Deep Learning via Hessian-free Optimization

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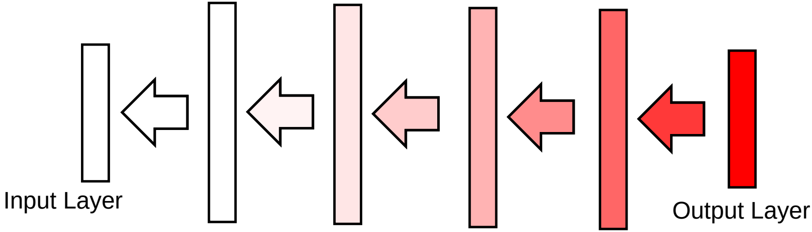

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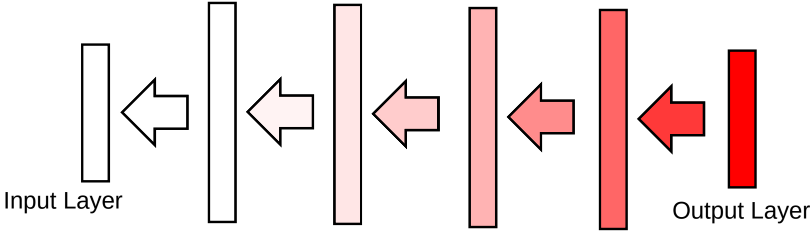
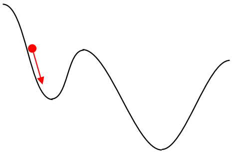


- the gradient is tiny for weights in early layers

Gradient descent is bad at deep learning (cont.)

Two hypotheses for why gradient descent fails:

- increased frequency and severity of bad local minima:



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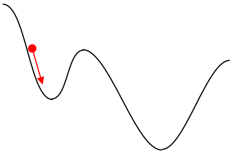
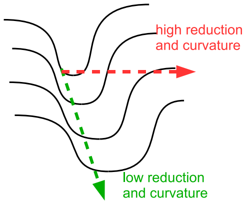
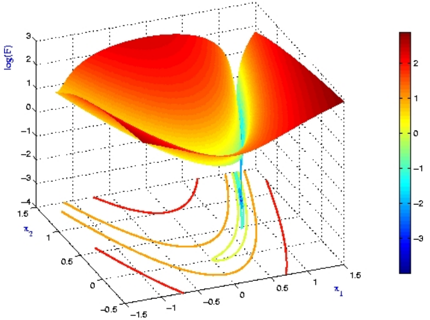


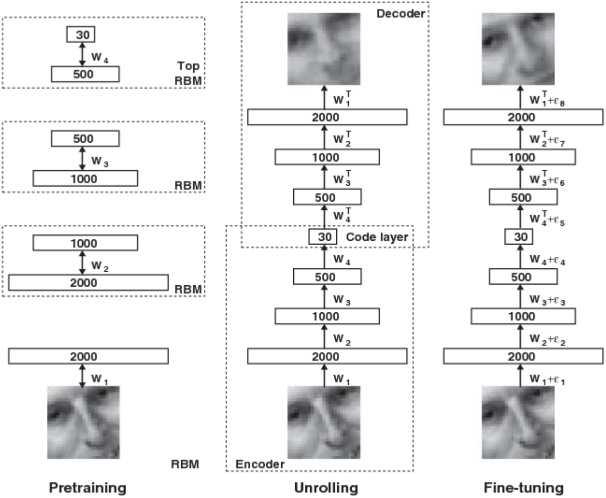
- pathological curvature, like the type seen in the well-known Rosenbrock function:

$$f(x,y) = (1-x)^2 + 100(y-x^2)^2$$





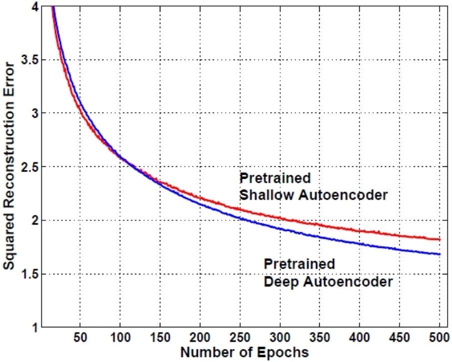
Pre-training for deep auto-encoders



(from Hinton and Salakhutdinov, 2006)

Pre-training (cont.)

- doesn't generalize to all the sorts of deep-architectures we might wish to train
- does it get full power out of deep auto-encoders?



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  - no pre-training required!

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- we show that it can achieve significantly lower test-set reconstruction errors on the deep auto-encoder problems considered in Hinton and Salakhutdinov
  - no pre-training required!
- using pre-training still lowers *generalization* error on 2 of the 3 problems
  - *but critically there isn't a significant benefit on the training set*
- our method provides a better solution to the underfitting problem in deep networks and can be applied to a much larger set of models

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General framework

- model the objective function by the local approximation:

$$f(\theta + p) \approx q_\theta(p) \equiv f(\theta) + \nabla f(\theta)^\top p + \frac{1}{2} p^\top \mathrm{B} p$$

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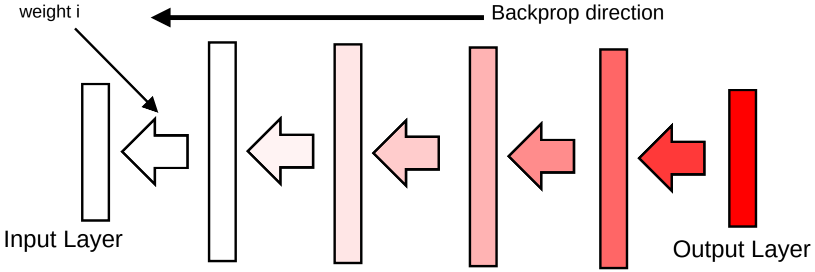
- in Newton's method, $\mathrm{B} = \mathrm{H}$ or $\mathrm{H} + \lambda I$
- fully optimizing $q_\theta(p)$ this w.r.t. p gives: $p = -\mathrm{B}^{-1} \nabla f(\theta)$
- update is: $\theta \leftarrow \theta + \alpha p$ for some $\alpha \leq 1$ determined by a line search

Vanishing Curvature

- define the direction d by $d_k = \delta_{ik}$
- low reduction along d: $-\nabla f^\top d = -(\nabla f)_i \approx 0$
- but also low curvature: $d^\top \mathrm{H} d = -\mathrm{H}_{ii} = \frac{\partial^2 f}{\partial \theta_i^2} \approx 0$



- so a 2nd-order optimizer will pursue d at a reasonable rate, an elegant solution to the vanishing gradient problem of 1st-order optimizers

Practical Considerations for 2nd-order optimization

Hessian size problem

- for machine learning models the number of parameter N can be **very** large
- we can't possibly calculate or even store a $N \times N$ matrix, let alone invert one

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Quasi-Newton Methods

- non-linear conjugate gradient (NCG) - a hacked version of the quadratic optimizer linear CG
- limited-memory BFGS (L-BFGS) - a low rank Hessian approximation
- approximate diagonal or block-diagonal Hessian

Unfortunately these don't seem to resolve the deep-learning problem

Hessian-free optimization

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- $\mathrm{H}v$ is computed for the *exact* value of H, there is no low-rank or diagonal approximation here!

Hessian-free optimization (cont.)

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- but we actually care about the quadratic, so this is good
- requires $N = \dim(\theta)$ iterations to converge in general, but makes a lot of progress in *far* fewer iterations than that

Standard Hessian-free Optimization

Pseudo-code for a simple variant of damped Hessian-free optimization:

---

for $n = 1$ to max-epochs **do**
    compute gradient $g_n = \nabla f(\theta_n)$
    choose/adapt λ_n according to some heuristic
    define the function $\mathrm{B}_n(v) = \mathbf{H}v + \lambda_n v$
    $p_n = \text{CGMinimize}(B_n, -g_n)$
    $\theta_{n+1} = \theta_n + p_n$
end for

In addition to choosing λ_n, the stopping criterion for the CG algorithm is a critical detail.

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- there are many aspects of the algorithm that are ill-defined in the basic approach which we need to address:
  - how can deal with negative curvature?
  - how should we choose λ?
  - how can we handle large data-sets
  - when should we stop the CG iterations?
  - can CG be accelerated?

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- technique generalizes to almost any twice-differentiable function that is tractable to compute
- can be automated (like automatic differentiation)

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- and we can compute $\mathrm{G}v$ using an algorithm similar to the one for $\mathrm{H}v$

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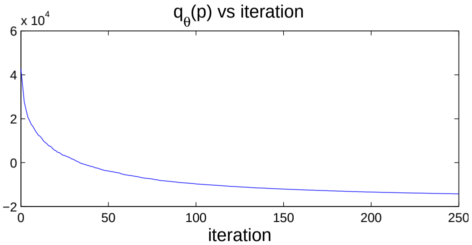
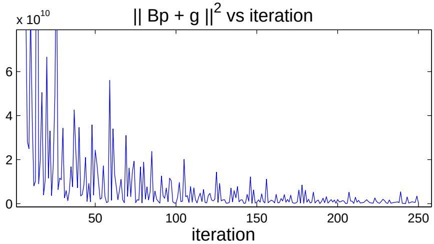
- strictly speaking $\|r\|$ is *not* the quantity that CG minimizes, nor is it the one we really care about





CG stopping conditions (cont.)

- we found that terminating CG once the relative per-iteration reduction rate fell below some tolerance ϵ worked best

$$\frac{\Delta q}{q} < \epsilon$$

(Δq is the change in the quadratic model averaged over some window of the last k iterations of CG)

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- size is related to model and qualitative aspects of the dataset, but critically not its size
  - for very large datasets, mini-batches might be a tiny fraction of the whole
- gradient and line-searches can be computed using even larger mini-batches since they are needed much less often

Other enhancements

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- (see the paper for further details)

Results

Experimental parameters (K = mini-batch size)

Name	size	K	encoder dims
CURVES	20000	5000	784-400-200-100-50-25-6
MNIST	60000	7500	784-1000-500-250-30
FACES	103500	5175	625-2000-1000-500-30

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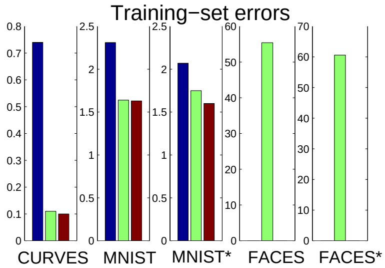
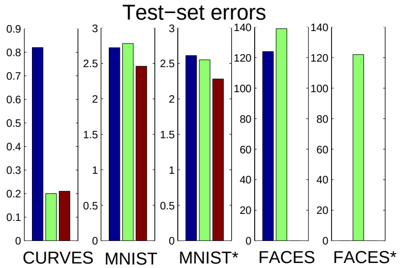
- all methods were run using GPU implementations. H&S's pre-training plus NCG fine-tuning method was run for a *lot* longer

Results (cont.)

- **PT + NCG** = pre-trained initialization with non-linear CG optimizer
- **RAND+HF** = random initialization with our Hessian-free method
- **PT + HF** = pre-trained initialization with our Hessian-free method
- * indicates an ℓ_2 prior was used

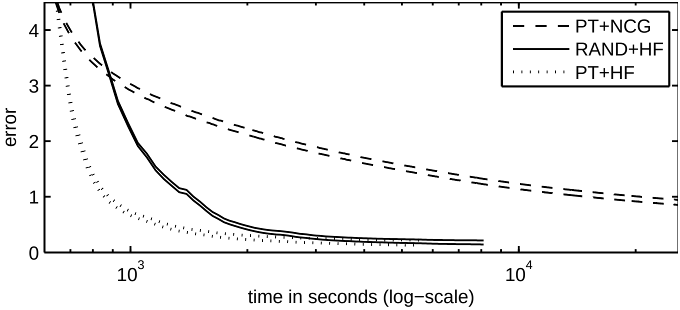




	PT + NCG	RAND+HF	PT + HF	NO EARLY STOP
CURVES	0.74, 0.82	0.11, 0.20	0.10, 0.21	0.1
MNIST	2.31, 2.72	1.64, 2.78	1.63, 2.46	1.4
MNIST*	2.07, 2.61	1.75, 2.55	1.60, 2.28	
FACES	-, 124	55.4, 139	-,-	12.9!
FACES*	-,-	60.6, 122	-,-	

Our HF method is practical

- error on the CURVES task versus GPU time:



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