r_1, r_2, ..., r_K$ in the output layer as illustrated in Fig. 2.

However, in contrast to CORAL, CORN estimates a series of conditional probabilities using conditional training subsets (described in Section 3.4) such that the output of the $k-$th binary task $f_k\left(\mathbf{x}^{[i]}\right)$ represents the conditional probability[1]

$$f_k\left(\mathbf{x}^{[i]}\right) = \hat{P}\left(y^{[i]} > r_k \,|\, y^{[i]} > r_{k-1}\right), \tag{2}$$

where the events are nested: $\left\{y^{[i]} > r_k\right\} \subseteq \left\{y^{[i]} > r_{k-1}\right\}$.

The transformed, unconditional probabilities can then be computed by applying the chain rule for probabilities to the model outputs:

$$\hat{P}\left(y^{[i]} > r_k\right) = \prod_{j=1}^{k} f_j\left(\mathbf{x}^{[i]}\right). \tag{3}$$

Since $\forall j,\ 0 \leq f_j\left(\mathbf{x}^{[i]}\right) \leq 1$, we have

$$\hat{P}\left(y^{[i]} > r_1\right) \geq \hat{P}\left(y^{[i]} > r_2\right) \geq ... \geq \hat{P}\left(y^{[i]} > r_{K-1}\right), \tag{4}$$

which guarantees rank consistency among the $K - 1$ binary tasks.

CORN Method 2/3

3.4. Conditional Training Subsets

Our model aims to estimate $f_1\left(\mathbf{x}^{[i]}\right)$ and the conditional probabilities $f_2\left(\mathbf{x}^{[i]}\right), ..., f_{K-1}\left(\mathbf{x}^{[i]}\right)$. Estimating $f_1\left(\mathbf{x}^{[i]}\right)$ is a classic binary classification task under the extended binary classification framework with the binary labels $y_1^{[i]}$. To estimate the conditional probabilities such as $\hat{P}\left(y^{[i]} > r_2 \,|\, y^{[i]} > r_1\right)$, we focus only on the subset of the training data where $y^{[i]} > r_1$. As a result, when we minimize the binary cross-entropy loss on these conditional subsets, for each binary task, the estimated output probability has a proper conditional probability interpretation[2].

In order to model the conditional probabilities in Eq. 3, we construct conditional training subsets for training, which are used in the loss function (Section 3.5) that is minimized via backpropagation. The conditional training subsets are obtained from the original training set as follows:

$$
\begin{aligned}
&S_1 : \text{ all } \left\{\left(\mathbf{x}^{[i]}, y^{[i]}\right)\right\}, \text{ for } i \in \{1, ..., N\},\\
&S_2 : \left\{(\mathbf{x}^{[i]}, y^{[i]}) \mid y^{[i]} > r_1\right\},\\
&\ldots\\
&S_{K-1} : \left\{(\mathbf{x}^{[i]}, y^{[i]}) \mid y^{[i]} > r_{k-2}\right\},
\end{aligned}
$$

where $N = |S_1| \geq |S_2| \geq ... \geq |S_{K-1}|$, and $|S_k|$ denotes the size of S_k. Note that the labels $y^{[i]}$ are subject to the binary label extension as described in Section 3.3. Each conditional training subset S_k is used for training the conditional probability prediction $\hat{P}\left(y^{[i]} > r_k \,|\, y^{[i]} > r_{k-1}\right)$ for $k \geq 2$.

CORN Method 3/3

3.5. Loss Function

Let $f_j(\mathbf{x}^{[i]})$ denote the predicted value of the j-th node in the output layer of the network (Fig. 2), and let $|S_j|$ denote the size of the j-th conditional training set. To train a CORN neural network using backpropagation, we minimize the following loss function:

$$L(\mathbf{X}, \mathbf{y}) = -\frac{1}{\sum_{j=1}^{K-1}|S_j|}\sum_{j=1}^{K-1}\sum_{i=1}^{|S_j|}\Big[\log\left(f_j(\mathbf{x}^{[i]})\right)\cdot \mathbb{1}\left\{y^{[i]} > r_j\right\} + \log\left(1 - f_j\left(\mathbf{x}^{[i]}\right)\right)\cdot \mathbb{1}\left\{y^{[i]} \leq r_j\right\}\Big], \quad (5)$$

We note that in $f_j(\mathbf{x}^{[i]})$, $\mathbf{x}^{[i]}$ represents the i-th training example in S_j. To simplify the notation, we omit an additional index j to distinguish between $\mathbf{x}^{[i]}$ in different conditional training sets.

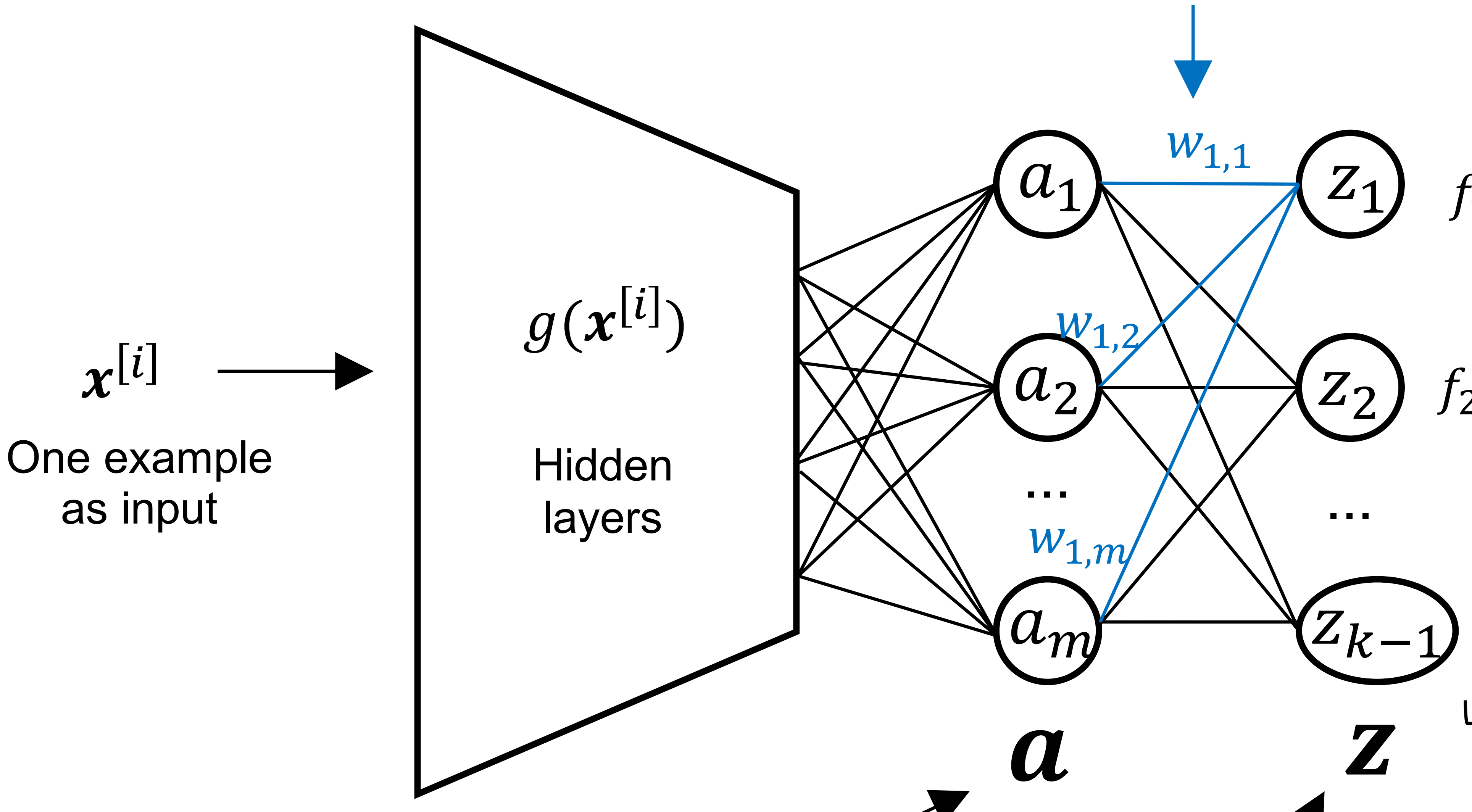
To improve the numerical stability of the loss gradients during training, we implement the following alternative formulation of the loss, where $\mathbf{Z}$ are the net inputs of the last layer (aka logits), as shown in Fig. 2, and $\log\left(\sigma\left(\mathbf{z}^{[i]}\right)\right) = \log\left(f_j\left(\mathbf{x}^{[i]}\right)\right)$:

$$L(\mathbf{Z}, \mathbf{y}) = -\frac{1}{\sum_{j=1}^{K-1}|S_j|}\sum_{j=1}^{K-1}\sum_{i=1}^{|S_j|}\Big[\log\left(\sigma\left(\mathbf{z}^{[i]}\right)\right)\cdot \mathbb{1}\left\{y^{[i]} > r_j\right\} + \left(\log\left(\sigma\left(\mathbf{z}^{[i]}\right)\right) - \mathbf{z}^{[i]}\right)\cdot \mathbb{1}\left\{y^{[i]} \leq r_j\right\}\Big]. \quad (6)$$

CORN Architecture

Weight parameters of the last layer (bias units $b_1 \dots b_{k-1}$ not shown)

$\mathbf{w}_1 = [w_{1,1} \;\; w_{1,2} \;\; \dots \;\; w_{1,m}]$



Logistic sigmoid function

$$f_1(\mathbf{x}^{[i]}) = \sigma\left(z_1^{[i]}\right) \quad \text{where} \quad z_1^{[i]} = \mathbf{a}^{[i]} \mathbf{w}_1^T + b_1$$

$$f_2(\mathbf{x}^{[i]}) = \sigma\left(z_2^{[i]}\right) \quad \text{where} \quad z_2^{[i]} = \mathbf{a}^{[i]} \mathbf{w}_2^T + b_2$$

$$\dots$$

$$f_{K-1}(\mathbf{x}^{[i]}) = \sigma\left(z_{K-1}^{[i]}\right) \quad \text{where} \quad z_{K-1}^{[i]} = \mathbf{a}^{[i]} \mathbf{w}_{K-1}^T + b_{K-1}$$

Outputs

where $\sigma\left(z_{K-1}^{[i]}\right) = \hat{P}\left(y^{[i]} > r_{K-1} \mid y^{[i]} > r_{K-2}\right)$

Activations of penultimate layer

$\mathbf{a} = [a_1 \;\; a_2 \;\; \dots \;\; a_m]$

Net inputs of output layer

$\mathbf{z} = [z_1 \;\; z_2 \;\; \dots \;\; z_{K-1}]$

Predicted rank $q^{[i]} = 1 + \sum_{k=1}^{K-1} \mathbb{1}\left\{\hat{P}\left(y^{[i]} > r_k\right) > 0.5\right\}$

where $\hat{P}\left(y^{[i]} > r_k\right) = \hat{P}\left(y^{[i]} > r_1\right) \cdot \hat{P}\left(y^{[i]} > r_2 \mid y^{[i]} > r_1\right) \cdots \hat{P}\left(y^{[i]} > r_k \mid y^{[i]} > r_{k-1}\right)$

CORN Performance 1/2

Table 1. Prediction errors on the test sets. Best results are highlighted in bold.

Method	Seed	MORPH-2 (Balanced)		AFAD (Balanced)		AES		FIREMAN	
		MAE	RMSE	MAE	RMSE	MAE	RMSE	MAE	RMSE
CE-NN	0	3.81	5.19	3.31	4.27	0.43	0.68	0.80	1.14
	1	3.60	4.8	3.28	4.19	0.43	0.69	0.80	1.14
	2	3.61	4.84	3.32	4.22	0.45	0.71	0.79	1.13
	3	3.85	5.21	3.24	4.15	0.43	0.70	0.80	1.16
	4	3.80	5.14	3.24	4.13	0.42	0.68	0.80	1.15
	AVG±SD	3.73 ± 0.12	5.04 ± 0.20	3.28 ± 0.04	4.19 ± 0.06	**0.43 ± 0.01**	0.69 ± 0.01	0.80 ± 0.01	1.14 ± 0.01
OR-NN [11]	0	3.21	4.25	2.81	3.45	0.44	0.70	0.75	1.07
	1	3.16	4.25	2.87	3.54	0.43	0.69	0.76	1.08
	2	3.16	4.31	2.82	3.46	0.43	0.69	0.77	1.10
	3	2.98	4.05	2.89	3.49	0.44	0.70	0.76	1.08
	4	3.13	4.27	2.86	3.45	0.43	0.69	0.74	1.07
	AVG±SD	3.13 ± 0.09	4.23 ± 0.10	2.85 ± 0.03	3.48 ± 0.04	**0.43 ± 0.01**	0.69 ± 0.01	**0.76 ± 0.01**	**1.08 ± 0.01**
CORAL [1]	0	2.94	3.98	2.95	3.60	0.47	0.72	0.82	1.14
	1	2.97	4.03	2.99	3.69	0.47	0.72	0.83	1.16
	2	3.01	3.98	2.98	3.70	0.48	0.73	0.81	1.13
	3	2.98	4.01	3.00	3.78	0.44	0.70	0.82	1.16
	4	3.03	4.06	3.04	3.75	0.46	0.72	0.82	1.15
	AVG±SD	2.99 ± 0.04	4.01 ± 0.03	2.99 ± 0.03	3.70 ± 0.07	0.46 ± 0.02	0.72 ± 0.01	0.82 ± 0.01	1.15 ± 0.01
CORN (ours)	0	2.98	4	2.80	3.45	0.41	0.67	0.75	1.07
	1	2.99	4.01	2.81	3.44	0.44	0.69	0.76	1.08
	2	2.97	3.97	2.84	3.48	0.42	0.68	0.77	1.10
	3	3.00	4.06	2.80	3.48	0.43	0.69	0.76	1.08
	4	2.95	3.92	2.79	3.45	0.43	0.69	0.74	1.07
	AVG±SD	**2.98 ± 0.02**	**3.99 ± 0.05**	**2.81 ± 0.02**	**3.46 ± 0.02**	**0.43 ± 0.01**	**0.68 ± 0.01**	**0.76 ± 0.01**	**1.08 ± 0.01**

CORN Performance 2/2

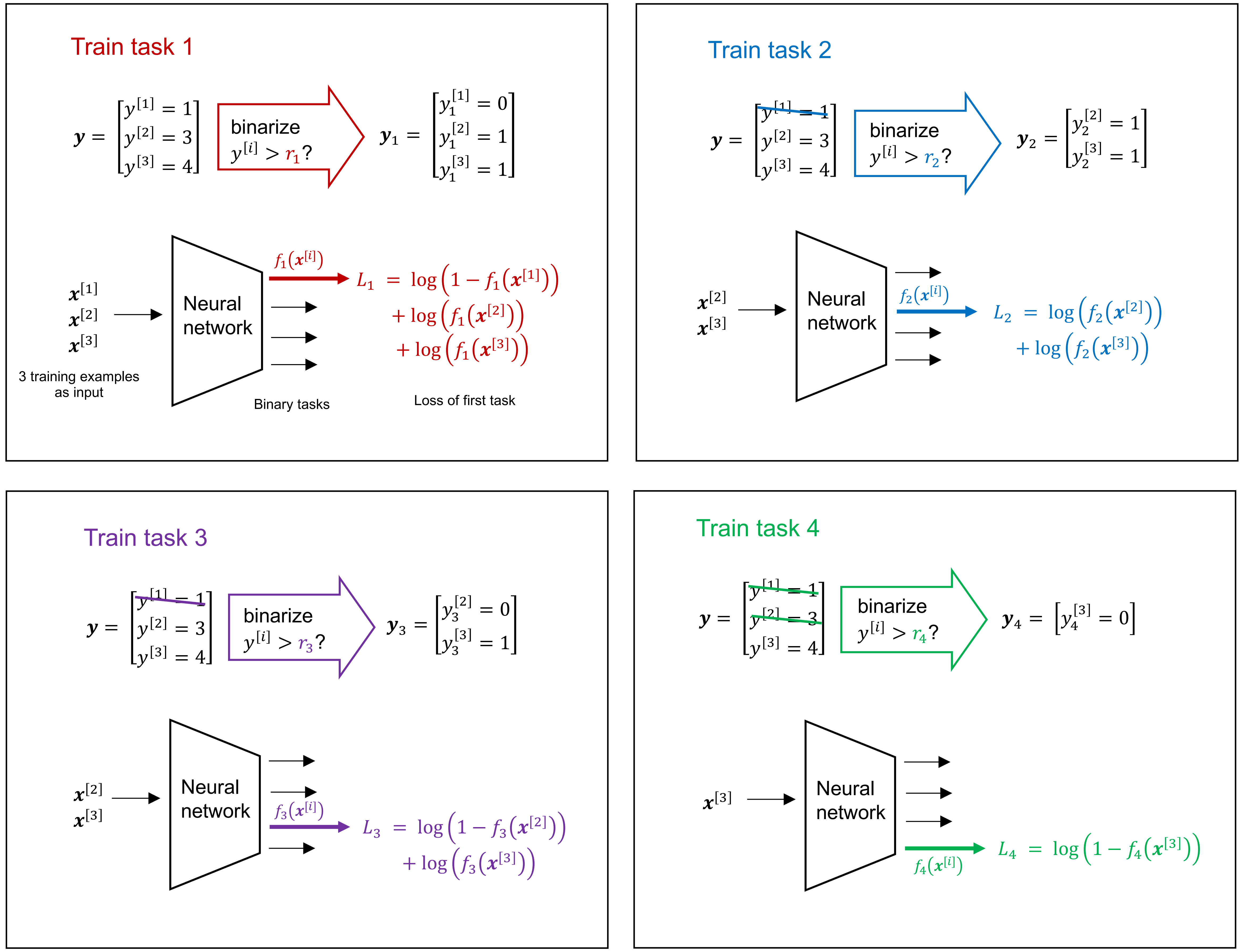
Table S1. Prediction errors on the test sets. Best results are highlighted in bold.

Method	Seed	TripAdvisor (Balanced)		Coursera (Balanced)	
		MAE	RMSE	MAE	RMSE
CE-RNN	0	1.13	1.56	1.01	1.48
	1	1.04	1.53	0.97	1.05
	2	1.05	1.54	1.12	1.65
	3	1.23	1.81	1.18	1.76
	4	1.03	1.52	0.84	1.26
	AVG±SD	1.10 ± 0.09	1.59 ± 0.12	1.02 ± 0.13	1.53 ± 0.19
OR-RNN [11]	0	1.06	1.53	0.98	1.34
	1	1.09	1.50	0.93	1.24
	2	1.11	1.53	1.12	1.47
	3	1.23	1.52	1.11	1.53
	4	1.07	1.40	0.85	1.16
	AVG±SD	1.11 ± 0.07	1.50 ± 0.06	1.00 ± 0.12	1.35 ± 0.15
CORAL [1]	0	1.15	1.58	0.99	1.29
	1	1.14	1.49	1.03	1.39
	2	1.16	1.46	1.14	1.40
	3	1.19	1.41	1.20	1.40
	4	1.13	1.47	0.82	1.11
	AVG±SD	1.15 ± 0.02	**1.48 ± 0.06**	1.04 ± 0.15	**1.33 ± 0.13**
CORN (ours)	0	1.09	1.55	0.95	1.37
	1	1.09	1.53	0.90	1.32
	2	1.01	1.45	1.07	1.49
	3	1.12	1.51	1.05	1.47
	4	1.03	1.46	0.78	1.14
	AVG±SD	**1.07 ± 0.05**	1.50 ± 0.04	**0.95 ± 0.12**	1.36 ± 0.14

CORN Loss

Assume 3 training examples $\boldsymbol{x}^{[1]}$, $\boldsymbol{x}^{[2]}$, and $\boldsymbol{x}^{[3]}$
with the following 3 rank labels:

$$\boldsymbol{y} = \begin{bmatrix} y^{[1]} = 1 \\ y^{[2]} = 3 \\ y^{[3]} = 4 \end{bmatrix}$$



Overall loss: $L(\boldsymbol{X}, \boldsymbol{y}) = \frac{1}{\sum_i |\boldsymbol{y}_i|} \sum_i L_i$

$$= \frac{1}{3 + 2 + 2 + 1} L_1 + L_2 + L_3 + L_4$$