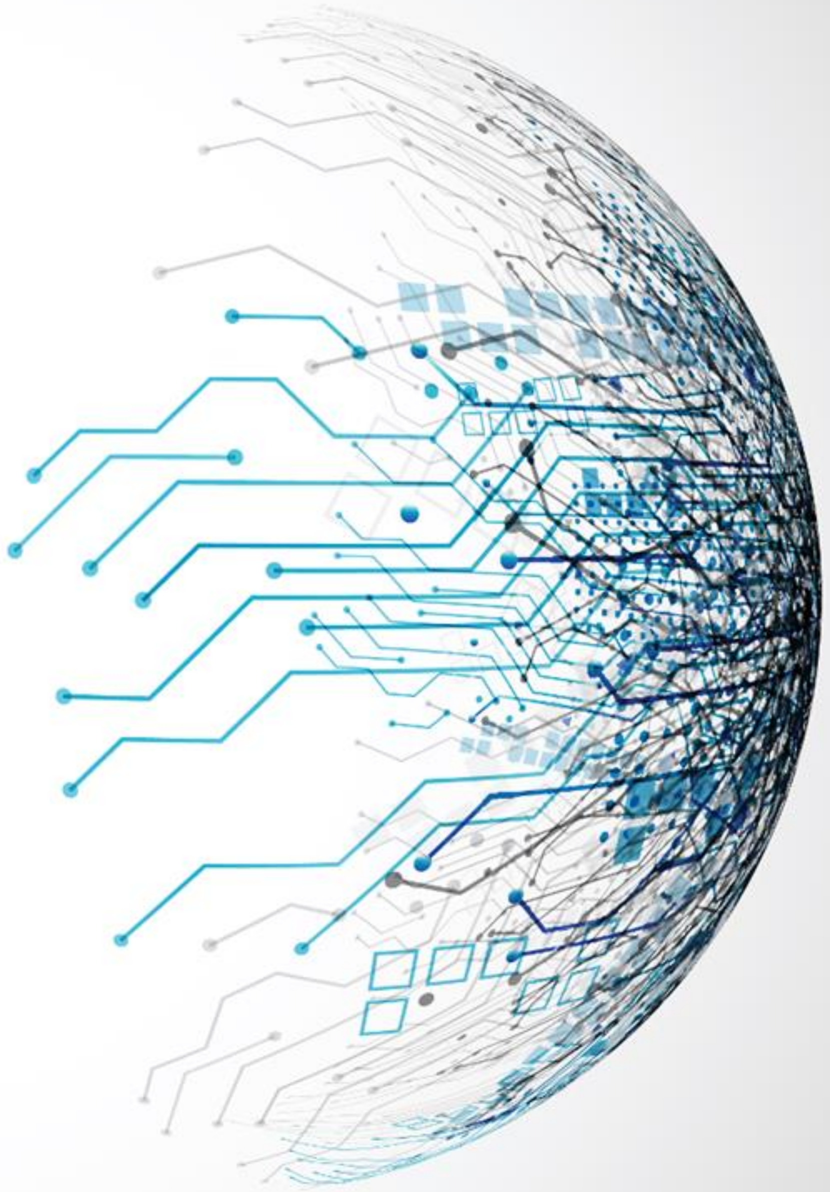
Deep Learning

Hyperparameter Optimization



Dr. Mohammed Salah Al-Radhi

(slides by: Dr. Tamás Gábor Csapó)

BME-VIK-TMIT

18 September 2024

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References

https://bit.ly/3AFIKuT

Deep Learning - BMEVITMMA19-EN | General | Microsoft Teams

Announcements

Project work

- Group and topic selection done

Milestone 1: data acquisition, data preparation (+ optional: containerization)

- Deadline: 7th week, **Oct 15**, Tuesday, 23:59, moodle, GitHub repo
- Oct 16, Wednesday class: consultation about projects (required for each group)

Milestone 2: baseline evaluation, baseline model

- Deadline: 11th week, **Nov 12**, Tuesday, 23:59, moodle, GitHub repo
- Nov 13, Wednesday class: consultation about projects (required for each group)

Final submission

- Deadline: end of 14th week, **Dec 6**, Friday, 23:59, moodle, GitHub repo and documentation

Outline

- Deep learning basics
- Incremental model development
- Initial model and manual fine-tuning
- Automatic hyperparameter optimization
- When is hyperopt not necessary?

Deep learning basics

Basic elements

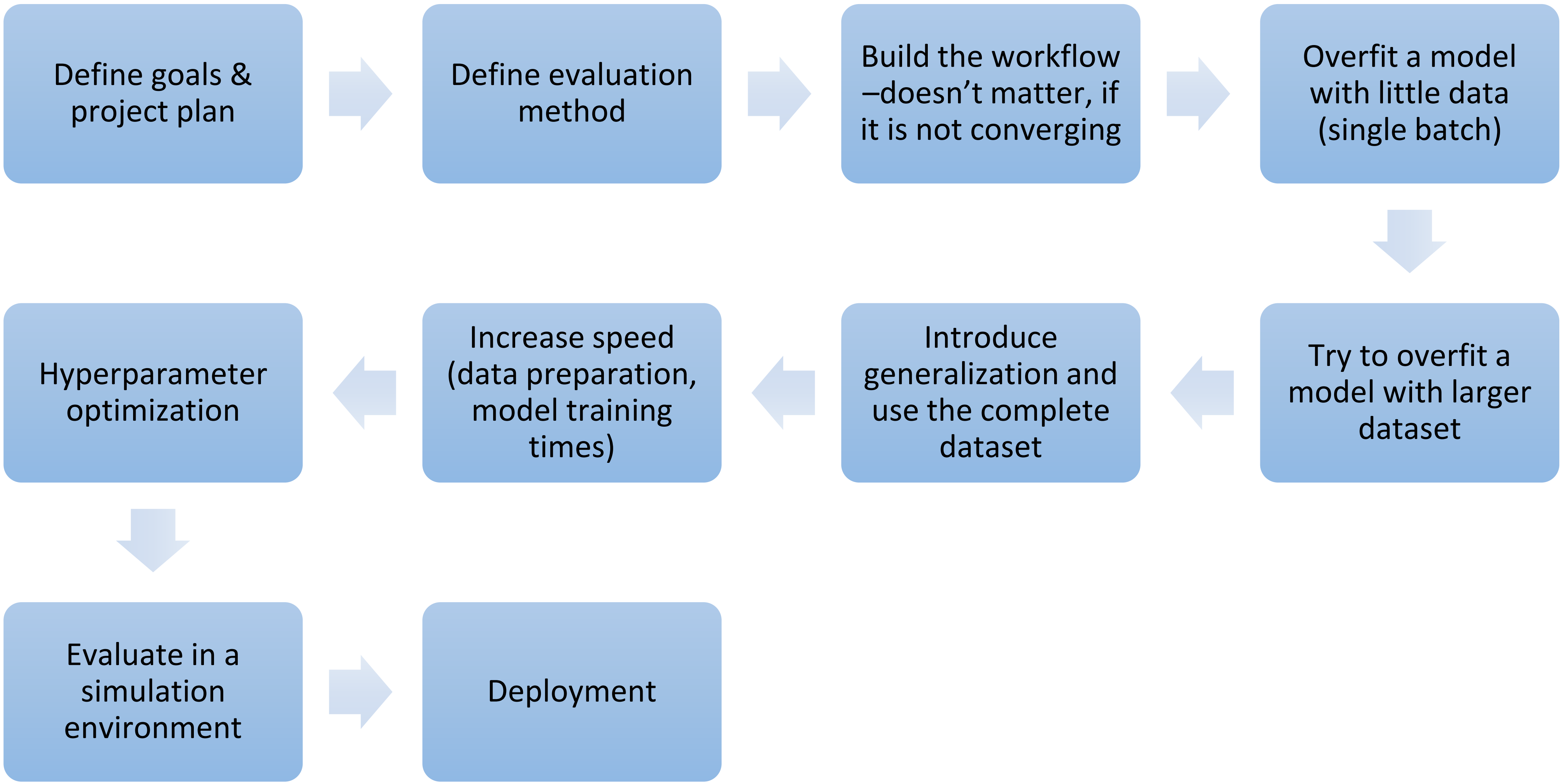
- **Architecture:**
  - FC: Fully Connected
  - RNN: Recurrent Neural Network
  - CNN: Convolutional Neural Network
- **Activation functions:** to become intelligent
- **Forward pass:** predict
- **Loss:** how good is my model?
- **Backward pass:** identify where the model can be improved
- **Optimizer:** improve the model
- **Regularization:** work on unseen data

References

- Fully connected networks and activation functions: https://cs231n.github.io/neural-networks-1/
- Recurrent Neural Networks: https://colah.github.io/posts/2015-08-Understanding-LSTMs/
- Convolutional neural networks: https://cs231n.github.io/convolutional-networks/
- Backpropagation (forward and backward pass): https://www.youtube.com/watch?v=bxe2T-V8XRs&list=PLiaHhY2iBX9hdHaRr6b7XevZtgZRa1PoU
- Loss functions and regularization: https://cs231n.github.io/neural-networks-2/
- Optimizers, early stopping, mini-batching: https://www.deeplearningbook.org/contents/optimization.html

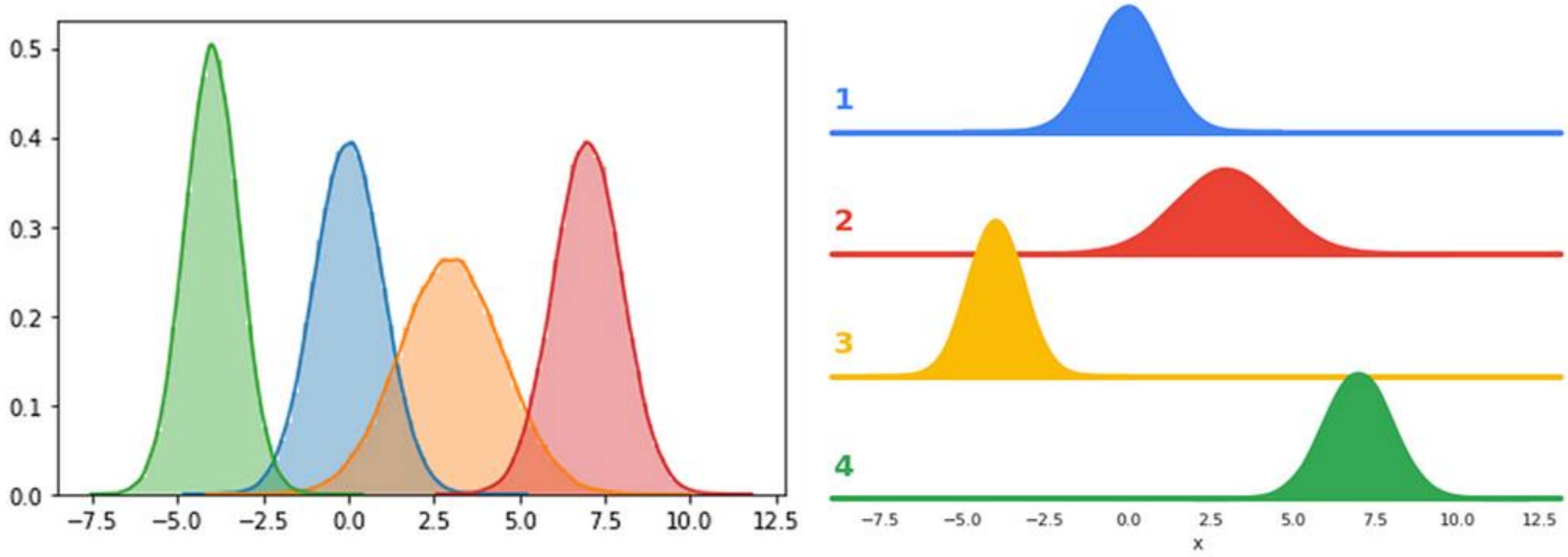
Incremental model development

Machine learning project main steps



Build the workflow

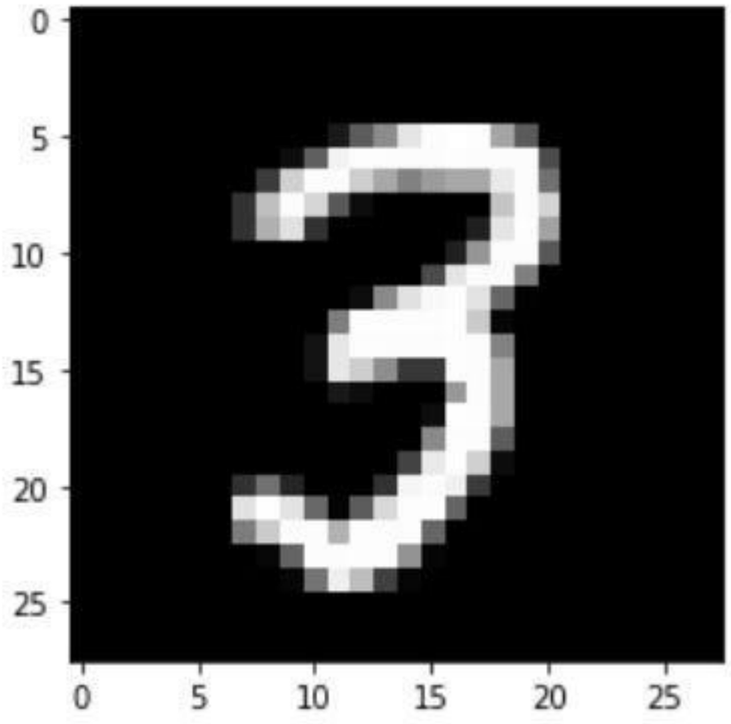
- Try to understand your data!
- Use a basic statistical model
- sns.displot



Source: https://towardsdatascience.com/sorry-but-sns-distplot-just-isnt-good-enough-this-is-though-ef2ddbf28078

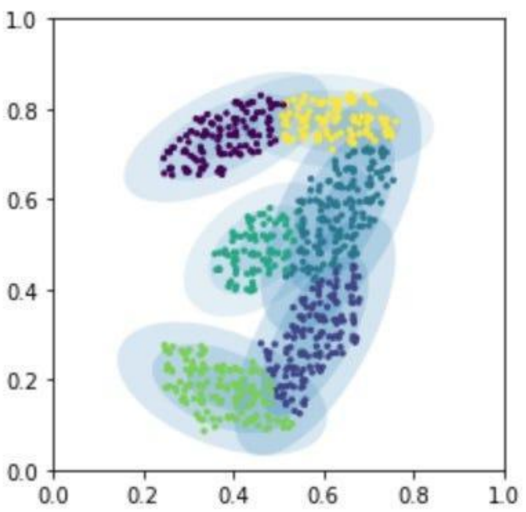
Start with a simple neural network

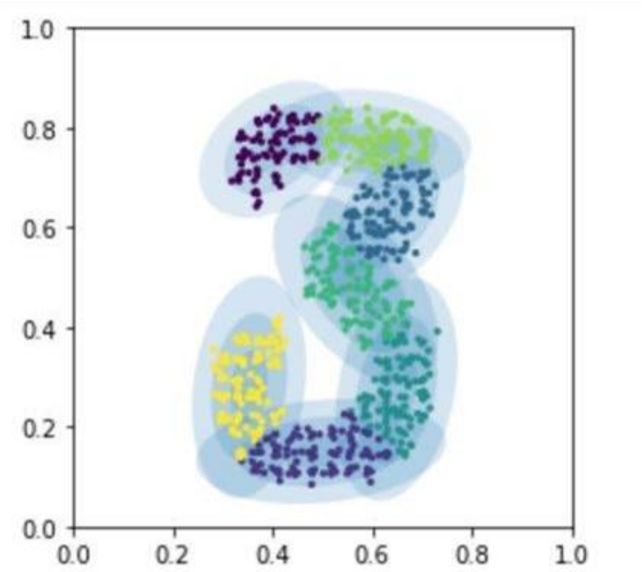
- What can you observe on the „MNIST” image with your eye?



Start with a simple neural network

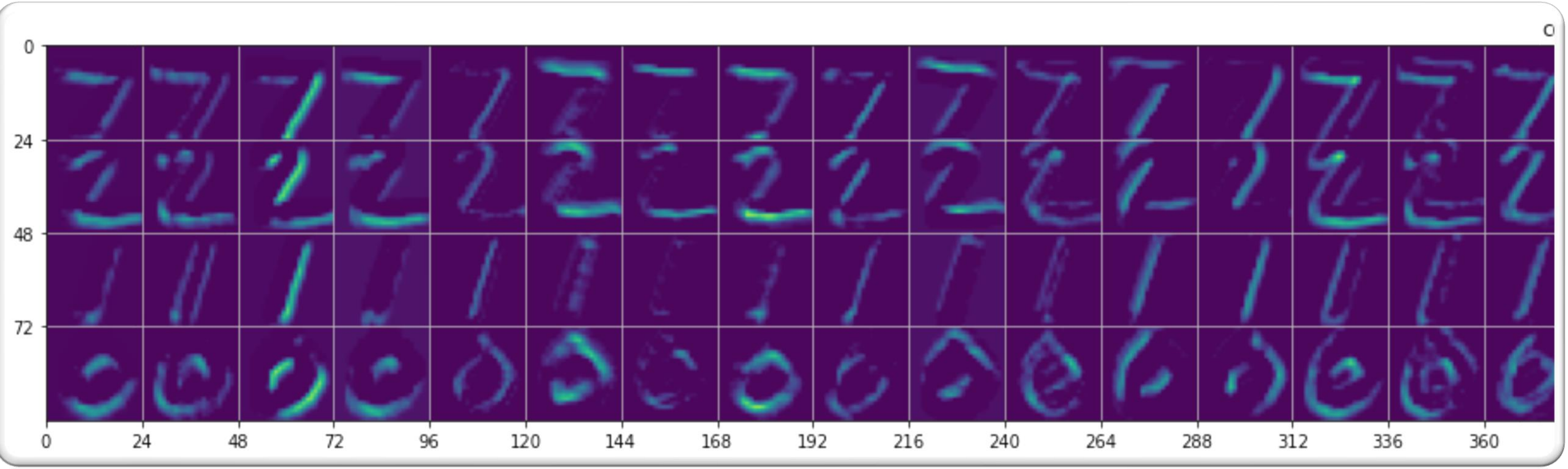
- What can a simple statistical model see?





Start with a simple neural network

- What can a simple CNN see? Check activations!



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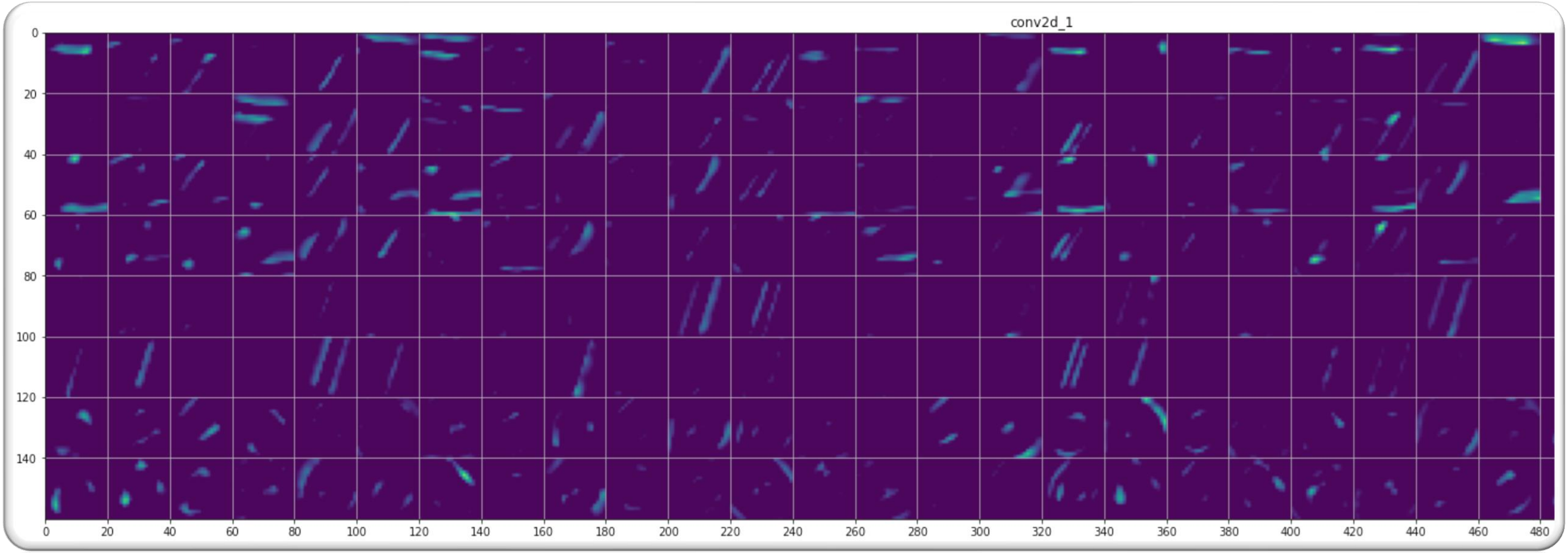


Simple model …. more complex

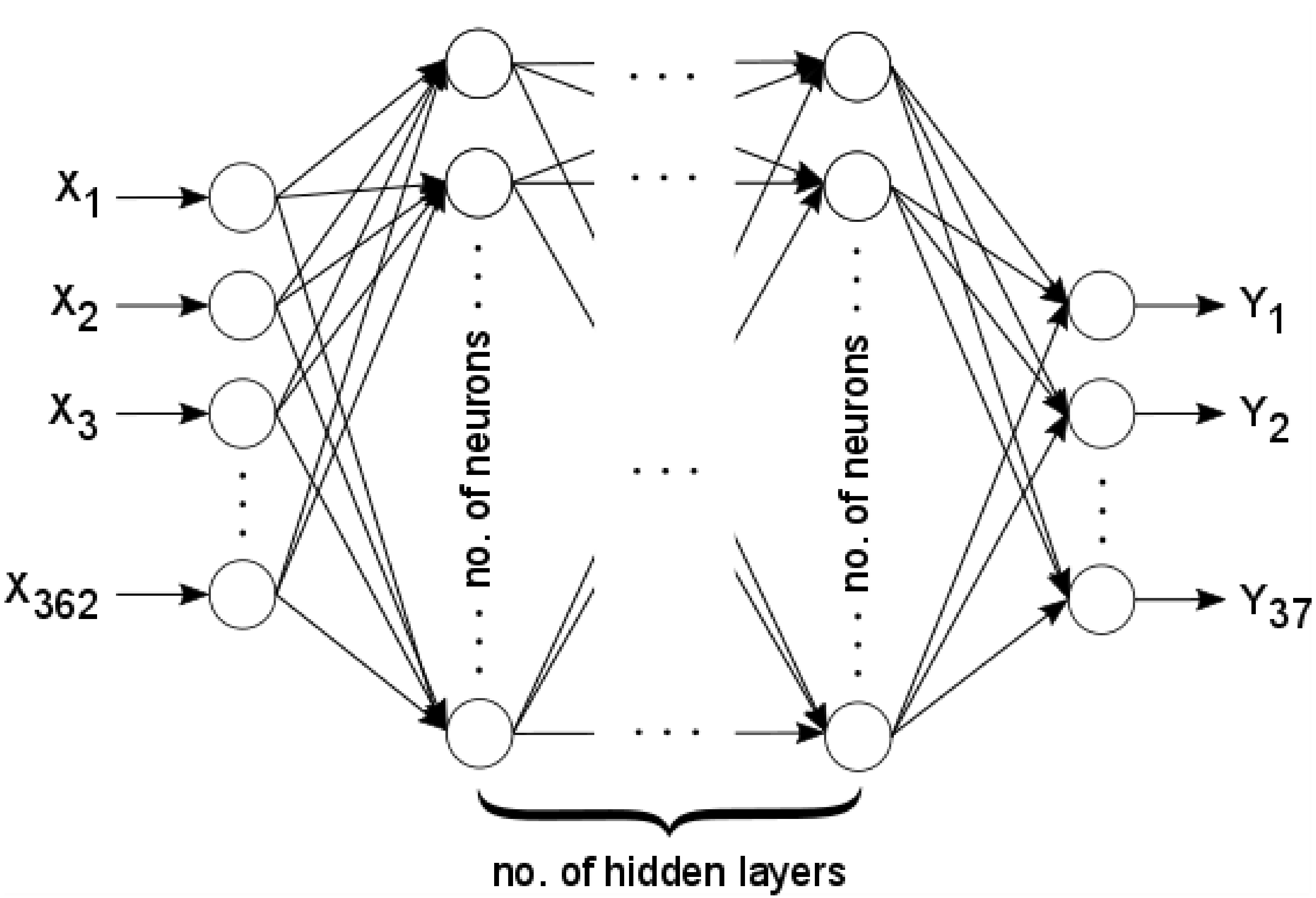
- Start from a simple model, single batch of data
- Add more data
- Try more complex models

Why automatic hyperopt?

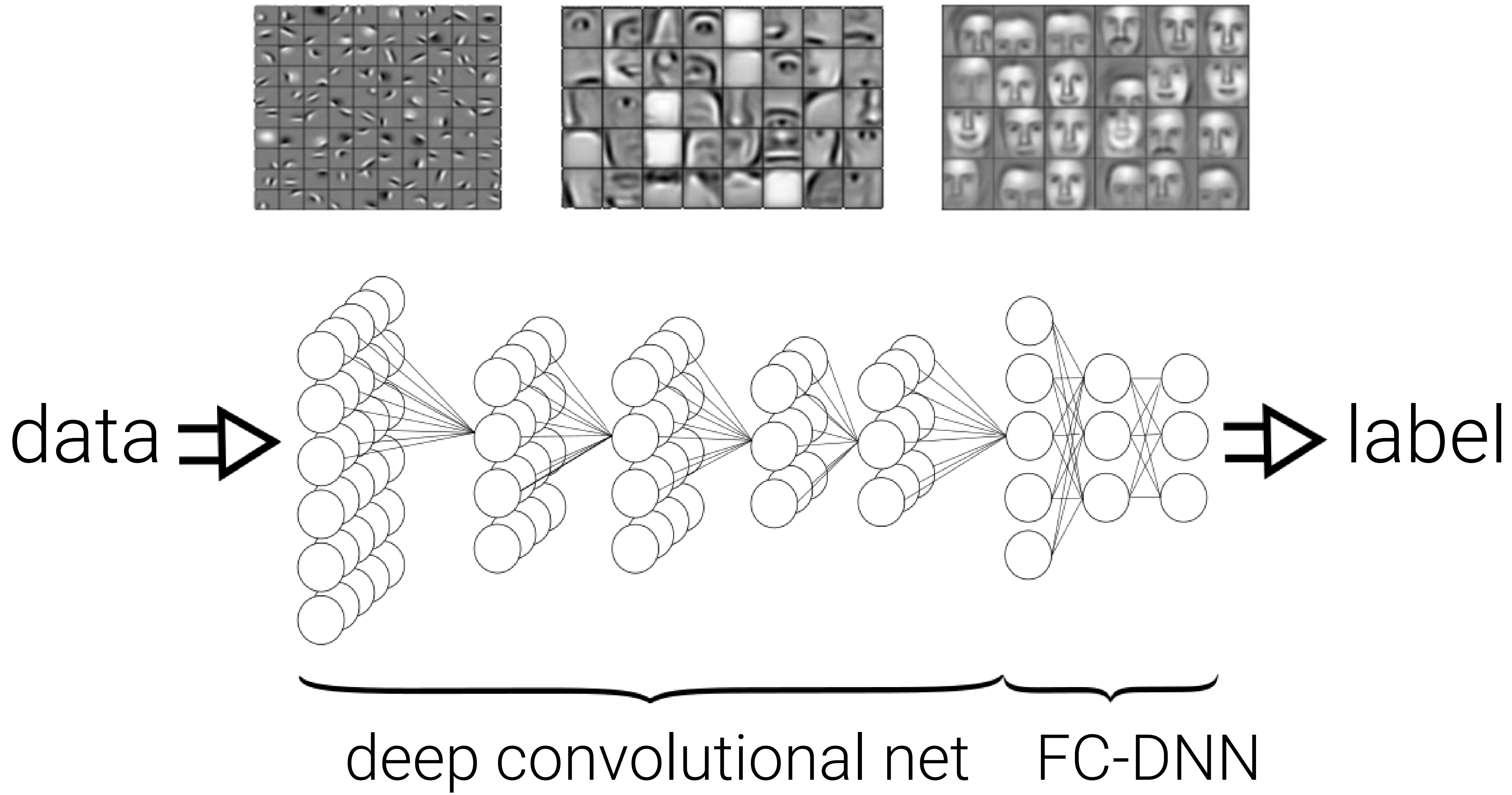
- When manual hyperopt isn’t feasible any more
- Tweak model performance
- Analyze several 1000 different parameter combinations

What to hyperopt / 1: Network architectures

FC = Fully Connected, Feed-forward

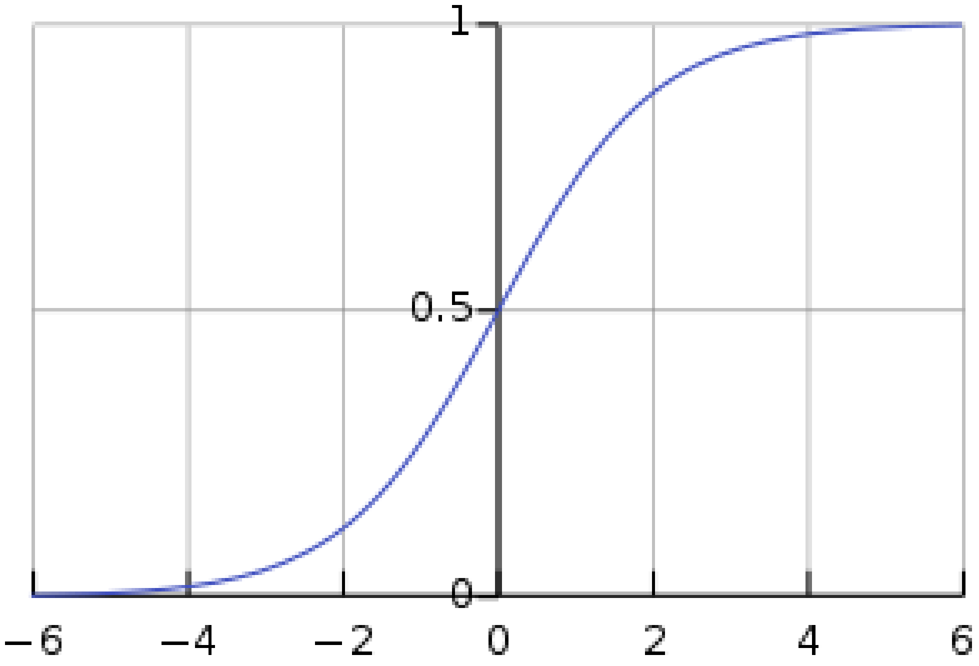


Convolutional: 2D-CNN



What to hyperopt / 2: activation functions

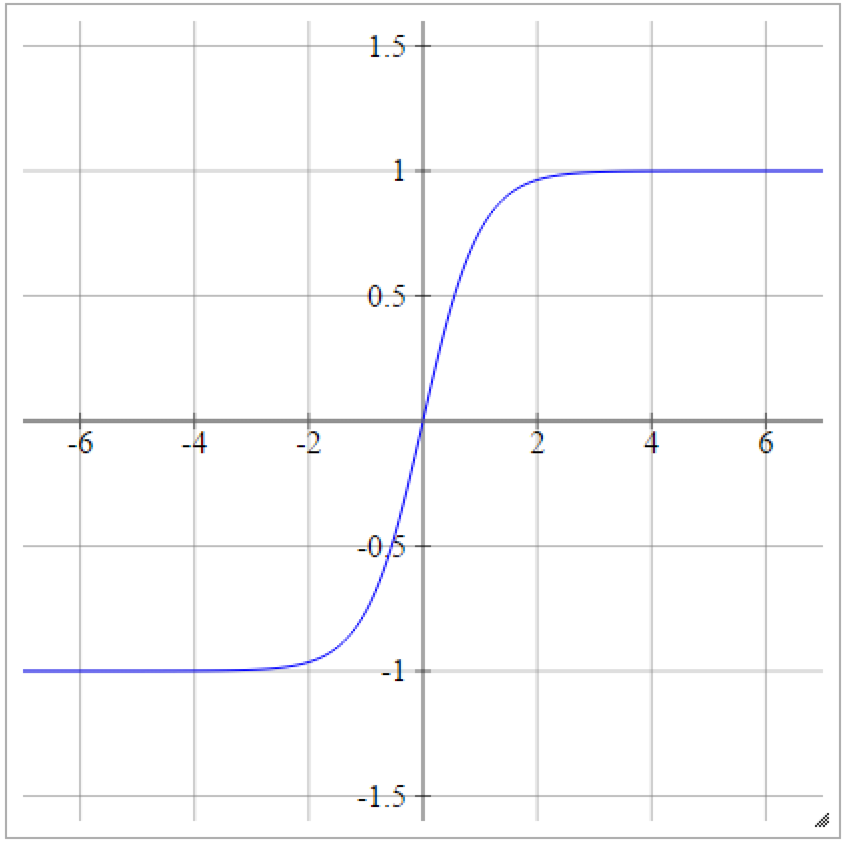
Sigmoid



$$f(x) = \sigma(x) = \frac{1}{1 + e^{-x}}$$

Source: https://en.wikipedia.org/wiki/Sigmoid_function

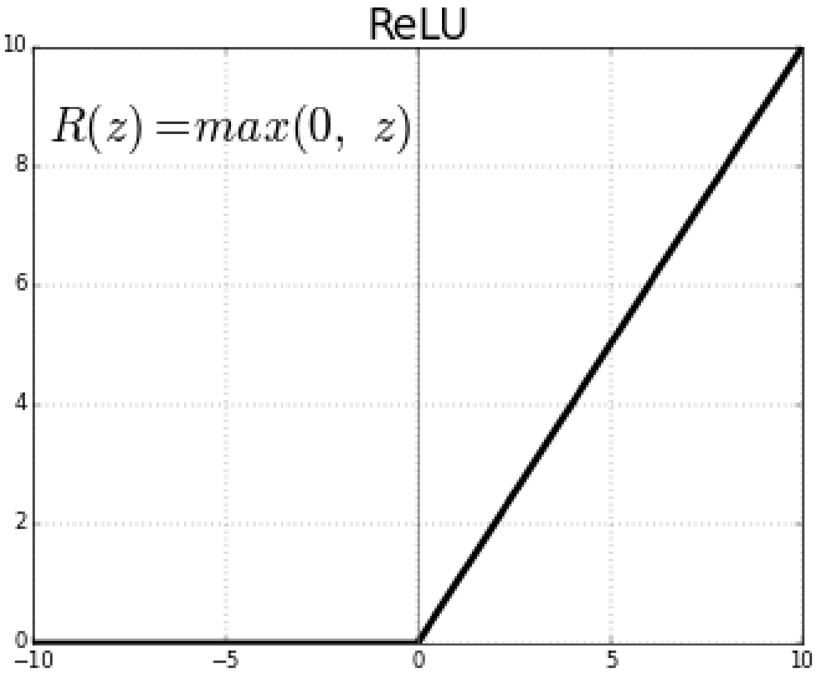
Tanh



$$f(x) = \tanh(x) = \frac{(e^x - e^{-x})}{(e^x + e^{-x})}$$

Source : https://stats.stackexchange.com/questions/115258/comprehensive-list-of-activation-functions-in-neural-networks-with-pros-cons

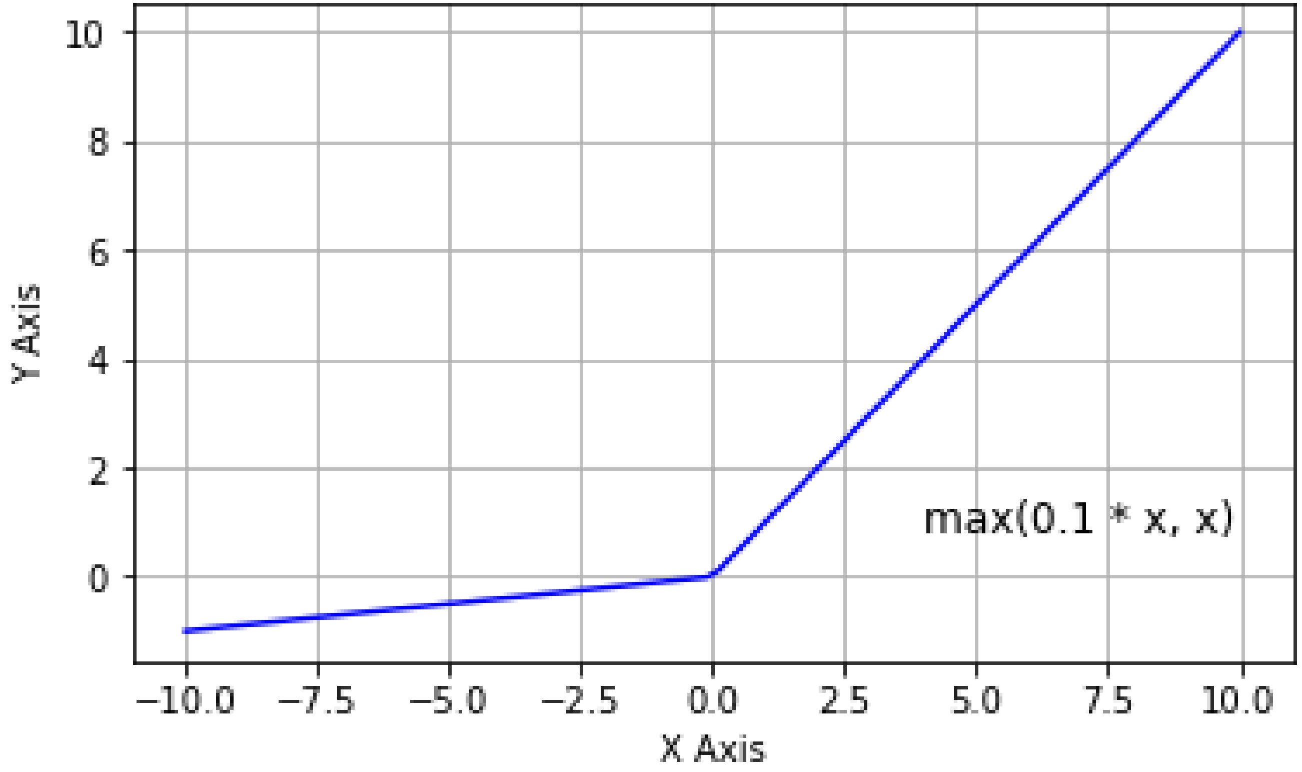
ReLU



$$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$$

Source : https://medium.com/@kanchansarkar/relu-not-a-differentiable-function-why-used-in-gradient-based-optimization-7fef3a4cecec

Leaky ReLU, PReLU

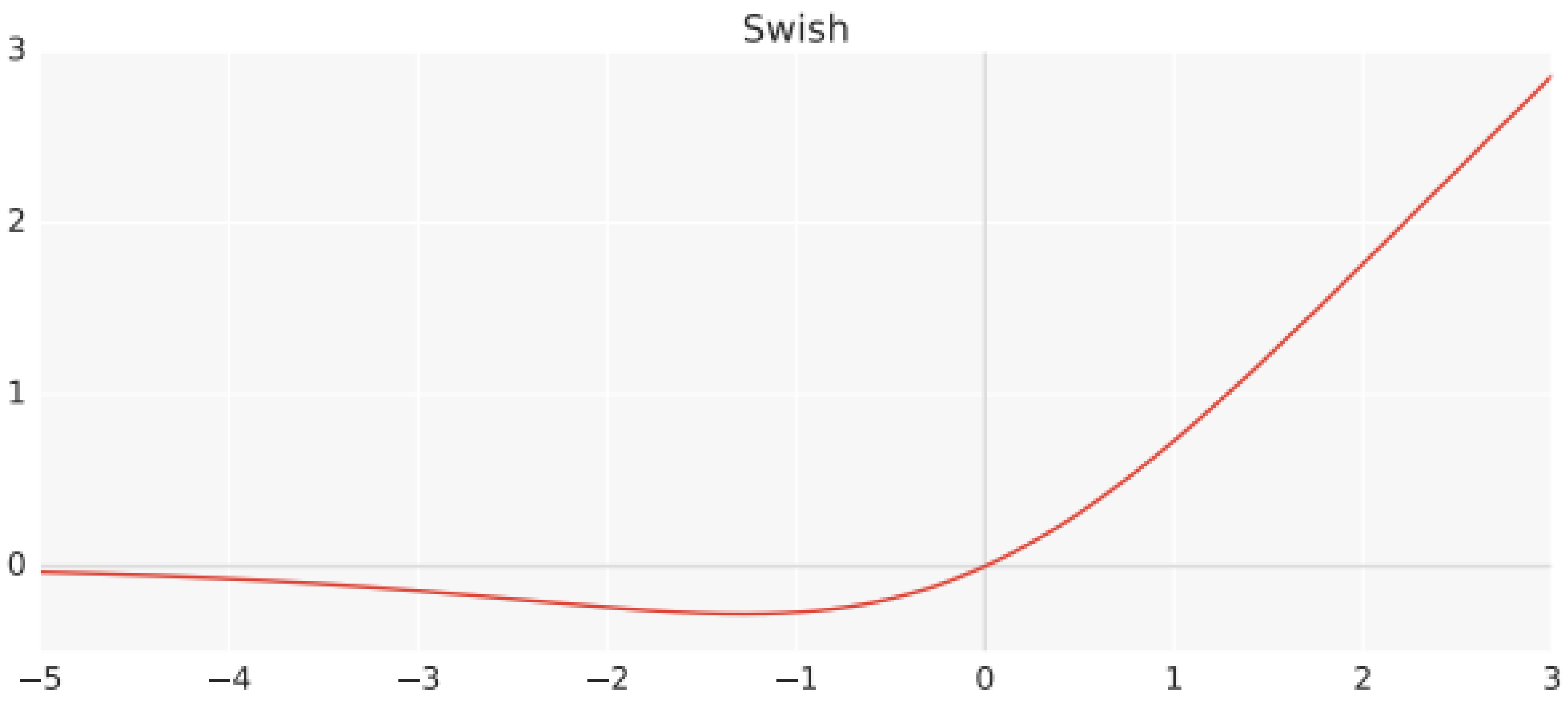


$$f(x) = \begin{cases} 0.01x & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$$

$$f(x) = \begin{cases} x & \text{if } x > 0 \\ ax & \text{otherwise} \end{cases}$$

Forrás: https://medium.com/@kanchansarkar/relu-not-a-differentiable-function-why-used-in-gradient-based-optimization-7fef3a4cecec

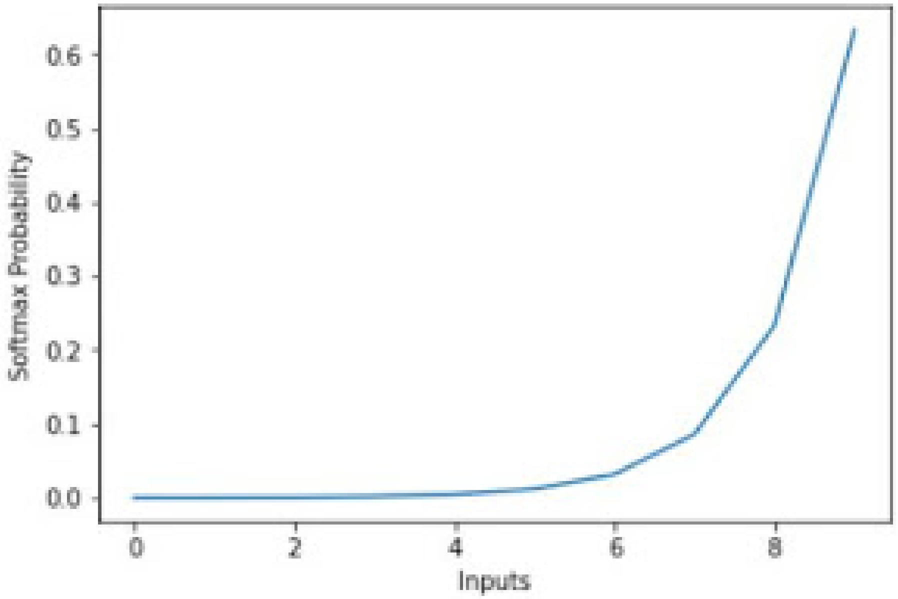
SWISH



$$f(x) = x * sigmoid(x)$$
$$= x * (1 + e^{-x})^{-1}$$

Source : https://medium.com/@neuralnets/swish-activation-function-by-google-53e1ea86f820

Softmax



z is a vector of the inputs to the output layer (if you have 10 output units, then there are 10 elements in z)

$$\sigma(z)_j = \frac{e^{z_j}}{\sum_{k=1}^{K} e^{z_k}}$$

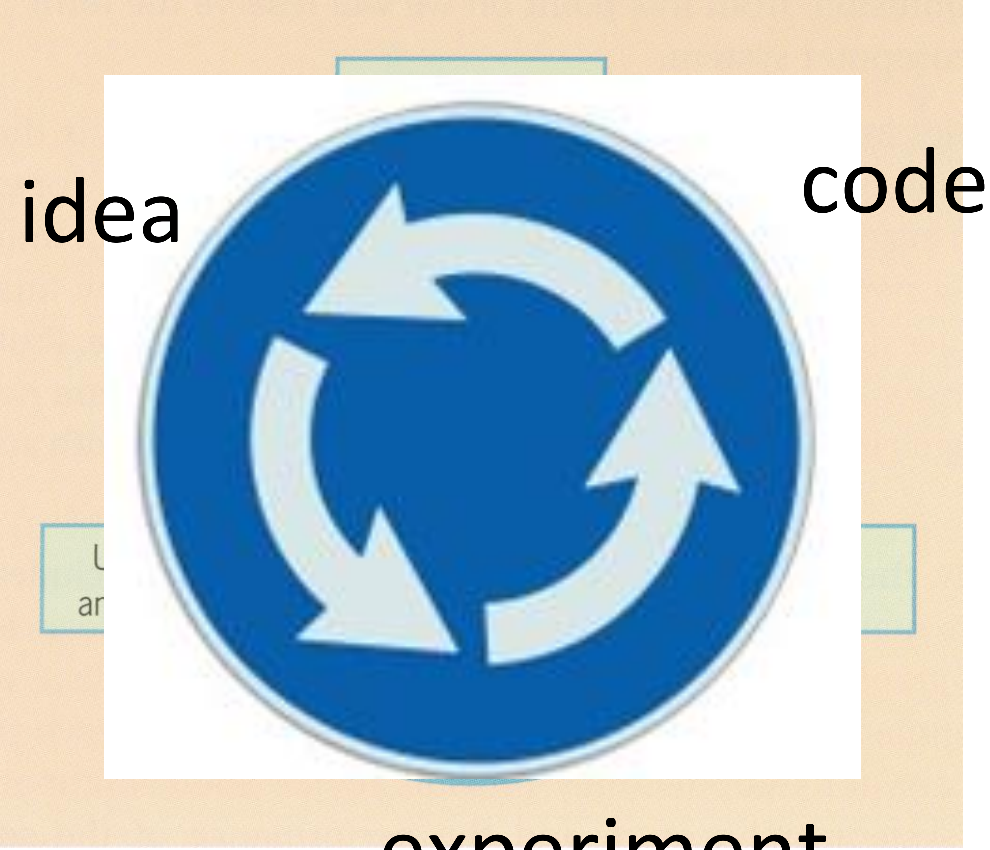
What to hyperopt / 3: optimizer algorithms

Optim

- torch.optim.
  - SGD
  - RMSprop
  - Adam
  - RAdam
  - NAdam
  - AdamW
  - Adadelta
  - Adagrad
  - Adamax

https://pytorch.org/docs/stable/optim.html

ML/ DL: iterative process...



Hyperparameters (for a simple FC-DNN)

- Epoch number
- Batch size
- Alpha Learning rate
- Beta Momentum
- Optimizer
- Number of layers
- Number of neurons
- Activation functions

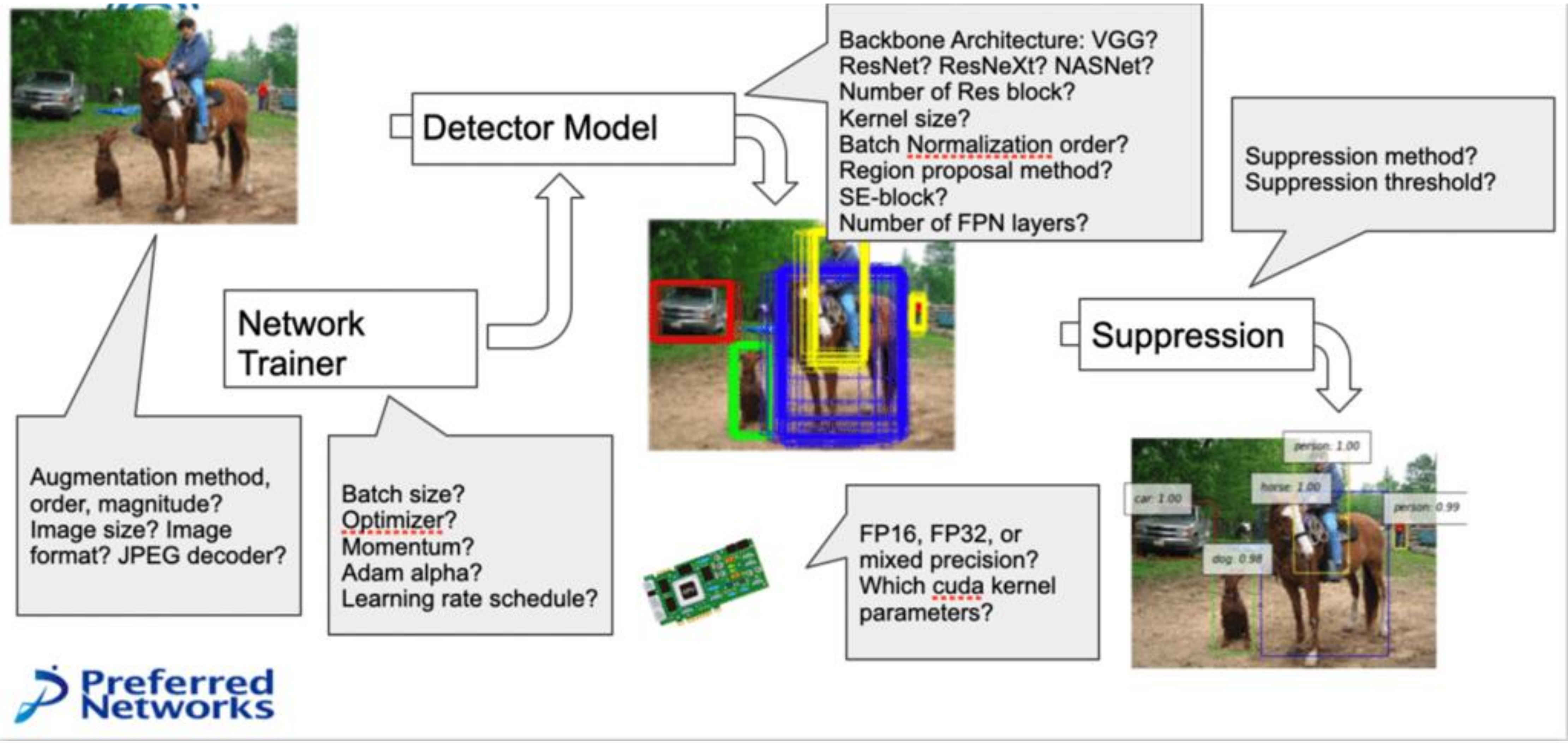
Hyperparameters, linear scale

- Layers: 2, 3, 4
- No. of neurons: 100, 200, 300, … 1000

Hyperparameters, what scale?

- Alpha: 0.0001, 0.001, … 1
- 10^{-4}, 10^{-3}, …10^{0}
- 10-base logarithm: back to linear scale, -4, -3, , … 0

… and even more hyperparameters!



Source: https://optuna.org

Generalization

Generalization

Training set (labels known)

Test set (labels unknown)

- How well does a learned model generalize from the data it was trained on to a new test set?

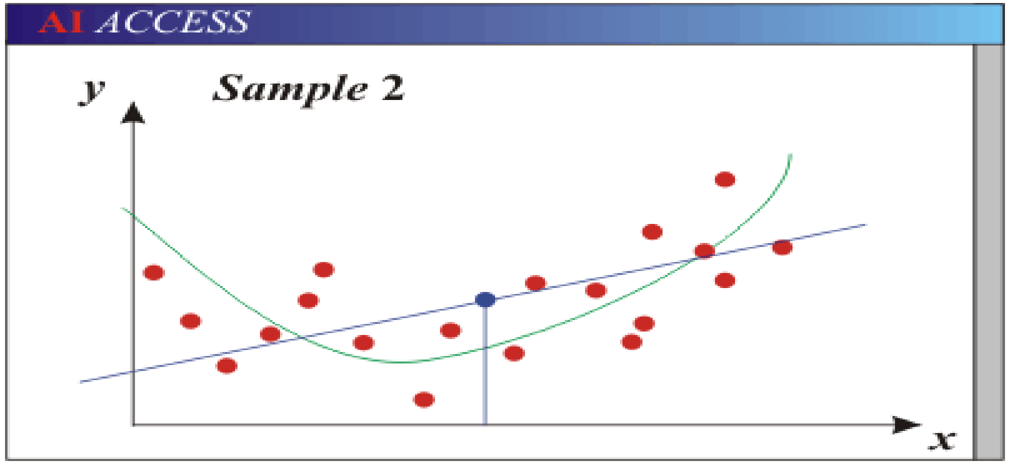
Slide credit: L. Lazebnik

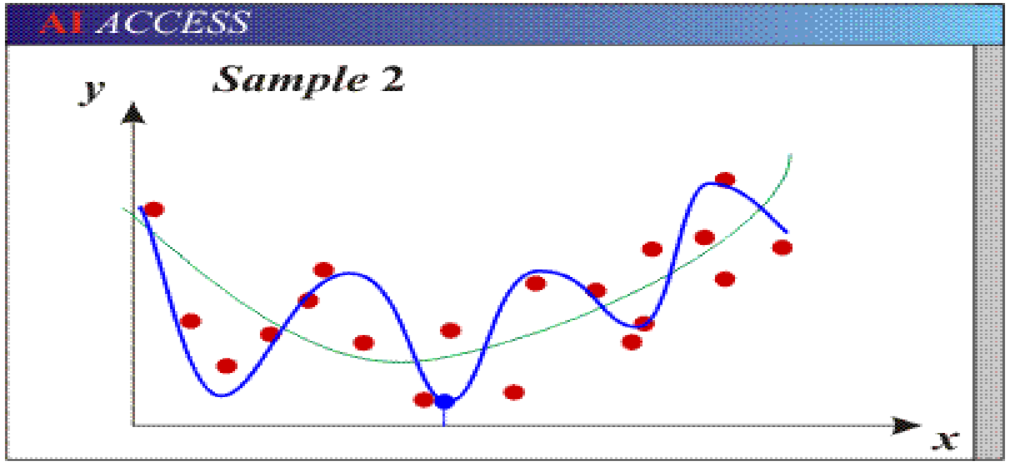
Generalization

- Components of generalization error
  - **Bias:** how much the average model over all training sets differ from the true model?
    - Error due to inaccurate assumptions/simplifications made by the model
  - **Variance:** how much models estimated from different training sets differ from each other
- **Underfitting:** model is too "simple" to represent all the relevant class characteristics
  - High bias and low variance
  - High training error and high test error
- **Overfitting:** model is too "complex" and fits irrelevant characteristics (noise) in the data
  - Low bias and high variance
  - Low training error and high test error

Slide credit: L. Lazebnik

Bias-Variance Trade-off

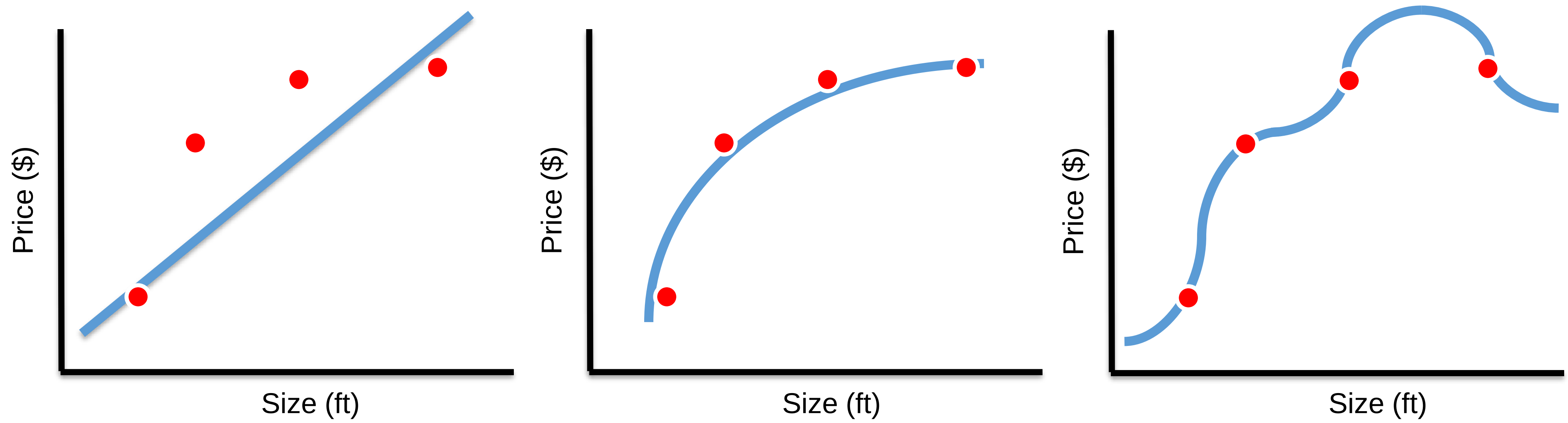




- Models with too few parameters are inaccurate because of a large bias (not enough flexibility).
- Models with too many parameters are inaccurate because of a large variance (too much sensitivity to the sample).

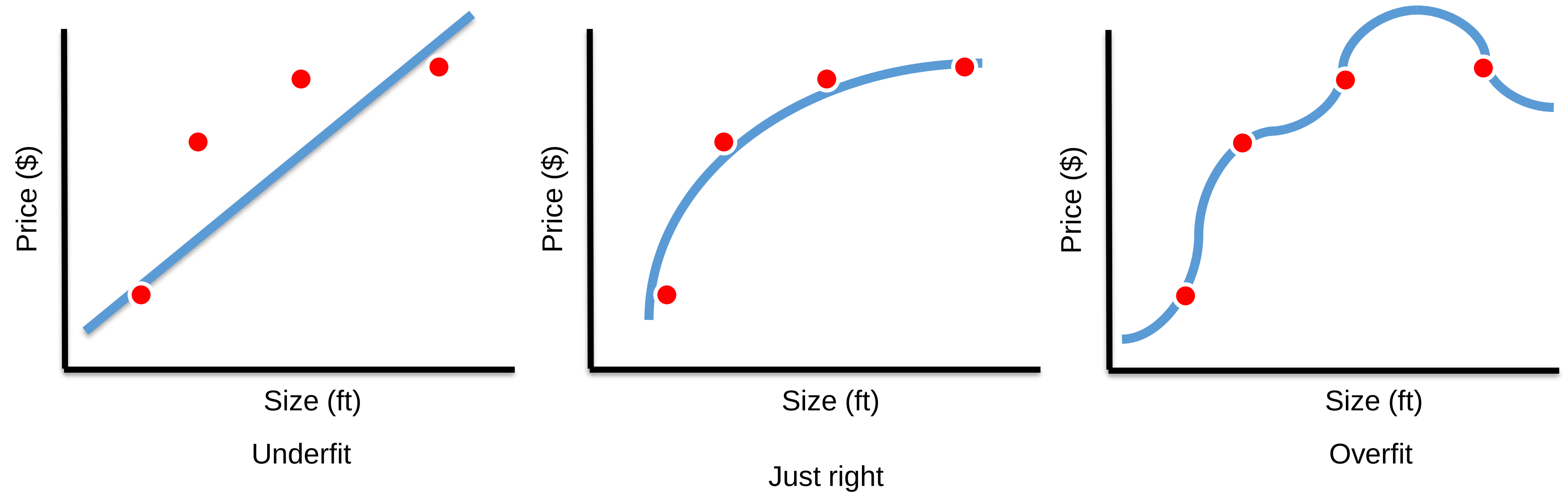
Slide credit: D. Hoiem

Bias/Variance Trade-off



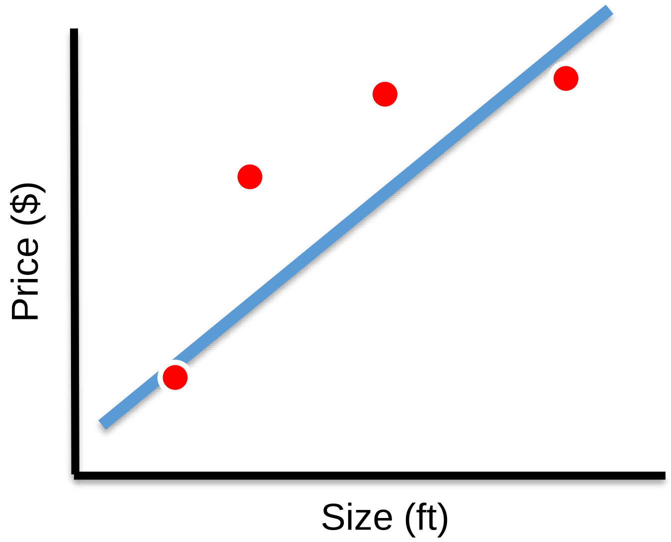
Source: Andrew Ng

Bias/Variance Trade-off

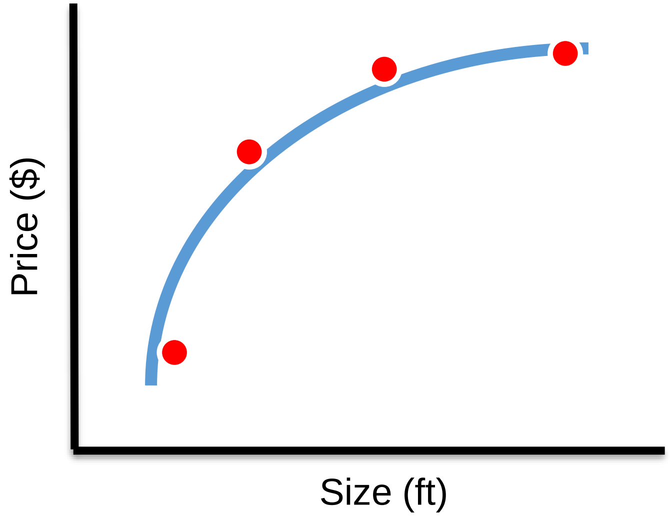


Source: Andrew Ng

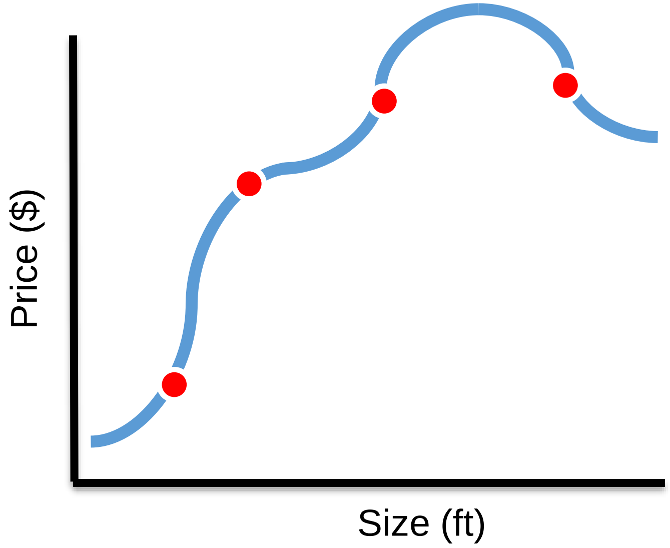
Linear Regression with Regularization



Underfit
High bias
Too simple
Too much regularization



Just right



Overfit
High Variance
Too Complex
Too little regularization

Source: Andrew Ng

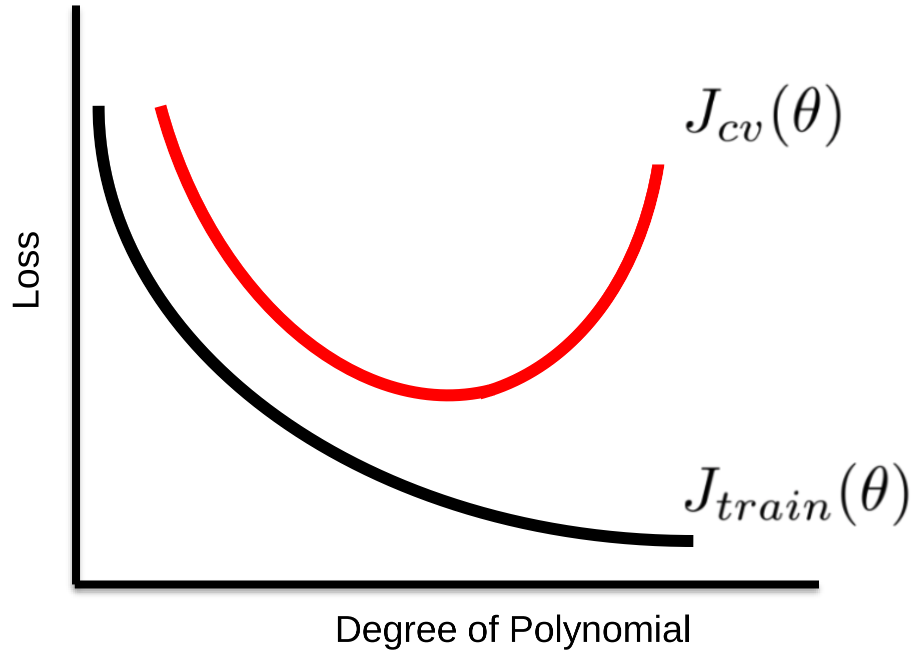
Bias / Variance Trade-off

- Training error

$$J_{train}(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

- Cross-validation error

$$J_{cv}(\theta) = \frac{1}{2m_{cv}}\sum_{i=1}^{m_{cv}}(h_\theta(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$$



Source: Andrew Ng

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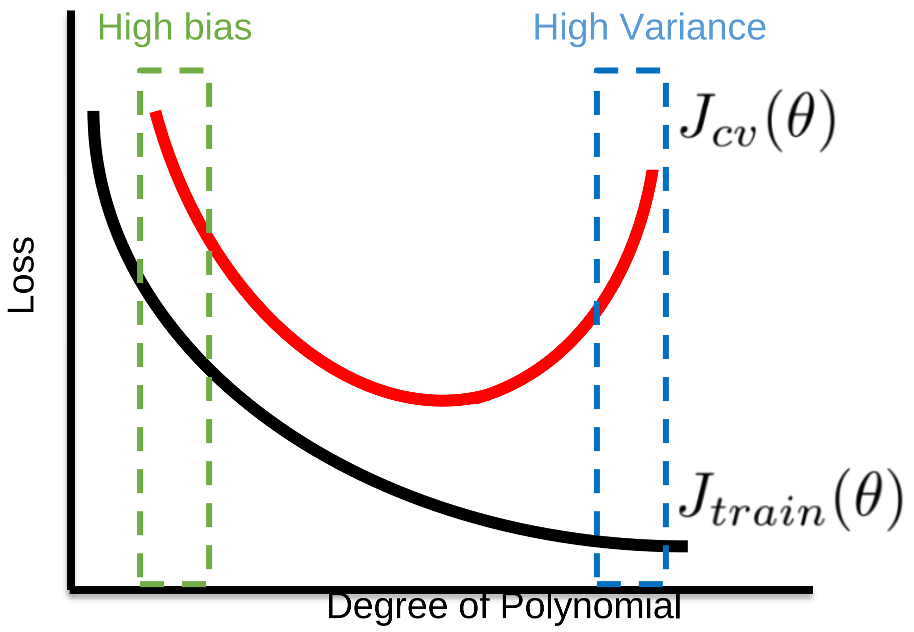
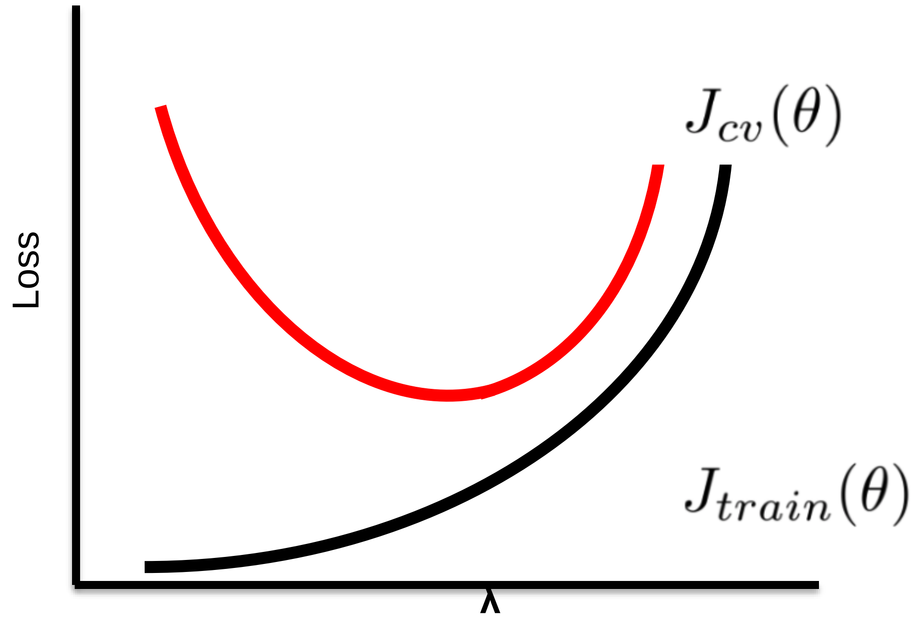


Bias / Variance Trade-off with Regularization

- Training error $$J_{train}(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \frac{\lambda}{2m}\sum_{j=1}^{m}\theta_j^2$$
- Cross-validation error $$J_{cv}(\theta) = \frac{1}{2m_{cv}}\sum_{i=1}^{m_{cv}}(h_\theta(x_{cv}^{(i)}) - y_{cv}^{(i)})^2 + \frac{\lambda}{2m_{cv}}\sum_{j=1}^{m_{cv}}\theta_j^2$$



Source: Andrew Ng

Bias / Variance Trade-off with Regularization

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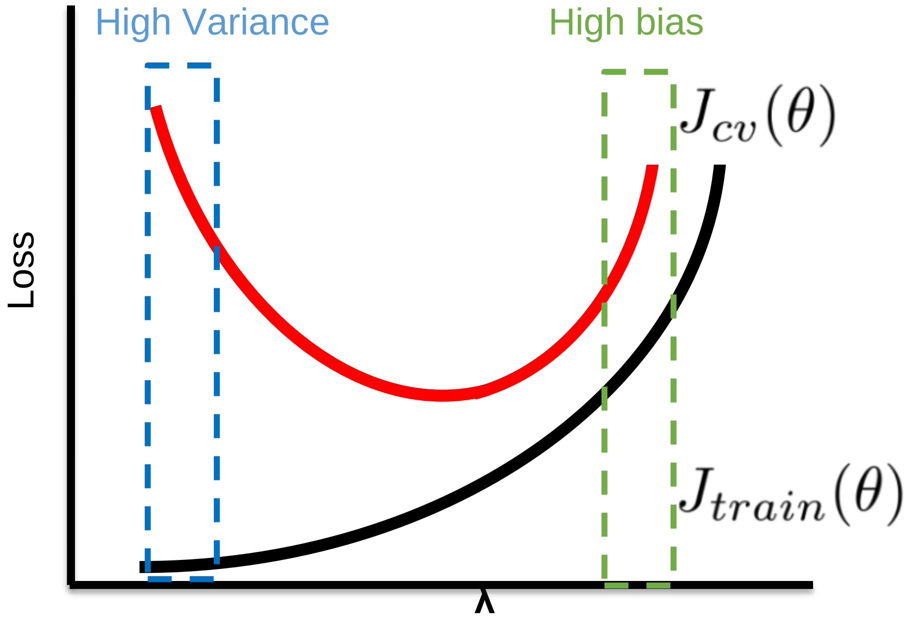

Source: Andrew Ng

Problem: Fail to Generalize

- Should we get more data?

Problem: Fail to Generalize

- Should we get more data?

- Getting more data does not always help

Problem: Fail to Generalize

- Should we get more data?
- Getting more data does not always help
- How do we know if we should collect more data?

Things You Can Try

- Get more data
  - When you have high variance
- Try different features
  - Adding feature helps fix high bias
  - Using smaller sets of feature fix high variance
- Try tuning your hyperparameter
  - Decrease regularization when bias is high
  - Increase regularization when variance is high

Things You Can Try

- Get more data
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Analyze your model before you act

Hyperparameter space

Manual search

1. experiment
- 5 hidden layers
- 1000 neurons
- Adam
- Accuracy=0.5

2. experiment
- 3 hidden layers
- 1000 neurons
- Adam
- Accuracy=0.4

3. experiment
- 6 hidden layers
- 1000 neurons
- Adam
- Accuracy=0.55

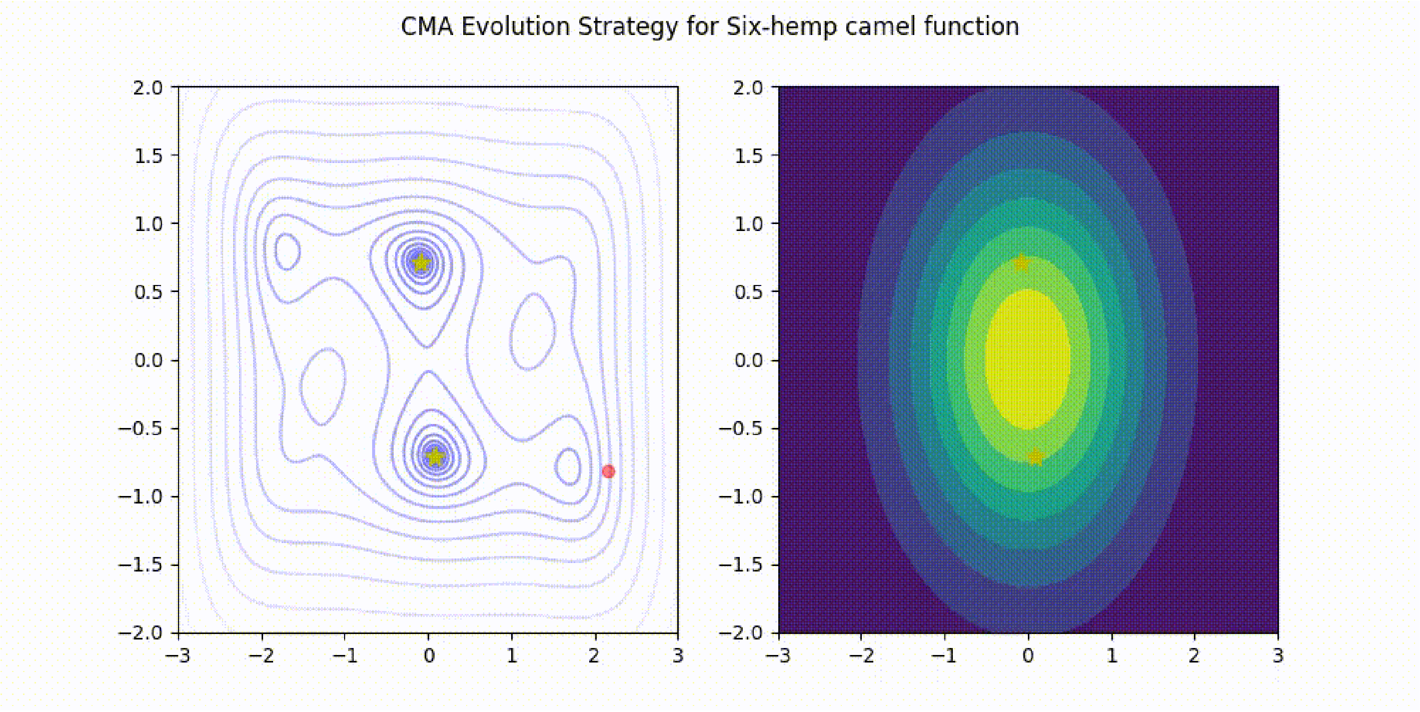
4. experiment
- 5 hidden layers
- 2000 neurons
- Adam
- Accuracy=0.56

….. ?????

Source: https://optuna.org

Bayesian hyperopt / other options

- GP: Gaussian Processes
- CMA-ES: Covariance Matrix Adaptation Evolution Strategy



Forrás: https://optuna.org & https://github.com/CyberAgentAILab/cmaes

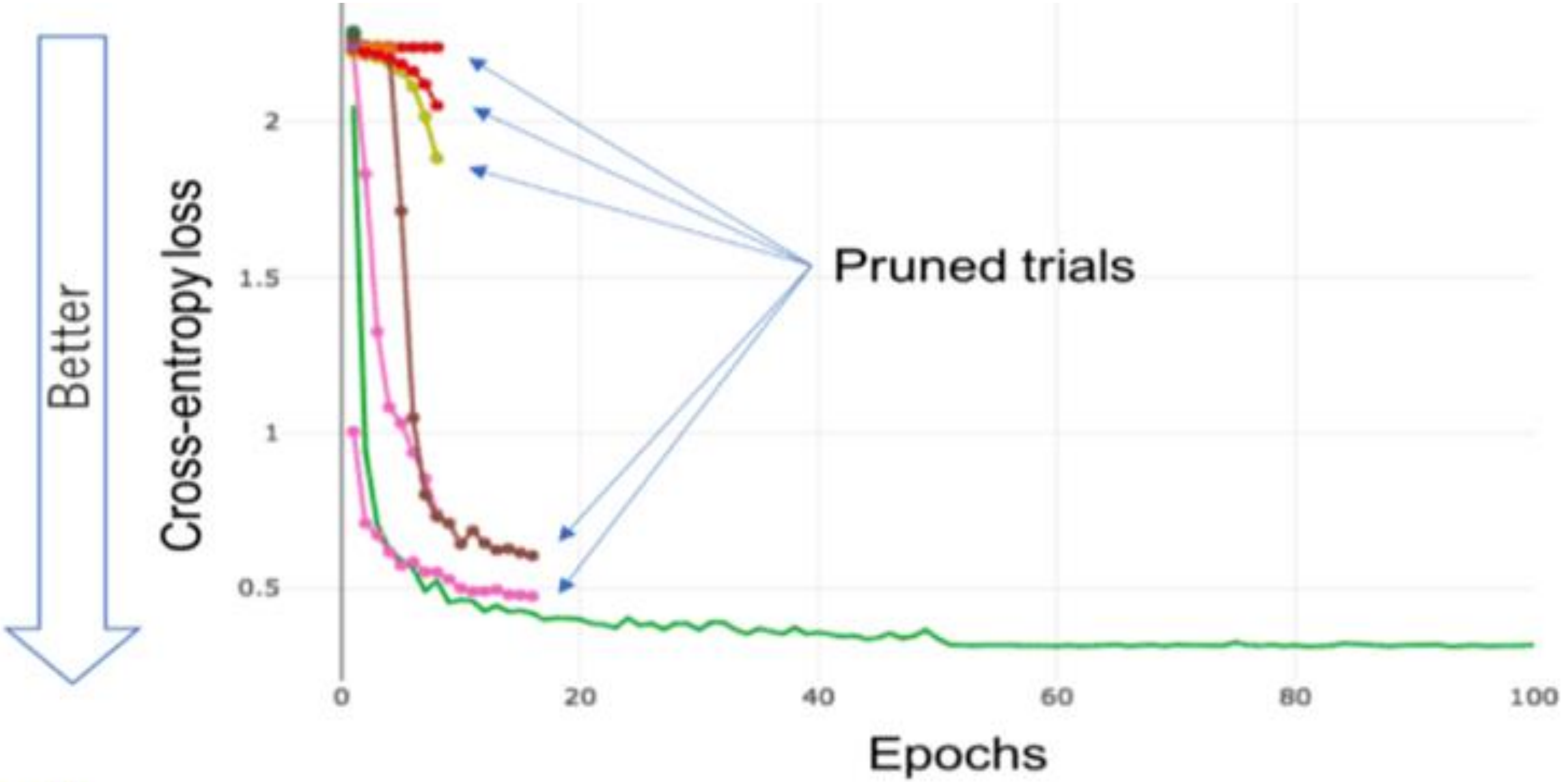
HyperBand / pruning

- Idea: don’t finish all the trainings!
- the trend can already be seen based on the first epochs
- training for several elements of the hyperparameter space, but only up to 2 epochs
- which of the alternatives could potentially be good?
- further training chosen ones for 2 additional epochs
- ... iterative narrowing of the parameter space

Source: https://optuna.org

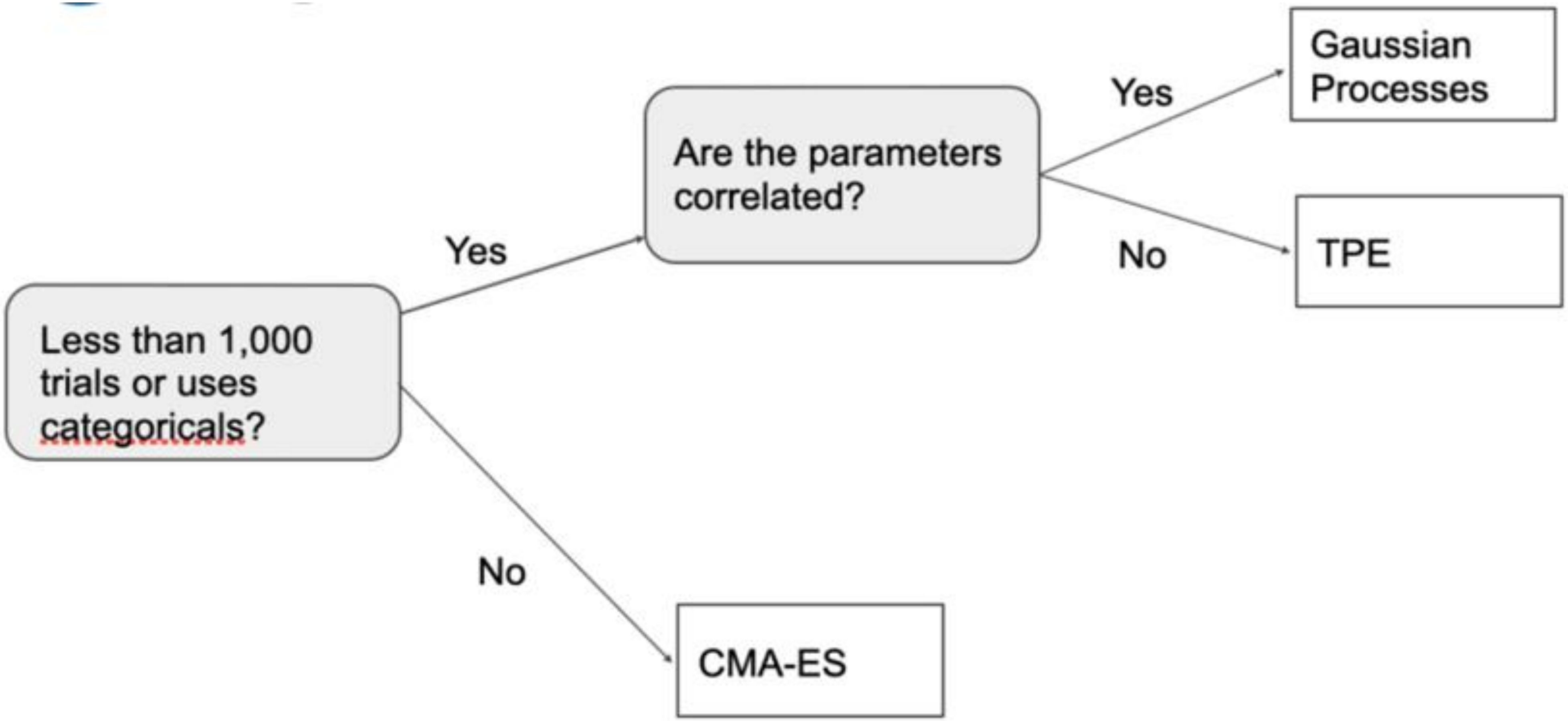
HyperBand / pruning

- … iterative narrowing of the parameter space



Source: https://optuna.org

Which hyperopt type to choose?



Source: https://optuna.org

Distributed hyperopt

```
$ python example.py
[I 2019-05-21 11:16:43,493] Using an existing study with name 'example-study' in
stead of creating a new one.
      total [############################......................] 57.17%
this epoch [####################################..............] 71.73%
       134 iter, 5 epoch / 10 epochs
    31.547 iters/sec. Estimated time to finish: 0:00:03.181785.
```

```
$ python example.py
[I 2019-05-21 11:16:42,393] Using an existing study with name 'example-stu
instead of creating a new one.
      total [##########################################........] 84.91%
this epoch [########################..........................] 49.07%
       199 iter, 8 epoch / 10 epochs
    44.127 iters/sec. Estimated time to finish: 0:00:00.801665.
```

```
$ python example.py
[I 2019-05-21 11:16:43,621] Using an existing study with name 'example-study' in
stead of creating a new one.
      total [########################..........................] 49.92%
this epoch [#################################################.] 99.20%
       117 iter, 4 epoch / 10 epochs
     27.85 iters/sec. Estimated time to finish: 0:00:04.214611.
```

```
$ python example.py
[I 2019-05-21 11:16:42,230] Using an existing study with name 'example-stu
instead of creating a new one.
      total [##########################........................] 53.76%
this epoch [##################................................] 37.60%
       126 iter, 5 epoch / 10 epochs
    26.211 iters/sec. Estimated time to finish: 0:00:04.134763.
```

```
$ python example.py
[I 2019-05-21 11:16:42,729] Using an existing study with name 'example-study' in
stead of creating a new one.
      total [#########################.........................] 51.63%
this epoch [########..........................................] 16.27%
       121 iter, 5 epoch / 10 epochs
     25.56 iters/sec. Estimated time to finish: 0:00:04.435707.
```

```
$ python example.py
[I 2019-05-21 11:16:42,022] Using an existing study with name 'example-stu
instead of creating a new one.
      total [############################......................] 56.32%
this epoch [###############################...................] 63.20%
       132 iter, 5 epoch / 10 epochs
    26.968 iters/sec. Estimated time to finish: 0:00:03.796150.
```

Source: https://optuna.org

Analysis & visualization of hyperopt results

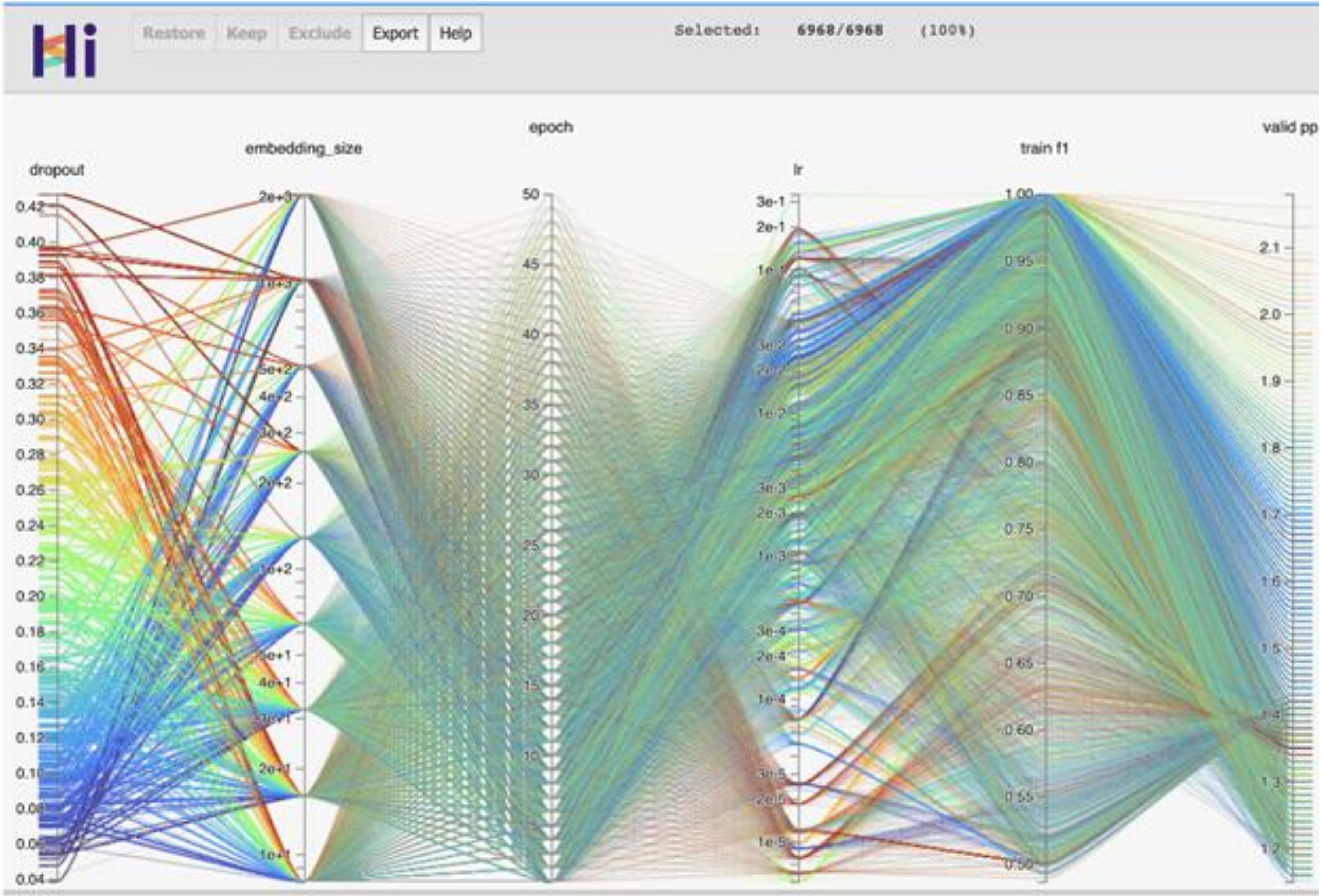
Hyperopt final result

```
[I 2020-09-11 17:26:10,217] Trial 98 pruned.
[I 2020-09-11 17:26:10,790] Trial 99 pruned.
Study statistics:
  Number of finished trials:  100
  Number of pruned trials:  67
  Number of complete trials:  33
Best trial:
  Value:  0.95390625
  Params:
    n_layers: 1
    n_units_l0: 115
    dropout_l0: 0.40951215992211487
    optimizer: Adam
    lr: 0.021951376926653072
```

Preferred Networks

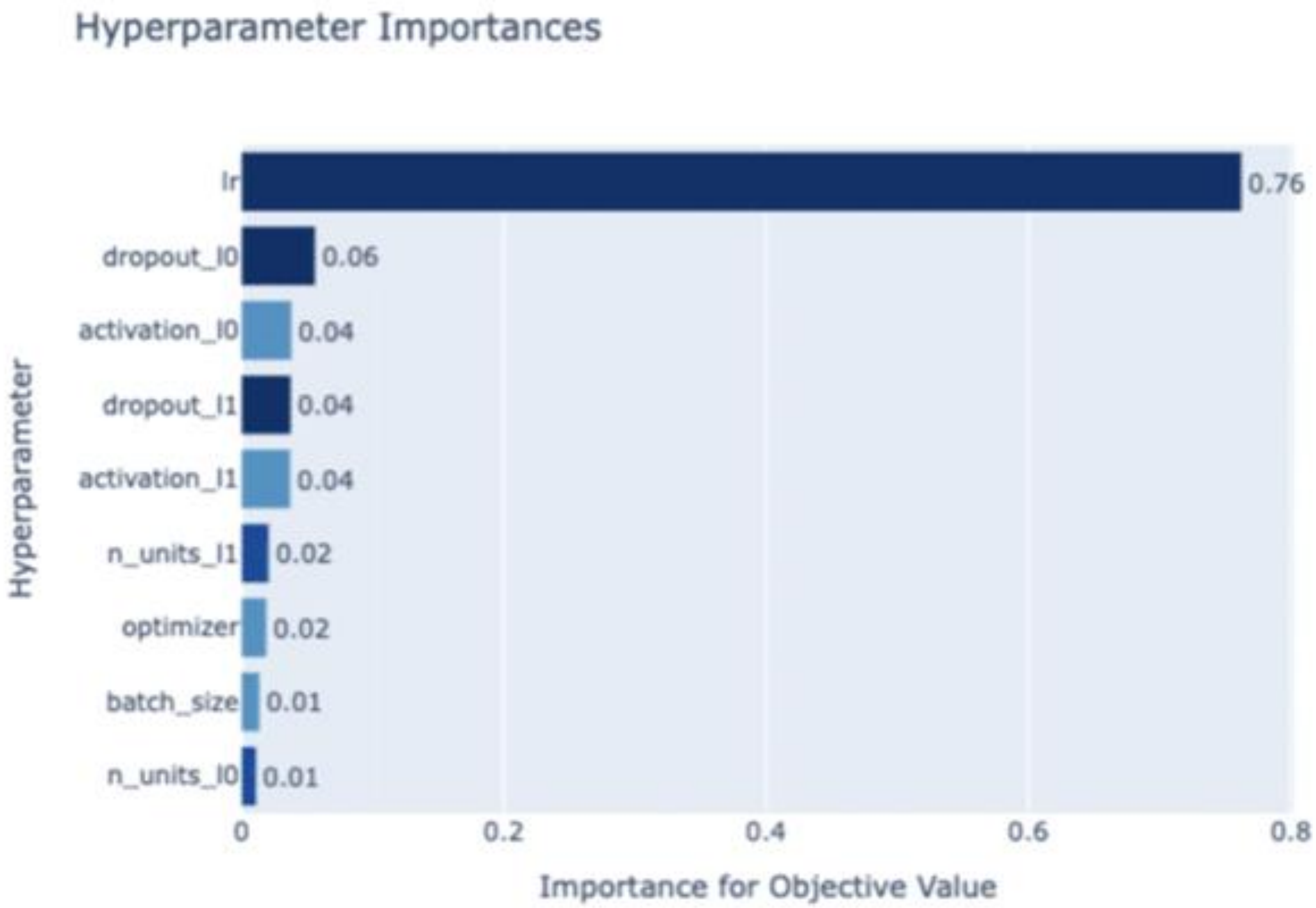
Source: https://github.com/optuna/optuna/blob/master/examples/pytorch_simple.py

Source: https://optuna.org



Forrás: https://github.com/facebookresearch/hiplot

Which hyperparameter is the most important?



Forrás: https://optuna.org

Weights and Biases

- Works fine in colab
- Can be installed locally using docker
  - https://hub.docker.com/r/wandb/local
  - https://docs.wandb.ai/guides/launch/docker
- Example for the visual result
  - https://wandb.ai/wandb/examples-keras-cnn-fashion/sweeps/us0ifmrf

Forrás: https://github.com/facebookresearch/hiplot

Weights and Biases - Sweeps

- https://docs.wandb.ai/guides/sweeps

Forrás: https://github.com/facebookresearch/hiplot

HyperOpt frameworks

- https://github.com/maxpumperla/hyperas
- https://github.com/keras-team/keras-tuner
- https://github.com/autonomio/talos
- https://github.com/sherpa-ai/sherpa

- https://github.com/optuna/optuna
- https://github.com/hyperopt/hyperopt
- https://github.com/Avsecz/kopt
- https://github.com/tobegit3hub/advisor
- https://github.com/AIworx-Labs/chocolate
- https://machinelearningmastery.com/grid-search-hyperparameters-deep-learning-models-python-keras/

General hyperopt code

```
import <hyper>

define objective(trial):
     <DNN definition, with hyperparams>

     return evaluation_score

study = <hyper>.create_space()
study.optimize(objective,
     search_algorithm,
     n_trials, …)
```

References

References

- https://optuna.org
- https://keras.io/keras_tuner/
- https://wandb.ai

Please, don't forget to send feedback:

https://bit.ly/bme-dl

Thank you
for your attention

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