Training DNNs: Tricks

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Recap: last lecture

Training DNNs

$$\min_{\boldsymbol{W}} \frac{1}{m}\sum_{i=1}^{m} \ell\left(\boldsymbol{y}_i, \mathrm{DNN}_{\boldsymbol{W}}\left(\boldsymbol{x}_i\right)\right) + \Omega\left(\boldsymbol{W}\right)$$

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This lecture: **additional tricks/heuristics that improve**

- **convergence speed**
- **task-specific (e.g., classification, regression, generation) performance**

Outline

Data Normalization

Regularization

Hyperparameter search, data augmentation

Suggested reading

Why scaling matters?

Consider a ML objective: $\min_{\boldsymbol{w}} \; f(\boldsymbol{w}) \doteq \frac{1}{m}\sum_{i=1}^{m} \ell(\boldsymbol{w}^\intercal \boldsymbol{x}_i; y_i)$, e.g.,

- Least-squares (LS): $\min_{\boldsymbol{w}} \; \frac{1}{m}\sum_{i=1}^{m} \|y_i - \boldsymbol{w}^\intercal \boldsymbol{x}_i\|_2^2$
- Logistic regression: $\min_{\boldsymbol{w}} \; -\frac{1}{m}\sum_{i=1}^{m} \left[y_i \boldsymbol{w}^\intercal \boldsymbol{x}_i - \log\left(1 + e^{\boldsymbol{w}^\intercal \boldsymbol{x}_i}\right)\right]$
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- Suppose the off-diagonal elements of $\boldsymbol{x}_i \boldsymbol{x}_i^\intercal$ are relatively small (e.g., when features are "independent").
- What happens when coordinates (i.e., features) of $\boldsymbol{x}_i$ have different orders of magnitude? Conditioning of $\nabla^2_{\boldsymbol{w}} f$ is bad, i.e., f is elongated

Fix the scaling: first idea

Normalization: make each feature zero-mean and unit variance, i.e., make each row of $\boldsymbol{X} = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m]$ zero-mean and unit variance, i.e.

$$\boldsymbol{X}' = \frac{\boldsymbol{X} - \boldsymbol{\mu}}{\boldsymbol{\sigma}} \quad (\boldsymbol{\mu}\text{—row means, } \boldsymbol{\sigma}\text{—row std, broadcasting applies})$$

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X = (X - X.mean(axis=1))/X.std(axis=1)
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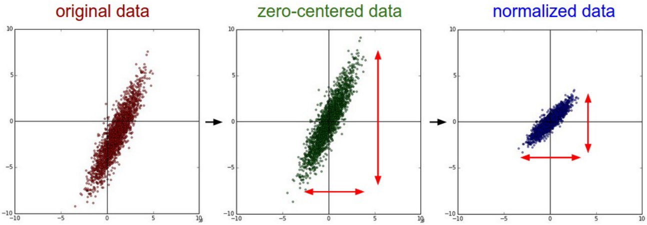

Credit: Stanford CS231N

NB: for data matrices, we often assume each column is a data point, and each row is a feature. This convention is different from that assumed in Tensorflow and PyTorch.

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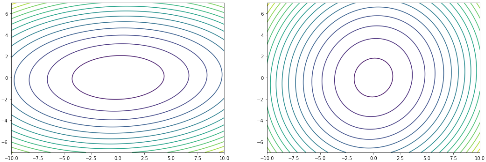
For LS, works well when features are approximately independent



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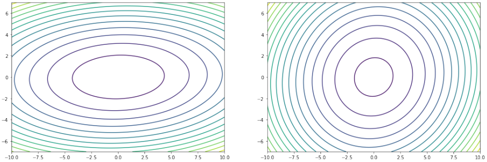

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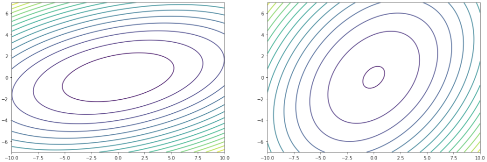
For LS, works not so well when features are highly dependent.



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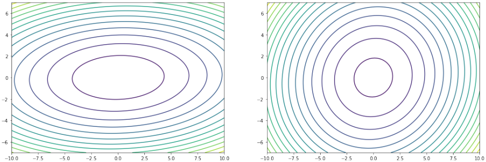

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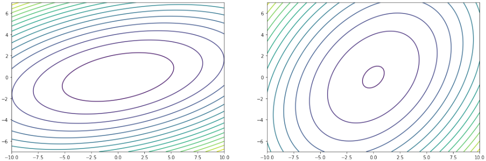

before vs. after the normalization

How to remove the feature dependency?

Fix the scaling: second idea

PCA and whitening

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PCA and whitening

PCA, i.e., zero-center and rotate the data to align principal directions to coordinate directions

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X -= X.mean(axis=1) #centering
U, S, VT = np.linalg.svd(X, full_matrices=False)
Xrot = U.T@X #rotate/decorrelate the data
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(math: $\boldsymbol{X} = \boldsymbol{U}\boldsymbol{S}\boldsymbol{V}^\intercal$, then $\boldsymbol{U}^\intercal \boldsymbol{X} = \boldsymbol{S}\boldsymbol{V}$)

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`Xwhite =1/(S+eps)*Xrot` # (math: $\boldsymbol{X}_{\mathrm{white}} = \boldsymbol{V}$)

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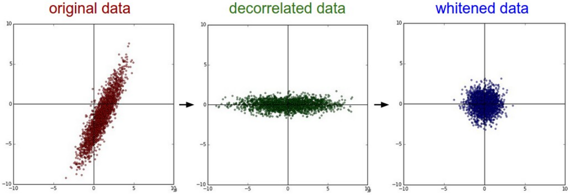

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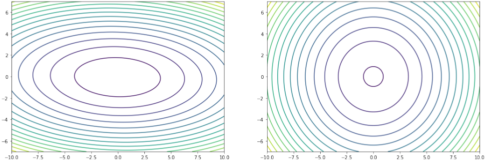

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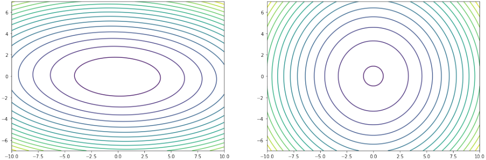

before vs. after the whitening

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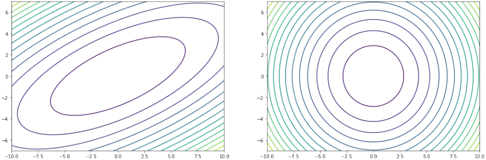

before vs. after the whitening

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- But recall our model objective $\min_{\boldsymbol{w}} \ f(\boldsymbol{w}) \doteq \frac{1}{m}\sum_{i=1}^{m} \ell(\boldsymbol{w}^\intercal \boldsymbol{x}_i; y_i)$ vs. DL objective

$$\min_{\boldsymbol{W}} \ \frac{1}{m}\sum_{i=1}^{m} \ell\left(\boldsymbol{y}_i, \sigma\left(\boldsymbol{W}_k \sigma\left(\boldsymbol{W}_{k-1} \ldots \sigma\left(\boldsymbol{W}_1 \boldsymbol{x}_i\right)\right)\right)\right) + \Omega\left(\boldsymbol{W}\right)$$

  - DL objective is much more complex
  - But $\sigma\left(\boldsymbol{W}_k \sigma\left(\boldsymbol{W}_{k-1} \ldots \sigma\left(\boldsymbol{W}_1 \boldsymbol{x}_i\right)\right)\right)$ is a composite version of $\boldsymbol{w}^\intercal \boldsymbol{x}_i$:

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- **Idea: also process the input data to some/all hidden layers**

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- Apply **normalization** to the outputs of the colored parts based on the statistics of a **mini-batch** of $\boldsymbol{x}_i$'s, e.g.,

$$\boldsymbol{W}_2\underbrace{\sigma\left(\boldsymbol{W}_1\boldsymbol{x}_i\right)}_{\doteq\boldsymbol{z}_i}\longrightarrow\boldsymbol{W}_2\underbrace{\mathrm{BN}\left(\sigma\left(\boldsymbol{W}_1\boldsymbol{x}_i\right)\right)}_{\mathrm{BN}(\boldsymbol{z}_i)}$$

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$$\boldsymbol{W}_2\underbrace{\sigma\left(\boldsymbol{W}_1\boldsymbol{x}_i\right)}_{\doteq\boldsymbol{z}_i}\longrightarrow\boldsymbol{W}_2\underbrace{\mathrm{BN}\left(\sigma\left(\boldsymbol{W}_1\boldsymbol{x}_i\right)\right)}_{\mathrm{BN}(\boldsymbol{z}_i)}$$

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Batch normalization

Apply normalization to the input data to some/all hidden layers

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  Flexibity restored by optional scaling γ_j's and shifting β_j's:

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Here, γ_j's and β's are trainable (optimization) variables!

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Question: how to perform training after plugging in the BN operations?

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  With BN: $\nabla_{\boldsymbol{W}} \frac{1}{|B|} \sum_{k=1}^{|B|} \ell\left(\boldsymbol{W}; \boldsymbol{x}_k, \boldsymbol{y}_k\right)$ has to be computed altogether, due to the inter-dependency across the summands

Batch normalization: implementation details

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In practice, collect the momentum-weighted running averages: e.g., for each hidden node with BN,

$$\overline{\mu} = (1-\eta)\,\overline{\mu}_{old} + \eta\mu_{new}$$
$$\overline{\sigma} = (1-\eta)\,\overline{\sigma}_{old} + \eta\sigma_{new}$$

with e.g., $\eta = 0.1$. In PyTorch, `torch.nn.BatchNorm1d`, `torch.nn.BatchNorm2d`, `torch.nn.BatchNorm3d` depending on the input shapes

Batch normalization: implementation details

Question: BN before or after the activation?

$$\boldsymbol{W}_2\sigma\left(\boldsymbol{W}_1\boldsymbol{x}_i\right) \longrightarrow \boldsymbol{W}_2\mathrm{BN}\left(\sigma\left(\boldsymbol{W}_1\boldsymbol{x}_i\right)\right) \quad \text{(after)}$$
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- But the "after" version is more intuitive as we have seen
- Both are used in practice and debatable which one is more effective
  - https://www.reddit.com/r/MachineLearning/comments/67gonq/d_batch_normalization_before_or_after_relu/
  - https://blog.paperspace.com/busting-the-myths-about-batch-normalization/
  - https://github.com/gcr/torch-residual-networks/issues/5
  - [Chen et al., 2019]

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- Yet another explanation from optimization perspective [Kohler et al., 2019]
- A good research topic

Batch PCA/whitening?

fixing the feature scaling makes the landscape "nicer"—derivatives and curvatures in all directions are roughly even in magnitudes. So for DNNs,

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    - zero-center
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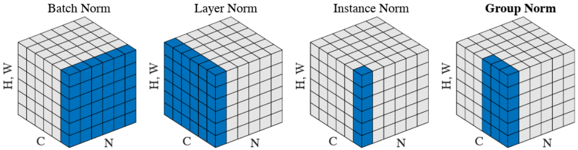
normalization is most popular due to the simplicity

Zoo of normalization



Normalization methods. Each subplot shows a feature map tensor, with N as the batch axis, C as the channel axis, and (H, W) as the spatial axes. The pixels in blue are normalized by the same mean and variance, computed by aggregating the values of these pixels.

Credit: [Wu and He, 2018]

normalization in different directions/groups of the data tensors

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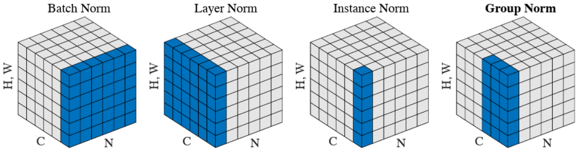

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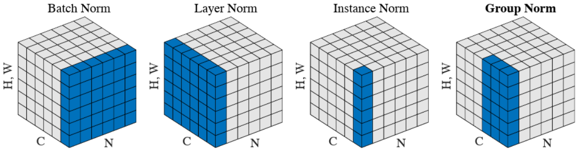

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An Overview of Normalization Methods in Deep Learning
https://mlexplained.com/2018/11/30/an-overview-of-normalization-methods-in-deep-learning/

Check out PyTorch normalization layers
https://pytorch.org/docs/stable/nn.html#normalization-layers

Outline

Regularization to avoid overfitting

Training DNNs $\min_{\boldsymbol{W}} \frac{1}{m}\sum_{i=1}^{m} \ell\left(\boldsymbol{y}_i, \mathrm{DNN}_{\boldsymbol{W}}\left(\boldsymbol{x}_i\right)\right) + \lambda\Omega\left(\boldsymbol{W}\right)$ with **explicit regularization** Ω. But which Ω?

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- $\Omega\left(\boldsymbol{W}\right) = \sum_k \left\|\boldsymbol{W}_k\right\|_F^2$ where k indexes the layers — penalizes large values in $\boldsymbol{W}$ and hence avoids steep changes (set `weight_decay` as λ in `torch.optim.xxxx`)

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- $\Omega\left(\boldsymbol{W}\right) = \sum_k \left\|\boldsymbol{W}_k\right\|_1$ — promotes sparse $\boldsymbol{W}_k$'s (i.e., many entries in $\boldsymbol{W}_k$'s to be near zero; good for feature selection)

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l1_reg = torch.zeros(1)
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Regularization to avoid overfitting

Training DNNs $\min_{\boldsymbol{W}} \frac{1}{m}\sum_{i=1}^{m} \ell\left(\boldsymbol{y}_i, \mathrm{DNN}_{\boldsymbol{W}}\left(\boldsymbol{x}_i\right)\right) + \lambda\Omega\left(\boldsymbol{W}\right)$ with **explicit regularization** Ω. But which Ω?

- $\Omega\left(\boldsymbol{W}\right) = \sum_k \|\boldsymbol{W}_k\|_F^2$ where k indexes the layers — penalizes large values in $\boldsymbol{W}$ and hence avoids steep changes (set `weight_decay` as λ in `torch.optim.xxxx`)
- $\Omega\left(\boldsymbol{W}\right) = \sum_k \|\boldsymbol{W}_k\|_1$ — promotes sparse $\boldsymbol{W}_k$'s (i.e., many entries in $\boldsymbol{W}_k$'s to be near zero; good for feature selection)

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for W in model.parameters():
  l1_reg += W.norm(1)
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- many others!

Implicit regularization

Training DNNs $\min_{\boldsymbol{W}} \ \frac{1}{m}\sum_{i=1}^{m} \ell\left(\boldsymbol{y}_i, \mathrm{DNN}_{\boldsymbol{W}}\left(\boldsymbol{x}_i\right)\right) + \lambda\Omega\left(\boldsymbol{W}\right)$ with **implicit regularization —** operation that is not built into the objective but avoids overfitting

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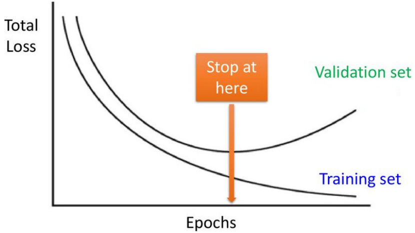
- early stopping
- batch normalization
- dropout
- ...

Early stopping

A practical/pragmatic stopping strategy: **early stopping**



... periodically check the validation error and stop when it doesn't improve

Early stopping

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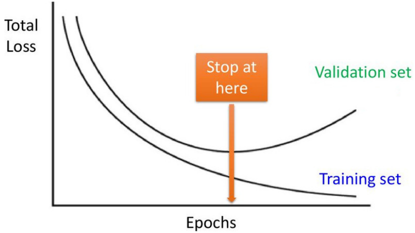
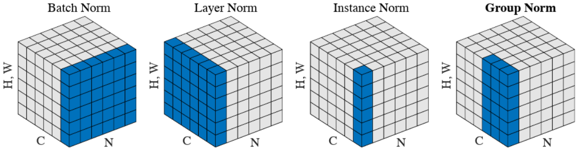


... periodically check the validation error and stop when it doesn't improve

Intuition: avoid the model to be too specialized/perfect for the training data

More concrete math examples: [Bishop, 1995, Sjöberg and Ljung, 1995]

Batch/general normalization



Normalization methods. Each subplot shows a feature map tensor, with N as the batch axis, C as the channel axis, and (H, W) as the spatial axes. The pixels in blue are normalized by the same mean and variance, computed by aggregating the values of these pixels.

Credit: [Wu and He, 2018]

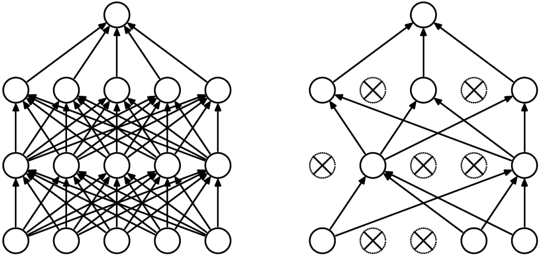
normalization in different directions/groups of the data tensors

weight normalization: decompose the weight as magnitude and direction $\boldsymbol{w} = g \frac{\boldsymbol{v}}{\|\boldsymbol{v}\|_2}$ and perform optimization in $(g, \boldsymbol{v})$ space

An Overview of Normalization Methods in Deep Learning

https://mlexplained.com/2018/11/30/an-overview-of-normalization-methods-in-deep-learning/

Dropout

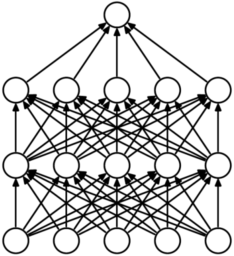


(a) Standard Neural Net (b) After applying dropout.

Credit: [Srivastava et al., 2014]

Idea: kill each non-output neuron with probability $1 - p$, called **Dropout**

Dropout



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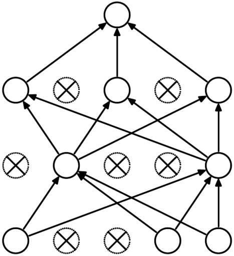

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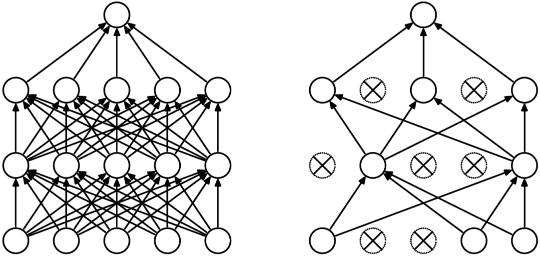

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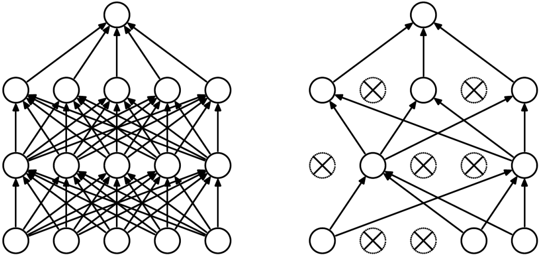

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- no Dropout at test time!

Dropout: implementation details

```python
p = 0.5 # probability of keeping a unit active. higher = less dropout

def train_step(X):
  # forward pass for example 3-layer neural network
  H1 = np.maximum(0, np.dot(W1, X) + b1)
  U1 = (np.random.rand(*H1.shape) < p) / p # first dropout mask. Notice /p!
  H1 *= U1 # drop!
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  U2 = (np.random.rand(*H2.shape) < p) / p # second dropout mask. Notice /p!
  H2 *= U2 # drop!
  out = np.dot(W3, H2) + b3

  # backward pass: compute gradients... (not shown)
  # perform parameter update... (not shown)

def predict(X):
  # ensembled forward pass
  H1 = np.maximum(0, np.dot(W1, X) + b1) # no scaling necessary
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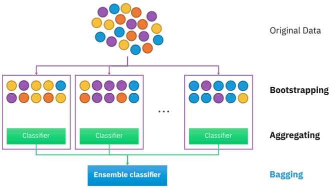
PyTorch: `torch.nn.Dropout`, `torch.nn.Dropout2d`, `torch.nn.Dropout3d`

Why Dropout?



Credit: Wikipedia

bagging can avoid overfitting

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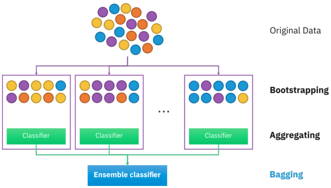

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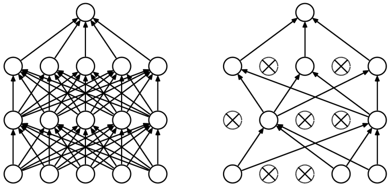

(a) Standard Neural Net (b) After applying dropout.

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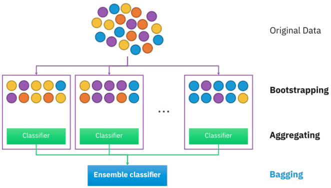

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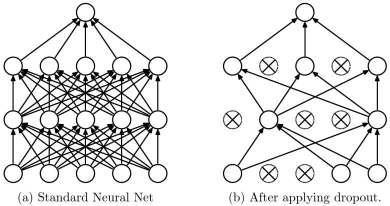

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For an n-node network, 2^n possible sub-networks.

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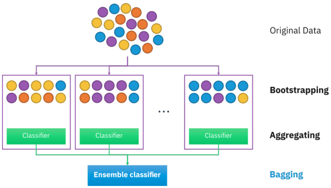

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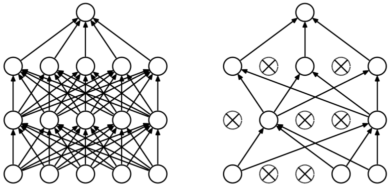

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Consider the average/ensemble prediction $\mathbb{E}_{\mathrm{SN}}\left[\mathrm{SN}\left(\boldsymbol{x}\right)\right]$ over 2^n of sub-networks and the new objective

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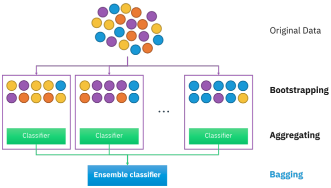

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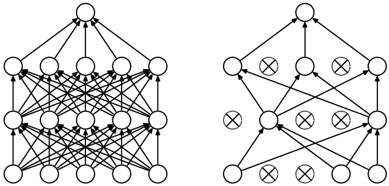

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Mini-batch SGD with Dropout samples data point and model simultaneously (stochastic composite optimization [Wang et al., 2016, Wang et al., 2017])

Outline

Hyperparameter search

...tunable parameters (vs. learnable parameters, or optimization variables)

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- Initialization schemes
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- etc

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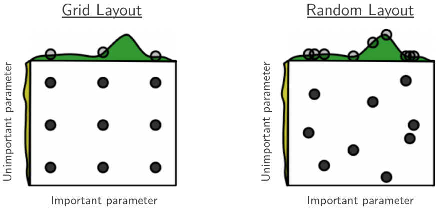
https://cs231n.github.io/neural-networks-3/#hyper



Credit: [Bergstra and Bengio, 2012]

Data augmentation

- More relevant data always help!

Data augmentation

- More relevant data always help!
- Fetch more external data

Data augmentation

- More relevant data always help!
- Fetch more external data
- Generate more internal data: generate based on whatever you want to be robust to
  - * vision: translation, rotation, background, noise, deformation, flipping, blurring, occlusion, etc

Credit: https://github.com/aleju/imgaug

See one example here https://pytorch.org/tutorials/beginner/transfer_learning_tutorial.html

Outline

Data Normalization

Regularization

Hyperparameter search, data augmentation

Suggested reading

Suggested reading

- Chap 7, Deep Learning (Goodfellow et al)
- Stanford CS231n course notes: Neural Networks Part 2: Setting up the Data and the Loss https://cs231n.github.io/neural-networks-2/
- Stanford CS231n course notes: Neural Networks Part 3: Learning and Evaluation https://cs231n.github.io/neural-networks-3/
- http://neuralnetworksanddeeplearning.com/chap3.html

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