Introduction to deep learning

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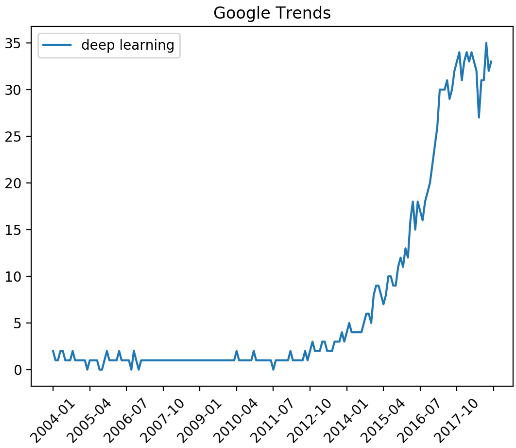
13 Dec. 2018

amazon.com

Starting with a cliché...



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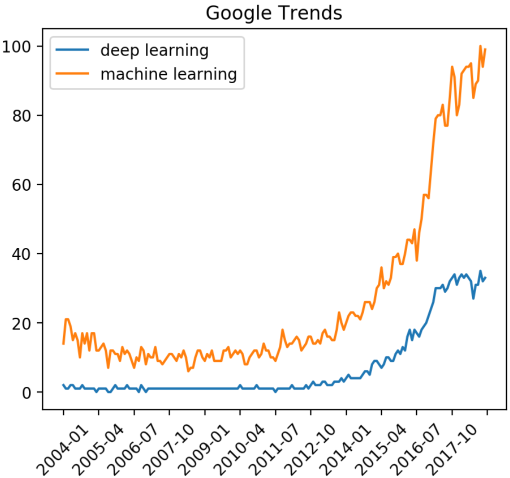

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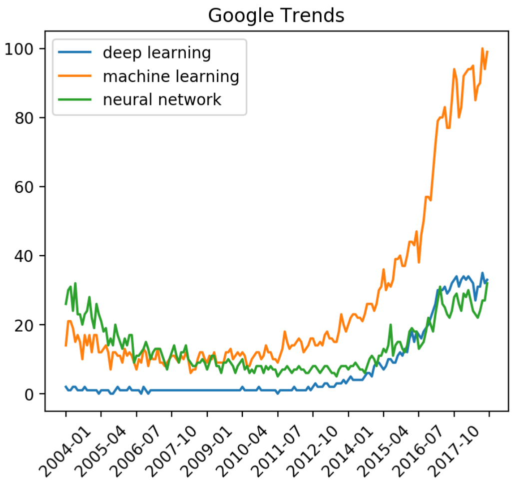

Deep neural networks: hierarchical function definitions

A neural network is a composition of functions (layers), each parameterized with a *weight vector* $\mathbf{w}_l$. E.g. for 2 layers:

$$f_{\mathsf{net}} = h_2(h_1(\mathbf{x}; \mathbf{w}_1); \mathbf{w}_2).$$

Generally $f_{\mathsf{net}} : \mathbf{x} \mapsto \mathbf{y}$ with:

$$\begin{aligned}
\mathbf{h}_1 &= \varphi(\mathbf{x}\mathbf{w}_1 + b_1) \\
\mathbf{h}_2 &= \varphi(\mathbf{h}_1\mathbf{w}_2 + b_2) \\
&\cdots \\
\hat{\mathbf{y}} &= \varphi(\mathbf{h}_{L-1}\mathbf{w}_L + b_L)
\end{aligned}$$

ϕ is the (non-linear) activation function.

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Defining the loss

- We have our function approximator $f_{\text{net}}(x) = \hat{y}$
- We have to define our loss (objective function) to relate this function outputs to the observed data.
- E.g. squared difference $\sum_n (y_n - \hat{y}_n)^2$ or cross-entropy

Probabilistic re-formulation

- Training minimizing loss:

$$\arg\min_{\mathbf{w}} \underbrace{\frac{1}{2}\sum_{i=1}^{N}(f_{\text{net}}(\mathbf{w}, x_i) - y_i)^2}_{\text{fit}} + \lambda \underbrace{\sum_i \parallel \mathbf{w}_i \parallel}_{\text{regularizer}}$$

- Equivalent probabilistic view for regression, maximizing posterior probability:

$$\arg\max_{\mathbf{w}} \underbrace{\log p(\mathbf{y}|\mathbf{x}, \mathbf{w})}_{\text{fit}} + \underbrace{\log p(\mathbf{w})}_{\text{regularizer}}$$

where $p(\mathbf{y}|\mathbf{x}, \mathbf{w}) \sim \mathcal{N}$ and $p(\mathbf{w}) \sim$ Laplace

- Optimization still done with back-prop (i.e. gradient descent).

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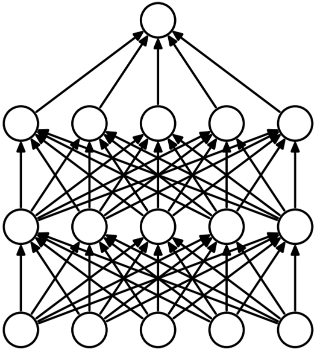
Graphical depiction



Optimization

One layer:

$$Loss = \frac{1}{2}(\mathbf{h} - \mathbf{y})^2$$
$$\mathbf{h} = \phi(\mathbf{x}\mathbf{w})$$
$$\frac{\vartheta Loss}{\vartheta \mathbf{w}} = \underbrace{(\mathbf{y} - \mathbf{h})}_{\epsilon} \frac{\vartheta \phi(\mathbf{x}\mathbf{w})}{\vartheta \mathbf{w}}$$

Two layers:

$$Loss = \frac{1}{2}(\mathbf{h}_2 - \mathbf{y})^2$$
$$\mathbf{h}_2 = \phi \left[\underbrace{\phi(\mathbf{x}\mathbf{w}_0)}_{\mathbf{h}_1} \mathbf{w}_1 \right]$$
$$\frac{\vartheta Loss}{\vartheta \mathbf{w}_0} = \cdots$$
$$\frac{\vartheta Loss}{\vartheta \mathbf{w}_1} = \cdots$$

Derivative w.r.t $\mathbf{w}_1$

$$\begin{aligned}
\frac{\vartheta(\mathbf{h}_2-\mathbf{y})^2}{\vartheta\mathbf{w}_1} &= -2\frac{1}{2}(\mathbf{h}_2-\mathbf{y})\frac{\vartheta\mathbf{h}_2}{\vartheta\mathbf{w}1} = \\
&= (\mathbf{y}-\mathbf{h}_2)\frac{\vartheta\phi(\mathbf{h}_1\mathbf{w}_1)}{\vartheta\mathbf{w}_1} = \\
&= (\mathbf{y}-\mathbf{h}_2)\frac{\vartheta\phi(\mathbf{h}_1\mathbf{w}_1)}{\vartheta\mathbf{h}_1\mathbf{w}_1}\frac{\vartheta\mathbf{h}_1\mathbf{w}_1}{\vartheta\mathbf{w}_1} = \\
&= \underbrace{(\mathbf{y}-\mathbf{h}_2)}_{\epsilon_2}\underbrace{\frac{\vartheta\phi(\mathbf{h}_1\mathbf{w}_1)}{\vartheta\mathbf{h}_1\mathbf{w}_1}}_{g_1}\mathbf{h}_1^T
\end{aligned}$$

$\mathbf{h}_1$ is computed during the *forward pass*.

Derivative w.r.t $\mathbf{w}_0$

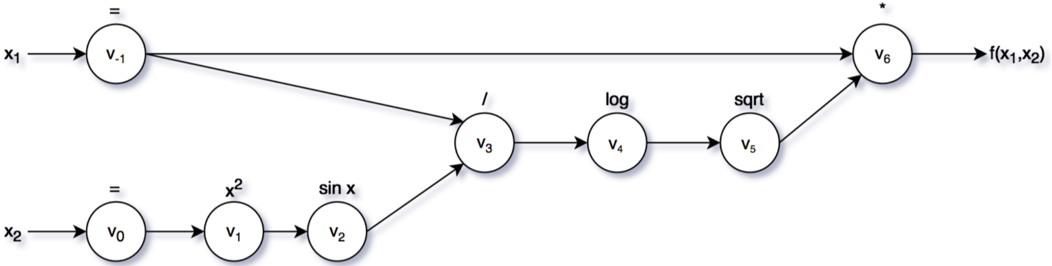
$$
\begin{aligned}
\frac{\vartheta(\mathbf{h}_2-\mathbf{y})^2}{\vartheta\mathbf{w}_0} &= -2\frac{1}{2}(\mathbf{h}_2-\mathbf{y})\frac{\vartheta\mathbf{h}_2}{\vartheta\mathbf{w}_0} = \\
&= (\mathbf{y}-\mathbf{h}_2)\frac{\vartheta\phi(\mathbf{h}_1\mathbf{w}_1)}{\vartheta\mathbf{h}_1\mathbf{w}_1}\frac{\vartheta\mathbf{h}_1\mathbf{w}_1}{\vartheta\mathbf{h}_1}\frac{\vartheta\mathbf{h}_1}{\vartheta\mathbf{w}_0} = \\
&= \epsilon_2\ g_1\ \mathbf{w}_1^T\ \frac{\vartheta\phi(\mathbf{x}\mathbf{w}_0)}{\mathbf{x}\mathbf{w}_0}\frac{\vartheta\mathbf{x}\mathbf{w}_0}{\vartheta\mathbf{w}_0} = \\
&= \epsilon_2\ g_1\ \mathbf{w}_1^T\ \underbrace{\frac{\vartheta\phi(\mathbf{x}\mathbf{w}_0)}{\vartheta\mathbf{x}\mathbf{w}_0}}_{g_0}\ \mathbf{x}^T
\end{aligned}
$$

Propagation of error is just the chain rule.

Go to notebook!

Automatic differentiation

Example: $f(x_1, x_2) = x_1 \sqrt{\log \frac{x_1}{sin(x_2^2)}}$ has *symbolic graph*:



(image: sanyamkapoor.com)

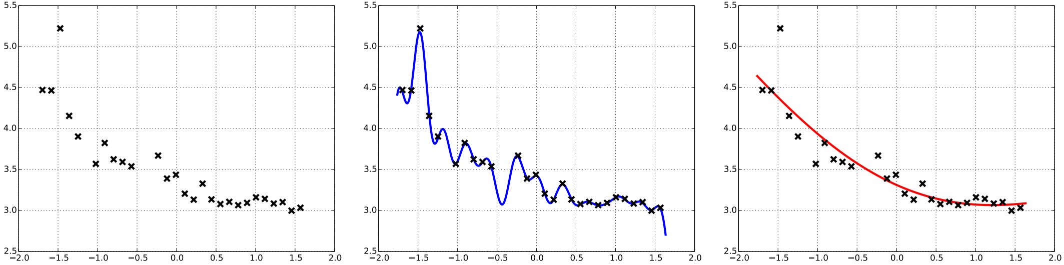
A NN in mxnet

Back to notebook!

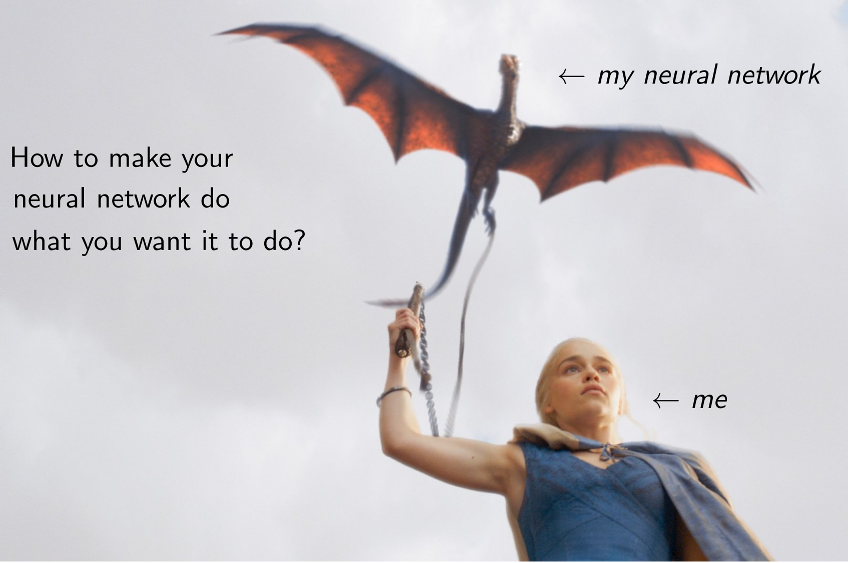
We're far from done...

- How to initialize the (so many) parameters?
- How to pick the right architecture?
- Layers and parameters co-adapt.
- Multiple local optima in optimization surface.
- Numerical problems.
- Bad behaviour of composite function (e.g. problematic gradient distribution).
- *OVERFITTING*

Curve fitting [skip]



Taming the dragon



Lottery ticket hypothesis

Might provide intuition for many of the tricks used.

- Optimization landscape: multiple optima and difficult to navigate
- Over-parameterized networks contain multiple sub-networks ("lottery tickets")
- "Winning ticket": a lucky sub-network found a good solution
- Over-parameterization: more tickets, higher winning probability
- Of course this means we have to prune or at least regularize.

(Frankle and Carbin (2018))

“Tricks”

- Smart initializations
- ReLU: better behaviour of gradients
- Early stopping: prevent overfitting
- Dropout
- Batch-normalization
- Transfer/meta-learning/BO: guide the training with another model
- many other “tricks”

Vanishing and exploding gradients

$$
\begin{aligned}
\frac{\vartheta(\mathbf{h}_2 - \mathbf{y})^2}{\vartheta \mathbf{w}_0} &= -2\frac{1}{2}(\mathbf{h}_2 - \mathbf{y})\frac{\vartheta \mathbf{h}_2}{\vartheta \mathbf{w}_0} = \\
&= (\mathbf{y} - \mathbf{h}_2)\frac{\vartheta \phi(\mathbf{h}_1\mathbf{w}_1)}{\vartheta \mathbf{h}_1\mathbf{w}_1}\frac{\vartheta \mathbf{h}_1\mathbf{w}_1}{\vartheta \mathbf{h}_1}\frac{\vartheta \mathbf{h}_1}{\vartheta \mathbf{w}_0} = \\
&= \epsilon_2 \; g_1 \; \mathbf{w}_1^T \; \frac{\vartheta \phi(\mathbf{x}\mathbf{w}_0)}{\mathbf{x}\mathbf{w}_0}\frac{\vartheta \mathbf{x}\mathbf{w}_0}{\vartheta \mathbf{w}_0} = \\
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\end{aligned}
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- ReLU: an activation function leading to well-behaved gradients.

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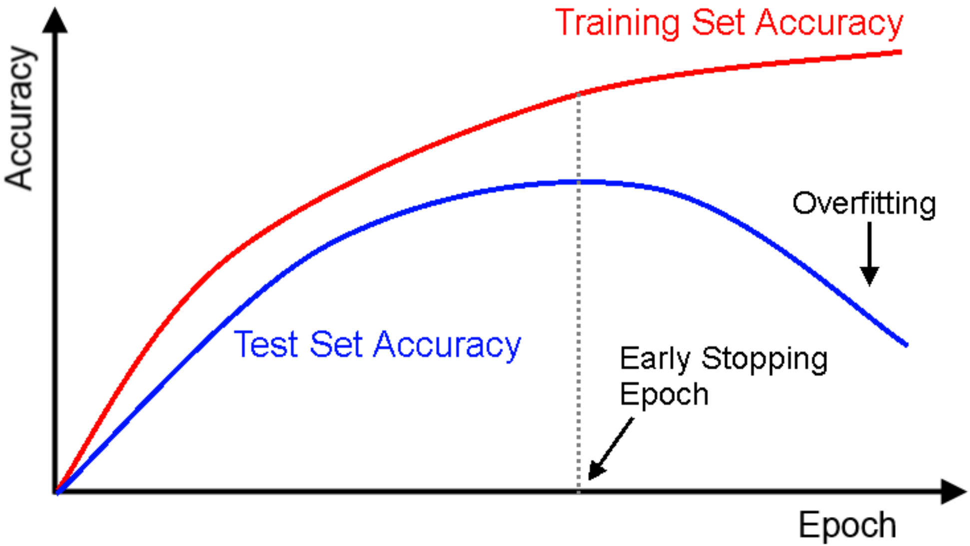
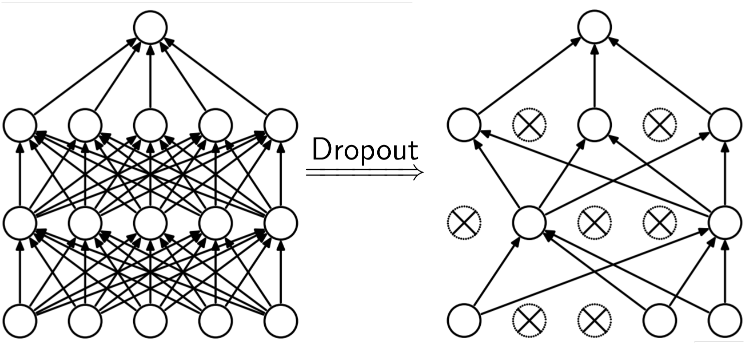
Early stopping



Dropout



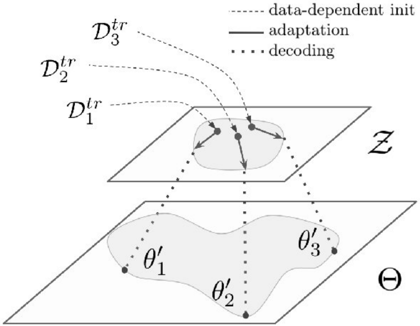
- Randomly drop units during training.
- Prevents units from co-adapting too much and prevents overfitting.

Batch-normalization

- Normalize each layer's output so e.g. $\mu = 0, \sigma = 1$
- Reduces covariate shift (data distribution changes)
- Less co-adaptation of layers
- Overall: faster convergence

Meta-learning

- Optimize the neural network model with the help of another model.
- The helper model might be allowed to learn from multiple datasets.

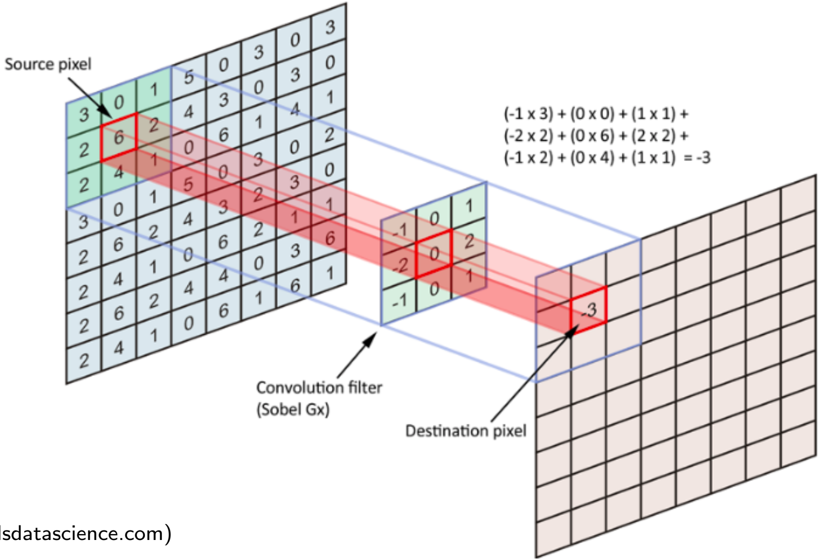


(image: Rusu et al. 2018 - LEO)

Bayesian HPO

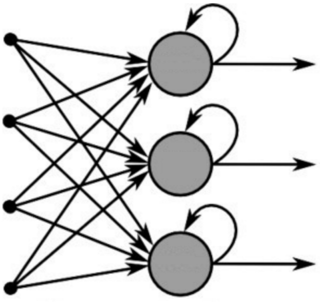
- Hyperparameters: learning rate, weight decay, architectures, learning protocols
- Optimize them using Bayesian optimization
- Prediction of learning curves. Can speed up HPO in a bandit setting
- Example: `https://xfer.readthedocs.io/en/master/demos/xfer-hpo.html`

Convolutional NN



(image: towardsdatascience.com)

Recurrent NN



Recurrent Neural Network   Feed-Forward Neural Network

image: towardsdatascience.com

Deployment: Transfer learning

Training neural networks from scratch is not practical as this requires:

- a lot of data
- expertise
- compute (e.g. GPU machines)

Solution:

- Transfer learning. Repurposing pre-trained neural networks to solve new tasks.
- A library for transfer learning: `https://github.com/amzn/xfer`

Go to Notebook!

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Bayesian deep learning

We saw that optimizing the parameters is a challenge.
Why not marginalize them out completely?

Probabilistic re-formulation

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Integrating out weights

$$D := (\mathbf{x}, \mathbf{y})$$

$$p(w|D) = \frac{p(D|w)p(w)}{p(D) = \int p(D|w)p(w)\mathsf{d}w}$$

Inference

- $p(D)$ (and hence $p(w|D)$) is difficult to compute because of the nonlinear way in which w appears through g.

- Attempt at *variational inference*:

$$\underbrace{\mathrm{KL}\left(q(w;\theta)\,\|\,p(w|D)\right)}_{\text{minimize}} = \log(p(D)) - \underbrace{\mathcal{L}(\theta)}_{\text{maximize}}$$

where

$$\mathcal{L}(\theta) = \underbrace{\mathbb{E}_{q(w;\theta)}[\log p(D,w)]}_{\mathcal{F}} + \mathbb{H}\left[q(w;\theta)\right]$$

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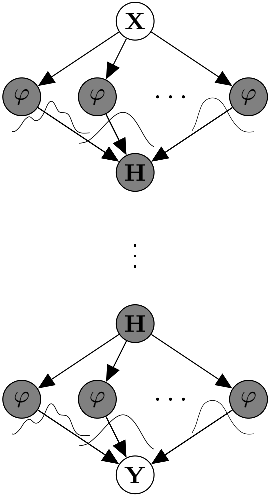
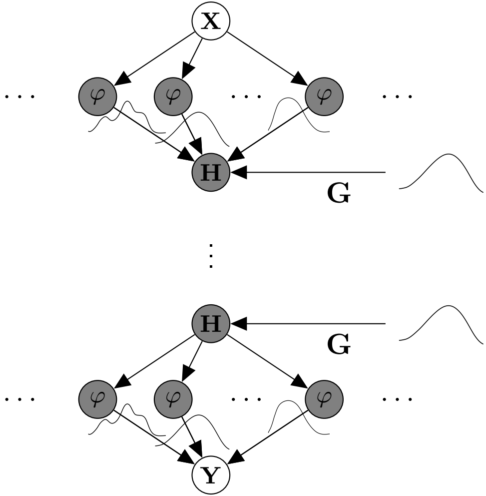
Bayesian neural network *(what we saw before)*



From NN to GP



- NN: $\mathbf{H}_2 = \mathbf{W}_2\phi(\mathbf{H}_1)$
- GP: ϕ is $\infty-$dimensional so:
  $$\mathbf{H}_2 = f_2(\mathbf{H}_1;\theta_2) + \epsilon$$
- NN: $p(\mathbf{W})$
- GP: $p(f(\cdot))$

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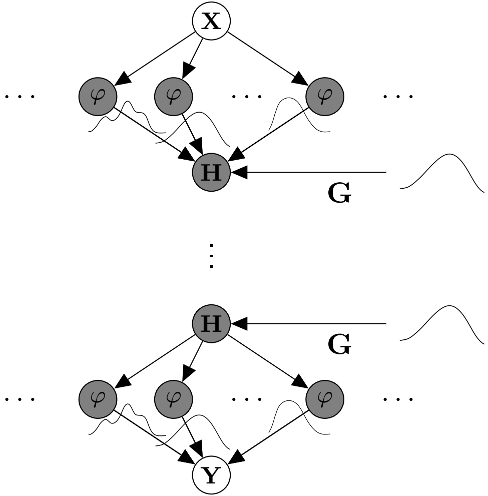

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Summary

- Vanilla feedforward NN with backpropabation (chain rule)
- Automatic differentiation
- Practical issues and solutions ("tricks")
- Understanding the challenges: optimization landscape and capacity
- ConvNets and RNNs
- Transfer Learning for practical use
- Bayesian NNs

Conclusions

- NNs are mathematically simple; challenge is in how to optimize them.
- Data efficiency? Uncertainty calibration? Interpretability? Safety? ...

APPENDIX

Inference: "Score function method"

$$
\begin{aligned}
\nabla_\theta \mathcal{F} &= \nabla_\theta \mathbb{E}_{q(w;\theta)}[\log p(D,w)] \\
&= \mathbb{E}_{q(w;\theta)}\left[p(D,w)\nabla_\theta \log q(w;\theta)\right] \\
&\approx \frac{1}{K}\sum_{i=1}^{K} p(D,w^{(k)})\nabla_\theta \log q(w^{(k)};\theta), \quad w^{(k)} \overset{iid}{\sim} q(w;\theta)
\end{aligned}
$$

(Paisley et al., 2012; Ranganath et al., 2014; Mnih and Gregor, 2014, Ruiz et al. 2016)

Inference: "Reparameterization gradient"

- Reparametrize w as a transformation $\mathcal{T}$ of a simpler variable ϵ: $w = \mathcal{T}(\epsilon;\theta)$
- $q(\epsilon)$ is now independent of θ

$$
\begin{aligned}
\nabla_\theta \mathcal{F} &= \nabla_\theta \mathbb{E}_{q(w;\theta)}[\log p(D,w)] \\
&= \mathbb{E}_{q(\epsilon)}\left[\nabla_w p(D,w)|_{w=\mathcal{T}(\epsilon;\theta)} \nabla_\theta \mathcal{T}(\epsilon;\theta)\right]
\end{aligned}
$$

- For example: $w \sim \mathcal{N}(\mu,\sigma) \xrightarrow{\mathcal{T}} w = \mu + \sigma \cdot \epsilon,\ \epsilon \sim \mathcal{N}(0,1)$
- MC by sampling from $q(\epsilon)$ (thus obtaining samples from w through $\mathcal{T}$)

(Salimans and Knowles, 2013; Kingma and Welling, 2014, Ruiz et al. 2016)

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- MC by sampling from $q(\epsilon)$ (thus obtaining samples from w through $\mathcal{T}$)

(Salimans and Knowles, 2013; Kingma and Welling, 2014, Ruiz et al. 2016)

We want the expectation $q(w;\theta)$ to appear on the left of ∇_θ, otherwise it's difficult. In score function we use a property of the log. In reparam. gradient we just reparameterize the main argument of the problematic $q(w;\theta)$ so then ∇_θ does not depend on this argument (the w) and can again be pushed.
The reparam. gradient has lower variance in practice, because it's a "richer" estimator, (e.g. has more info, like curvature about true gradient). But it's more restrictive, in that it works when w is continuous and [...].
Notice we can't do the fully naive MC where we bring the ∇ inside the integral and do: $\int q(w;\theta)\nabla_\theta p(D,w)dw$, because this doesn't make sense as the derivative for θ cannot be applied to $p(D,w)$ that does not contain θ!

$$
\begin{aligned}
&\nabla_\theta \mathcal{F}(\theta) = \\
&\nabla_\theta \int_w q(w;\theta) \log p(D,w) = && (1)\\
&\int_w \nabla_\theta q(w;\theta) \log p(D,w)] = && (2)\\
&\int_w q(w;\theta) \nabla_\theta \log q(w;\theta) \log p(D,w) = && (3)\\
&\int_w q(w;\theta) p(D,w) \nabla_\theta \log q(w;\theta) && (4)
\end{aligned}
$$

$$\text{setting: } w = \mathcal{T}(\epsilon;\theta) \Rightarrow \tag{5}$$

$$\int_w q(w;\theta) \log p(D,w) = \int_\epsilon q(\epsilon) \log p(D, \mathcal{T}(\epsilon;\theta)) \tag{6}$$

So:

$$\nabla_\theta \mathcal{F}(\theta) =$$

$$\nabla_\theta \int_w q(w;\theta) \log p(D,w) = \tag{7}$$

$$\int_\epsilon \nabla_\theta q(\epsilon) \log p(D, \mathcal{T}(\epsilon;\theta)) = \tag{8}$$

$$\int_\epsilon q(\epsilon) \nabla_\theta \log p(D, \mathcal{T}(\epsilon;\theta)) = \tag{9}$$

$$\int_\epsilon q(\epsilon) \nabla_w \log p(D, \mathcal{T}(\epsilon;\theta)) \nabla_\theta \mathcal{T}(\epsilon;\theta) \tag{10}$$

where last equality is from chain rule.