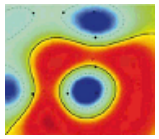
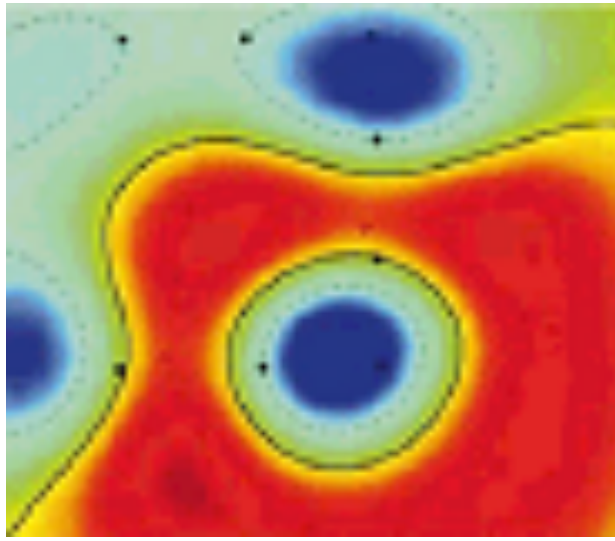


WiSe 2024/25

Deep Learning 1

Technische Universität Berlin



Lecture 4

Optimization (Part 2)

Outline

Recap Lecture 3

Post-Hoc Mitigation of Poor Conditioning

- Momentum
- Adam algorithm

Efficient Optimization

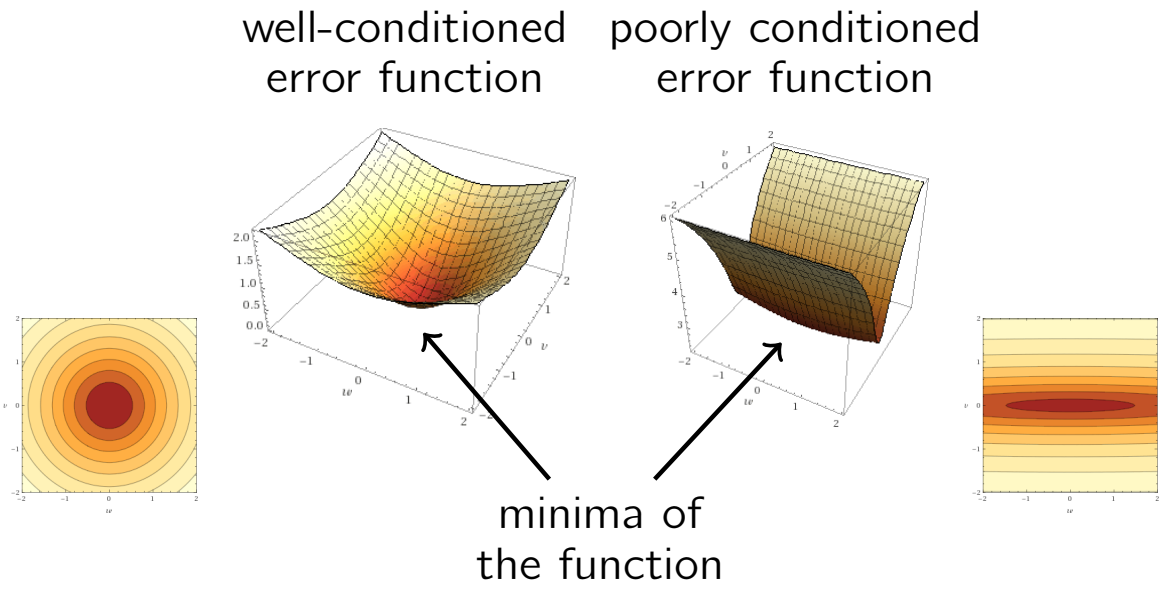
- Redundancies in the error function
- The stochastic gradient descent procedure
- Efficient networks
- Local connectivity

Implementation Aspects

- Computations as matrix-vector operations
- Training on specific hardware
- Distributed training schemes

Recap Lecture 3

Recap: Hessian-Based Analysis



Using the framework of Taylor expansions, any error function can be expanded at its minimum $\theta^\star$ by the quadratic function:

$$\mathcal{E}(\theta) = \mathcal{E}(\theta^\star) + 0 + \frac{1}{2}(\theta - \theta^\star)^\top H (\theta - \theta^\star) + \text{higher-order terms}$$

where H is the Hessian. The condition number is then the ratio of largest and smallest eigenvalues of the Hessian (the lower the better):

$$\boxed{\text{Condition number} = \lambda_{\max}/\lambda_{\min}}$$

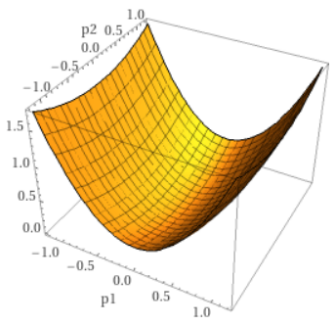
Better Conditioning $\mathcal{E}(\theta)$

Various techniques:

- Centering/whitening the data
- Centering the activations
- Properly scaling the weights
- Design the architecture appropriately (limited depth, shortcut connections, batch-normalization layers, no bottlenecks, ...)

Note:

- Despite all measures to reduce the condition number of $\mathcal{E}(\theta)$, the latter may still be poorly conditioned.
- We also need to adapt the optimization procedure in a way that it deals better with poor conditioning.



Part 1

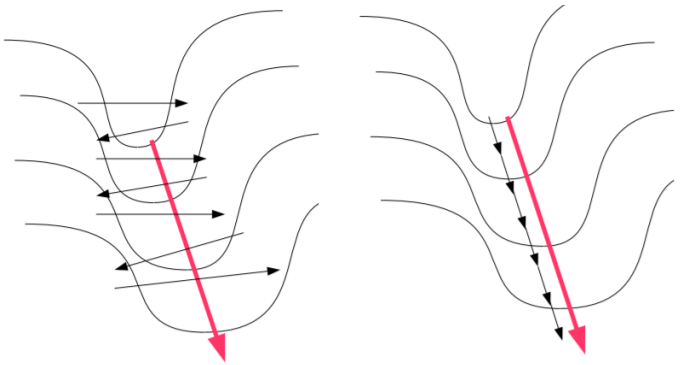
Post-Hoc Mitigations

Momentum

沿着低曲率方向下降可以加速收敛过程，通过模仿物理中的动量来实现这一点。简单来说，动量优化的核心思想是通过考虑之前的梯度累积来加速收敛，尤其是在一些平缓区域，这样可以有效避免梯度下降中的震荡。

左边图展示了普通梯度下降的路径，容易在曲率较大的地方发生震荡。

右边图显示了使用动量之后的路径，通过保留历史梯度的方向信息，能够更快速和稳定地到达最低点。



Idea:

- Descent along directions of low curvature can be accelerated by imitating a physical momentum.

Algorithm:

Δ 表示更新方向，μ 是动量系数，$\nabla E(\theta)$ 是损失函数 E 对参数 θ 的梯度。

- Compute the direction of descent as a cumulation of previous gradients:

$$\Delta \leftarrow \mu \cdot \Delta + (-\nabla \mathcal{E}(\theta))$$

  where $\mu \in [0, 1[$. The higher μ, the stronger the momentum.

- Update the parameters θ by performing a step along the obtained direction of descent.

$$\theta \leftarrow \theta + \gamma \cdot \Delta$$

动量方法的本质是在梯度下降过程中引入惯性，避免在曲率较大的方向上过度摆动，从而加速在低曲率方向上的收敛。

Momentum

Recall:

- Gradient descent with momentum proceeds as

$$\Delta \leftarrow \mu \cdot \Delta + (-\nabla \mathcal{E}(\theta))$$
$$\theta \leftarrow \theta + \gamma \cdot \Delta$$

Property:

If all gradient estimates $\nabla \mathcal{E}(\theta)$ coincide along a particular direction, then the effective learning rate along that direction becomes:

$$\gamma' = \gamma \cdot \frac{1}{1-\mu}$$

This can be derived as the closed form of a geometric series.

加速收敛：通过引入动量，更新时不仅仅依赖当前的梯度，还结合了之前的梯度信息。这种累积会在平缓区域（曲率小的区域）加速前进，使得沿这个方向的更新更加迅速。

累积效应：由于动量的累积效应，参数在同一方向上的更新会更加剧烈，相当于在这个方向上增加了步长。因此，沿这个方向的有效学习率 γ' 就变大了，相当于整体上加速了收敛过程。

几何级数累积：从公式推导来看，有效学习率是一个几何级数的封闭形式，反映了多次梯度累积的整体效果。因此，当动量系数 μ 较大时，累积效应更明显，使得有效学习率明显放大。

Heuristic:

- When error function is believed to be poorly conditioned, choose a momentum of 0.9 or 0.99.

The Adam Algorithm

Algorithm 1: *Adam*, our proposed algorithm for stochastic optimization. See section 2 for details, and for a slightly more efficient (but less clear) order of computation. g_t^2 indicates the elementwise square $g_t \odot g_t$. Good default settings for the tested machine learning problems are $\alpha = 0.001$, $\beta_1 = 0.9$, $\beta_2 = 0.999$ and $\epsilon = 10^{-8}$. All operations on vectors are element-wise. With β_1^t and β_2^t we denote β_1 and β_2 to the power t.

Require: α: Stepsize
Require: $\beta_1, \beta_2 \in [0, 1)$: Exponential decay rates for the moment estimates
Require: $f(\theta)$: Stochastic objective function with parameters θ
Require: θ_0: Initial parameter vector
  $m_0 \leftarrow 0$ (Initialize 1^{st} moment vector)
  $v_0 \leftarrow 0$ (Initialize 2^{nd} moment vector)
  $t \leftarrow 0$ (Initialize timestep)
  while θ_t not converged **do**
    $t \leftarrow t + 1$
    $g_t \leftarrow \nabla_\theta f_t(\theta_{t-1})$ (Get gradients w.r.t. stochastic objective at timestep t)
    $m_t \leftarrow \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot g_t$ (Update biased first moment estimate)
    $v_t \leftarrow \beta_2 \cdot v_{t-1} + (1 - \beta_2) \cdot g_t^2$ (Update biased second raw moment estimate)
    $\widehat{m}_t \leftarrow m_t / (1 - \beta_1^t)$ (Compute bias-corrected first moment estimate)
    $\widehat{v}_t \leftarrow v_t / (1 - \beta_2^t)$ (Compute bias-corrected second raw moment estimate)
    $\theta_t \leftarrow \theta_{t-1} - \alpha \cdot \widehat{m}_t / (\sqrt{\widehat{v}_t} + \epsilon)$ (Update parameters)
  end while
  return θ_t (Resulting parameters)

from Kingma'15

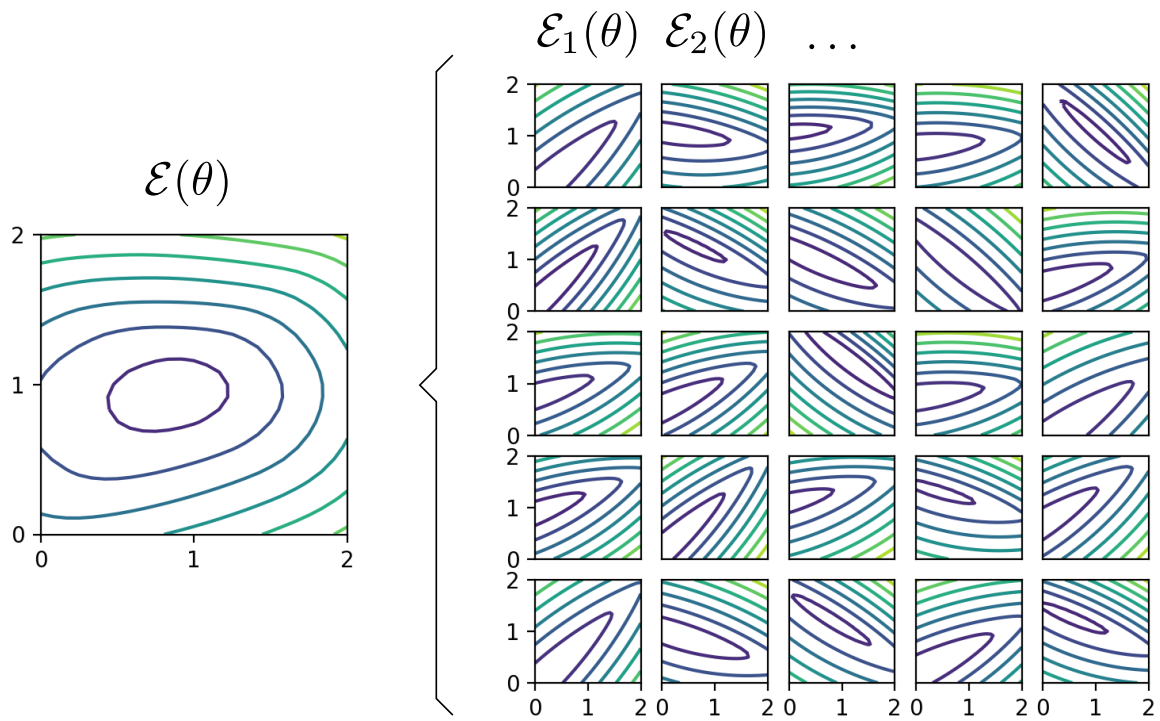
Part 2

Avoiding Redundancies

Data Redundancies

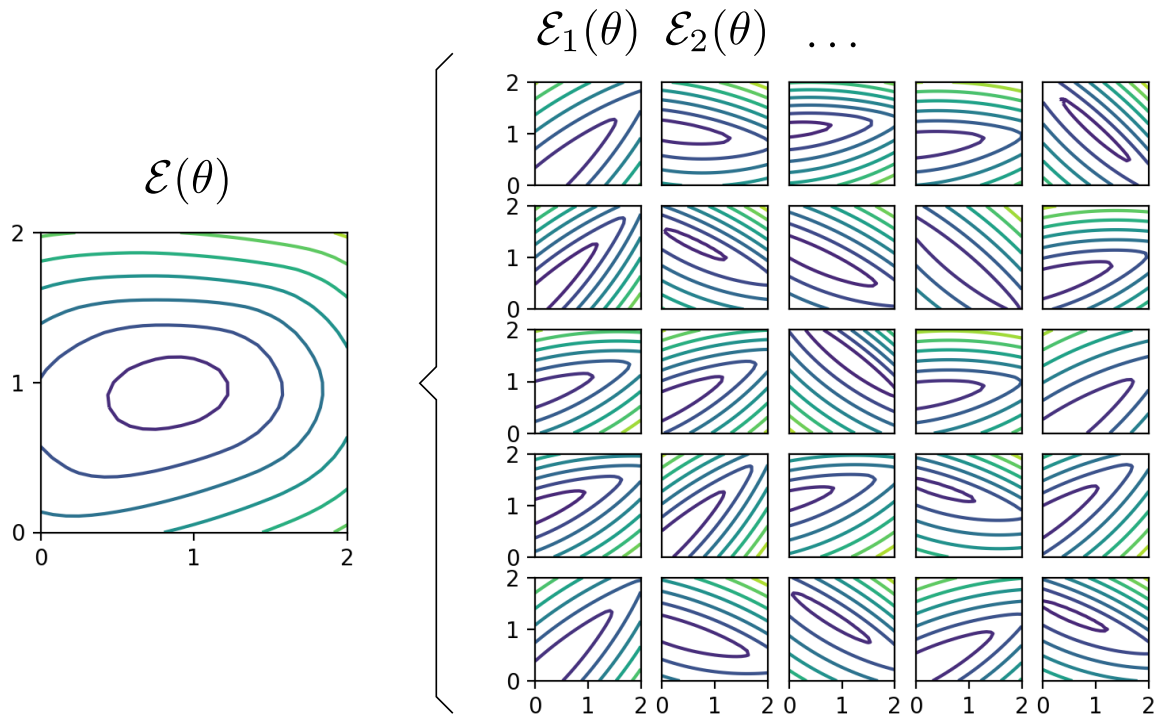
Observation:

- The error function can usually be decomposed as the sum of errors on individual data points, i.e. $\mathcal{E}(\theta) = \sum_{i=1}^{N} \mathcal{E}_i(\theta)$.
- Error terms associated to different data points have similar shapes, e.g. for a linear model $y = w \cdot x + b$ with $\theta = (w, b)$, the overall and individual error functions typically look like this:



右图分别是每个点的error 等高线,横纵坐标为theta1和theta2

Data Redundancies



Conclusion:

- It is redundant (and computationally inefficient) to compute the error function for every data point at each step of gradient descent.

Question:

- Can we perform gradient descent only on a subset of the data, or alternatively, pick at each iteration a random subset of data?

Stochastic Gradient Descent

Gradient descent:

for $t = 1 \dots T$ **do**

$$\theta \leftarrow \theta - \gamma \underbrace{\nabla\Big(\frac{1}{N}\sum_{i=1}^{N}\mathcal{E}_i(\theta)\Big)}_{\nabla\mathcal{E}(\theta)}$$

end for

Stochastic gradient descent:

for $t = 1 \dots T$ **do**

$$\mathcal{I} = \text{choose}(\{1, 2, \dots, N\}, K)$$

$$\theta \leftarrow \theta - \gamma \underbrace{\nabla\Big(\frac{1}{K}\sum_{i\in\mathcal{I}}\mathcal{E}_i(\theta)\Big)}_{\widehat{\nabla}\mathcal{E}(\theta)}$$

end for

- Gradient descent costs $O(N)$ at each iteration whereas stochastic gradient descent costs $O(K)$ where $K \ll N$.
- $\widehat{\nabla}$ is an unbiased estimator of ∇.
- SGD may never stabilize to a fixed solution due to the random sampling.

Stochastic Gradient Descent

Idea:

- Make the learning rate decrease over time, i.e., replace the fixed learning rate γ by a time-dependent learning rate $\gamma^{(t)}$.

Stochastic gradient descent (improved):

for $t = 1 \dots T$ **do**

$$\mathcal{I} = \text{choose}(\{1, 2, \dots, N\}, K)$$

$$\theta \leftarrow \theta - \gamma^{(t)} \underbrace{\nabla\Big(\frac{1}{K} \sum_{i \in \mathcal{I}} \mathcal{E}_i(\theta)\Big)}_{\widehat{\nabla}\mathcal{E}(\theta)}$$

end for

- SGD is guaranteed to converge if the learning rate satisfies the following two conditions:

$$\lim_{t \to \infty} \gamma^{(t)} = 0 \qquad \text{(i)}$$

$$\sum_{t=1}^{\infty} \gamma^{(t)} = \infty \qquad \text{(ii)}$$

Choosing the Learning Rate Schedule of SGD

	$\gamma^{(t)} = 1$	$\gamma^{(t)} = t^{-1}$	$\gamma^{(t)} = e^{-t}$
$\lim_{t\to\infty} \gamma^{(t)} = 0$	✗	✓	✓
$\sum_{t=1}^{\infty} \gamma^{(t)} = \infty$	✓	✓	✗

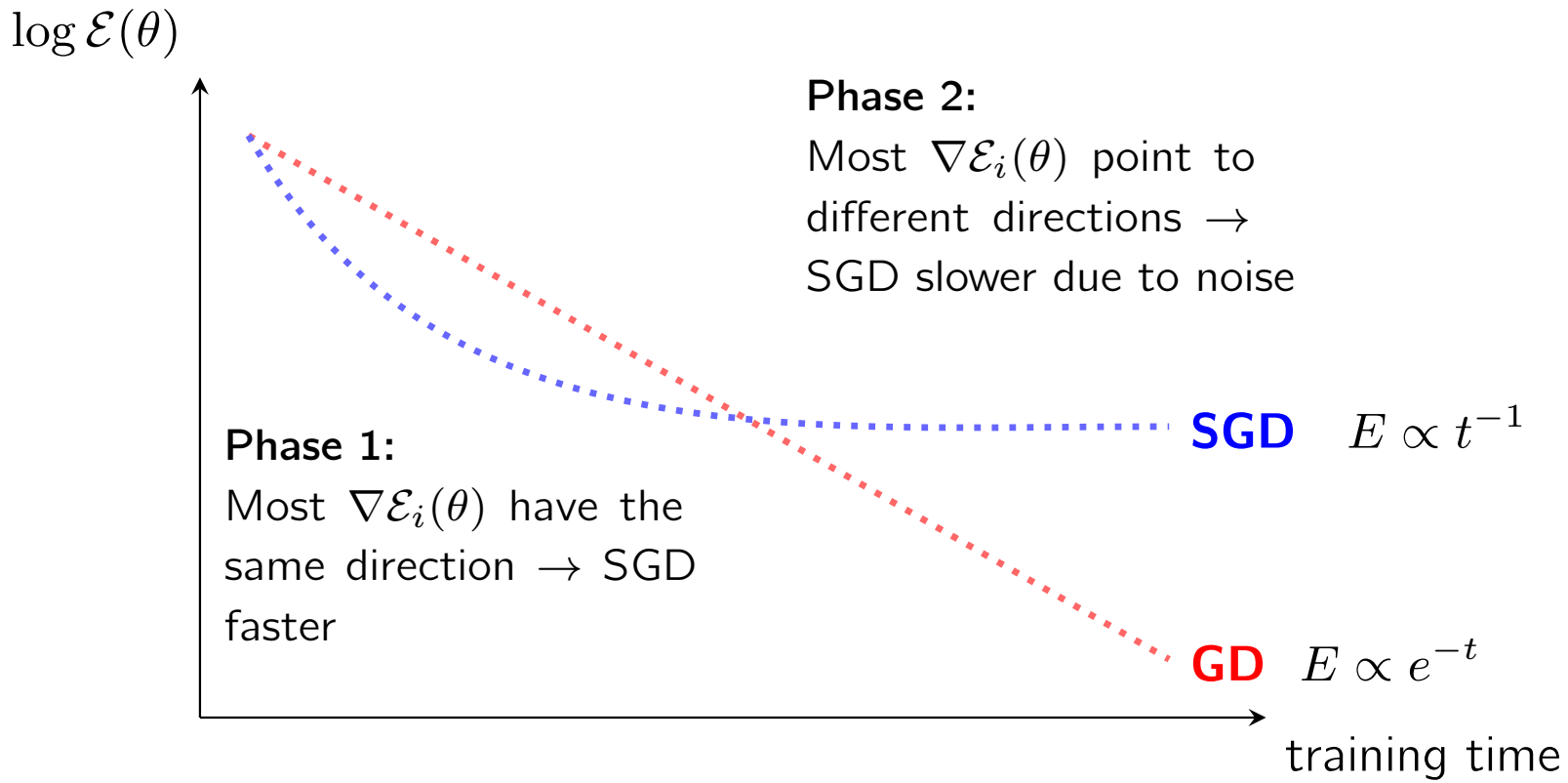
Observation:

- The learning rate should decay but not too quickly.
- Because of ths required slow decay, one also gets a slow convergence rate, e.g. t^{-1}. (Compare with the exponential convergence of GD near the optimum).

Question:

- Is SGD useful at all?

GD vs. SGD Convergence



Observations:

- In Phase 1, constants (K vs. N) matter. SGD moves way faster initially.
- Phase 2 is often irrelevant, because the model already starts overfitting before reaching it.
- K can be increased over the course of training in order to perform efficiency in both phases.

Further advantages of SGD vs. GD

- May escape local minima due to noise.
- May arrive at better generalizing solution (cf. Regularization in lectures 5–6).

Part 3

Model Efficiency

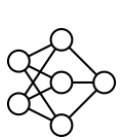
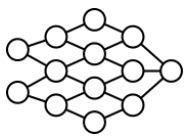
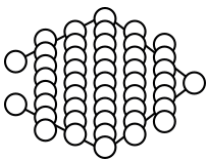
Model Efficiency

Observation:

- Another factor that can have a strong effect on training efficiency is how much time/resource it takes to produce one forward pass.

General guidelines:

- The number of neurons in the network should not be chosen larger than needed for the task.

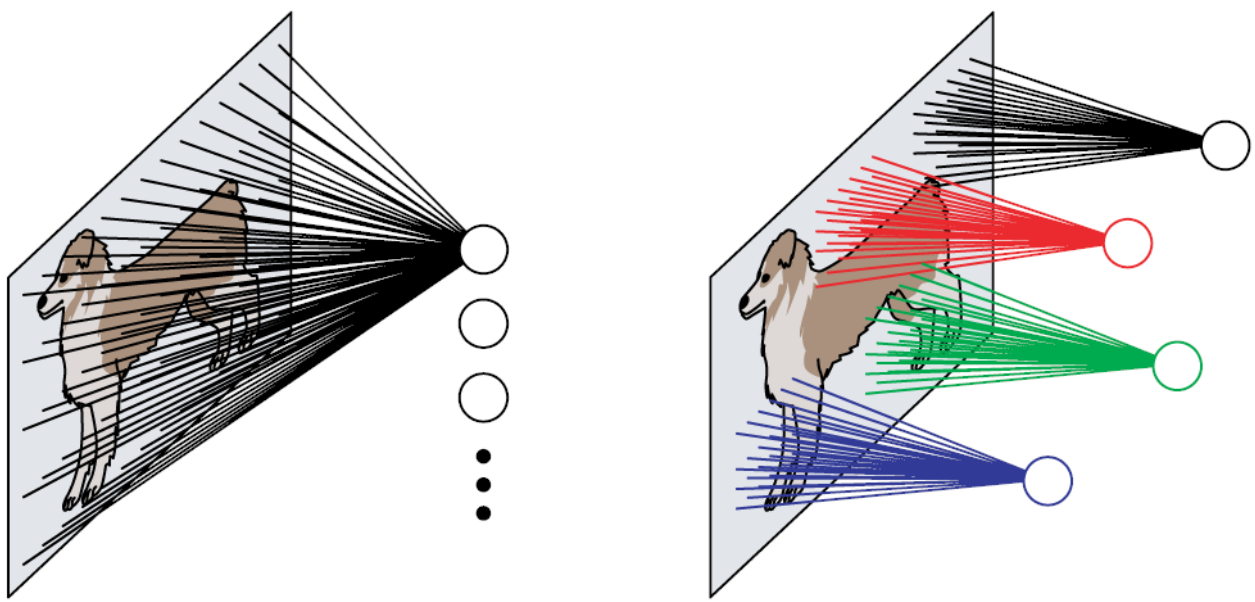
			
Solves the task	✗	✓	✓
Cheap to evaluate	✓	✓	✗

- The network should be organized in a way that only relevant computations are performed.

Model Efficiency

Global connectivity vs. local connectivity

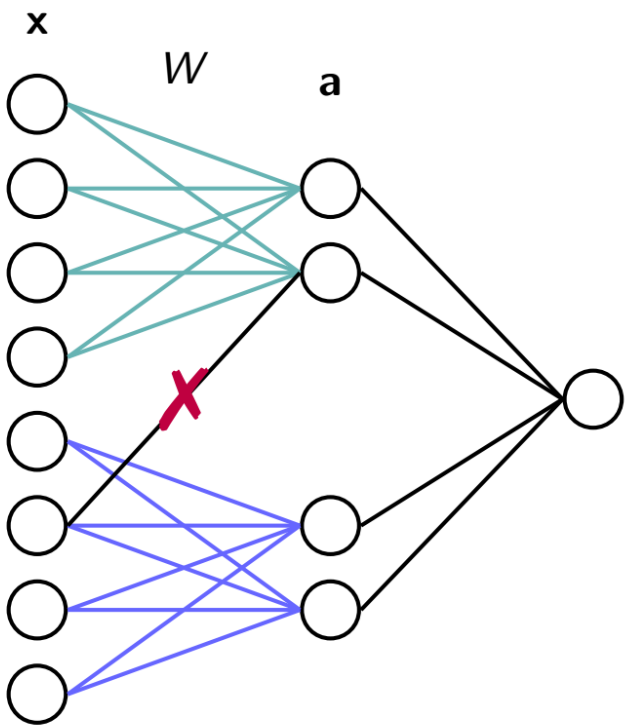
- Keeping only local connections can substantially reduce the number of computations for each neuron.
- Only works if the representation computed at a the layer does not require long-range interactions.



Adapted from B. Sick, O. Durr, Deep Learning Lecture, ETHZ.

Model Efficiency

Global connectivity vs. local connectivity

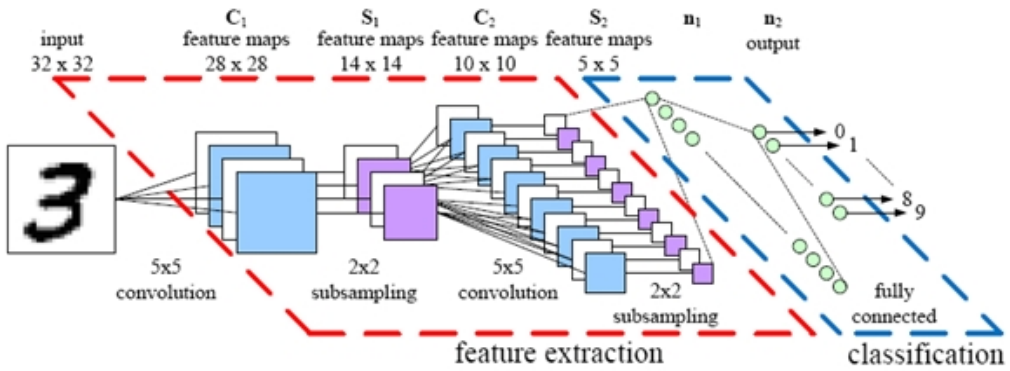


$$\mathbf{a} = \underbrace{W^\top \mathbf{x}}_{8\times 4=32 \text{ computations}} = \underbrace{W_\mathrm{A}^\top \mathbf{x}_\mathrm{A} + W_\mathrm{B}^\top \mathbf{x}_\mathrm{B}}_{2\times(2\times 4)=16 \text{ computations}}$$

$$W = \begin{pmatrix} W_\mathrm{A} & 0 \\ 0 & W_\mathrm{B} \end{pmatrix}$$

Avoiding Computational Bottlenecks

The CNN Architecture:



- Lower layers detect simple features at exact locations.
- Higher layers detect complex features at approximate locations.

空间信息

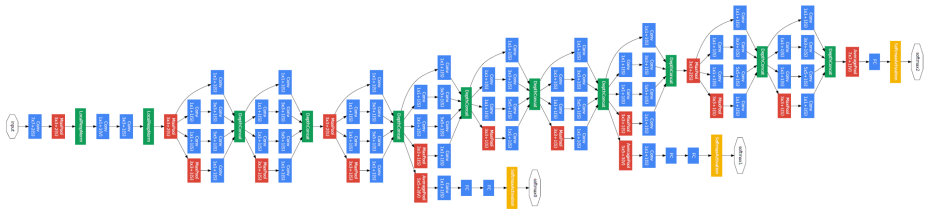
Key Computational Benefit of the CNN:

- Spatial information is progressively replaced by with semantic information as we move from the input layer to the top layer.
- The dimensionality and number of connections is never too high at any layer.

Avoiding Computational Bottlenecks

Example:

The Inception-v1 (GoogleNet) architecture



type	patch size/ stride	output size	output filters	depth	#1×1	#3×3 reduce	#3×3	#5×5 reduce	#5×5	pool proj	params	ops
convolution	7×7/2	112×112	64	1							2.7K	34M
max pool	3×3/2	56×56	64	0								
convolution	3×3/1	56×56	192	2		64	192				112K	360M
max pool	3×3/2	28×28	192	0								
inception (3a)		28×28	256	2	64	96	128	16	32	32	159K	128M
inception (3b)		28×28	480	2	128	128	192	32	96	64	380K	304M
max pool	3×3/2	14×14	480	0								
inception (4a)		14×14	512	2	192	96	208	16	48	64	364K	73M
inception (4b)		14×14	512	2	160	112	224	24	64	64	437K	88M
inception (4c)		14×14	512	2	128	128	256	24	64	64	463K	100M
inception (4d)		14×14	528	2	112	144	288	32	64	64	580K	119M
inception (4e)		14×14	832	2	256	160	320	32	128	128	840K	170M
max pool	3×3/2	7×7	832	0								
inception (5a)		7×7	832	2	256	160	320	32	128	128	1072K	54M
inception (5b)		7×7	1024	2	384	192	384	48	128	128	1388K	71M
avg pool	7×7/1	1×1	1024	0								
dropout (40%)		1×1	1024	0								
linear		1×1	1000	1							1000K	1M
softmax		1×1	1000	0								

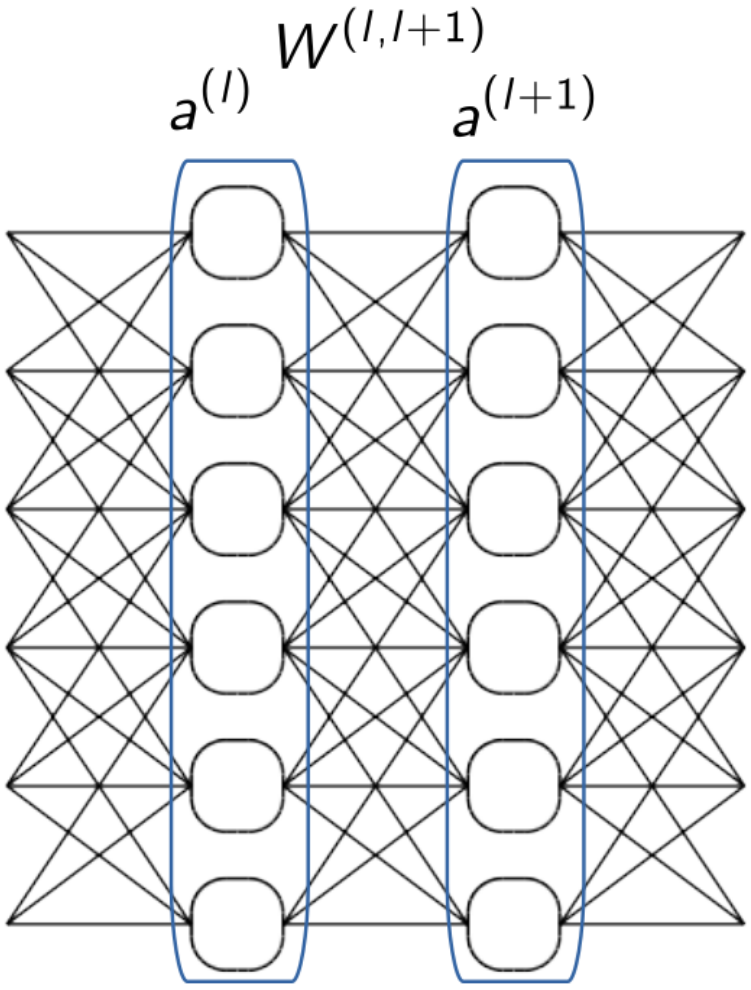
Observation:

- No specific layer strongly dominate in terms of number of operations.

Part 4

Systemize / Parallellize Computations

Systemize Computations



Per-neuron forward computations

$$\forall_j : a_j = g\left(\sum_i a_i w_{ij} + b_j\right)$$

Whole-layer computation

$$a^{(l+1)} = g\left(W^{(l,l+1)} \cdot a^{(l)} + b^{(l+1)}\right)$$

matrix-vector products (e.g. numpy.dot)

element-wise application of nonlinearity

Choosing Batch Size in SGD

Two factors enter into the decision of the batch size.

- Whether gradient of data points are redundant, typically, whether we are in phase 1 or phase 2 of training.
- Whether the machine used for training the model is sufficiently big so that the batch operation can be performed in $O(1)$ on that machine.

	Phase 1 of training (correlated gradients)	Phase 2 of training (decorrelated gradients)
small machine	small batch	medium batch
big machine	medium batch	large batch

Map Neural Network to Hardware

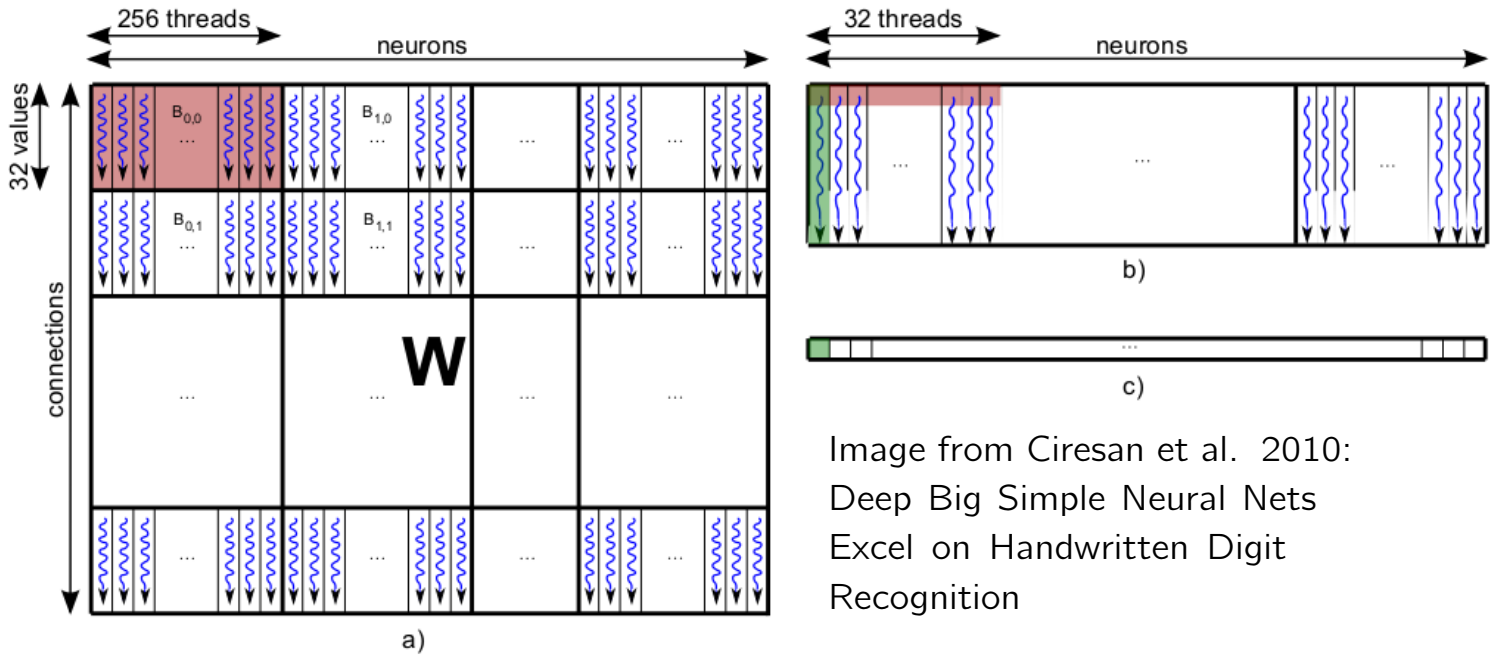


Image from Ciresan et al. 2010: Deep Big Simple Neural Nets Excel on Handwritten Digit Recognition

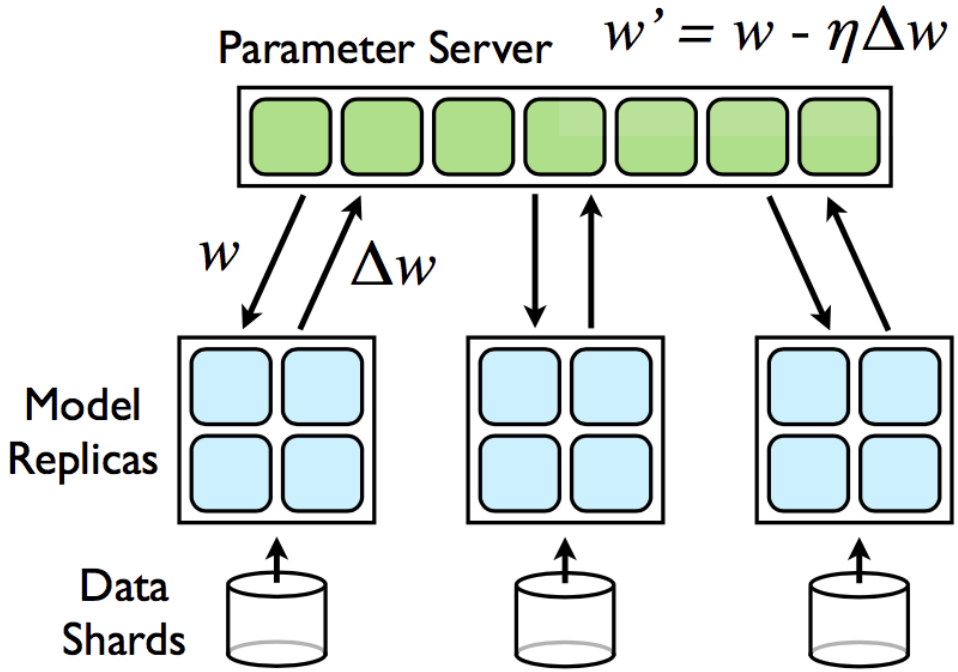
- In order for the training procedure to match the hardware specifications (e.g. CPU cache, GPU block size) optimally, neural network computations (e.g. batch computations) must be decomposed into blocks of appropriate size.
- These hardware-specific optimizations are already built in most fast neural network libraries (e.g. PyTorch, Tensorflow, cuDNN, ...).

Part 5

Distributed Training

Distributed Training

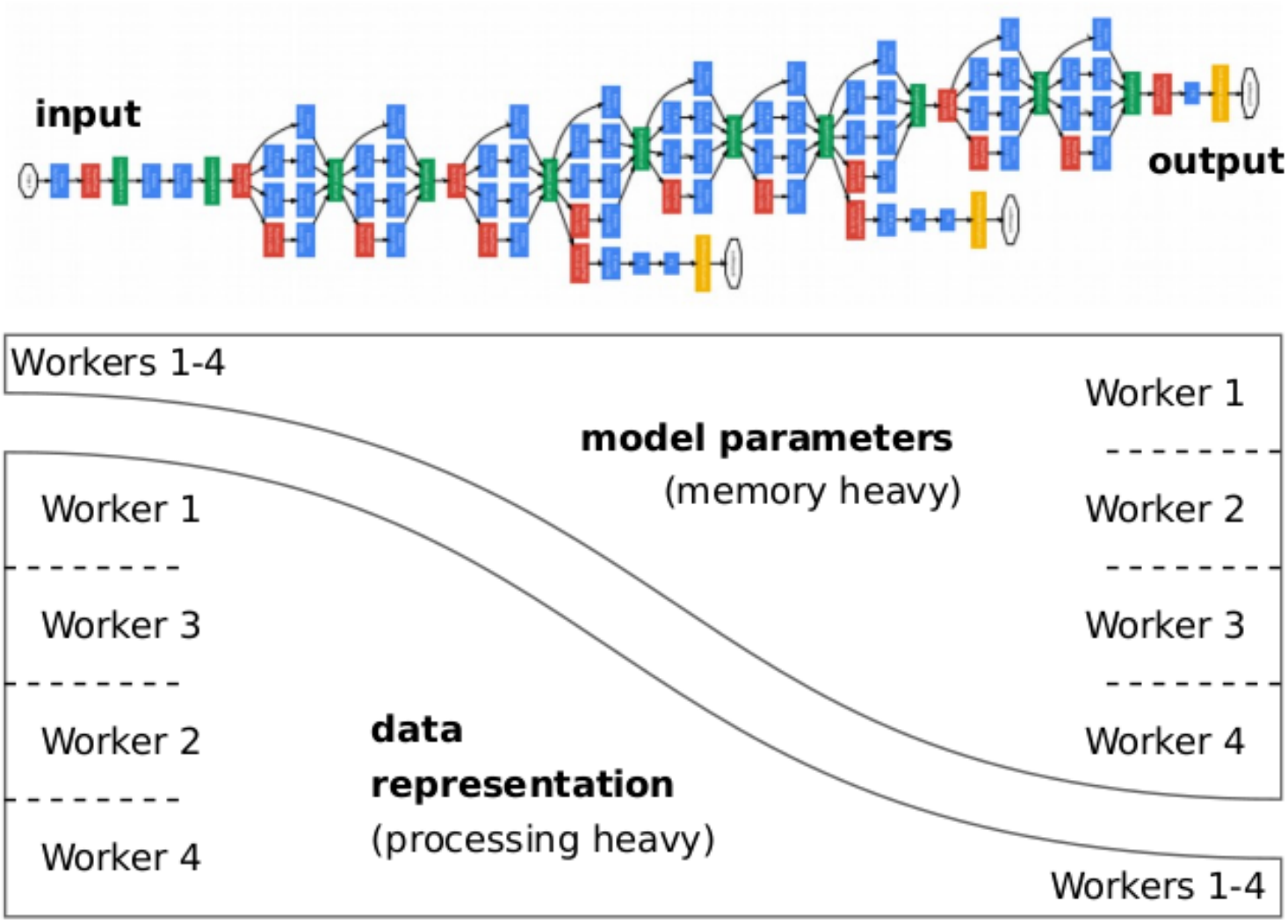
Example: Google's DistBelief Architecture [Dean'12]



Each model replica trains on its own data, and synchronizes the model parameters it has learned with other replica via a dedicated parameter server.

Distributed Training

Combining data-parallelism and model-parallelism



see also Krizhevsky'14: One weird trick for parallelizing convolutional neural networks

Summary

Summary

- Even with the best practices for shaping the error function $\mathcal{E}(\theta)$ such as data centering, designing a good architecture, etc., the optimization of $\mathcal{E}(\theta)$ remains computationally demanding.
- A poorly conditioned error function can be addressed by enhancing the simple gradient descent procedure with momentum.
- The contributions of different data points to the error function are initially highly correlated $\rightarrow$ it is beneficial to approximate the error gradient from only a random subset of points at each iteration (stochastic gradient descent).
- The model can be shaped in a way that avoids unnecessary computations (e.g. weights connecting features known to be unrelated), and in a way that avoids computational bottlenecks.
- For most efficient neural network training, it is important to consider what the hardware can achieve (e.g. what operation the hardware achieves in $O(1)$).
- Very large models and very large datasets do not fit on a single machine. In that case, we need to design distributed schemes, with appropriate use of data/model parallelism.