# Deep Learning via Hessian-free Optimization

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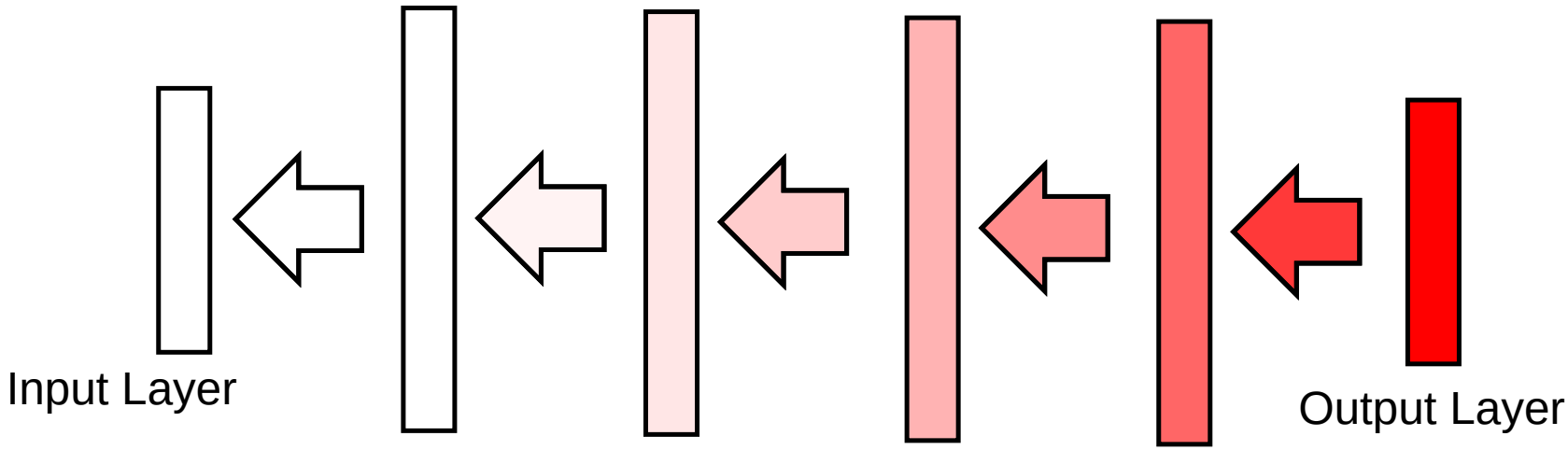

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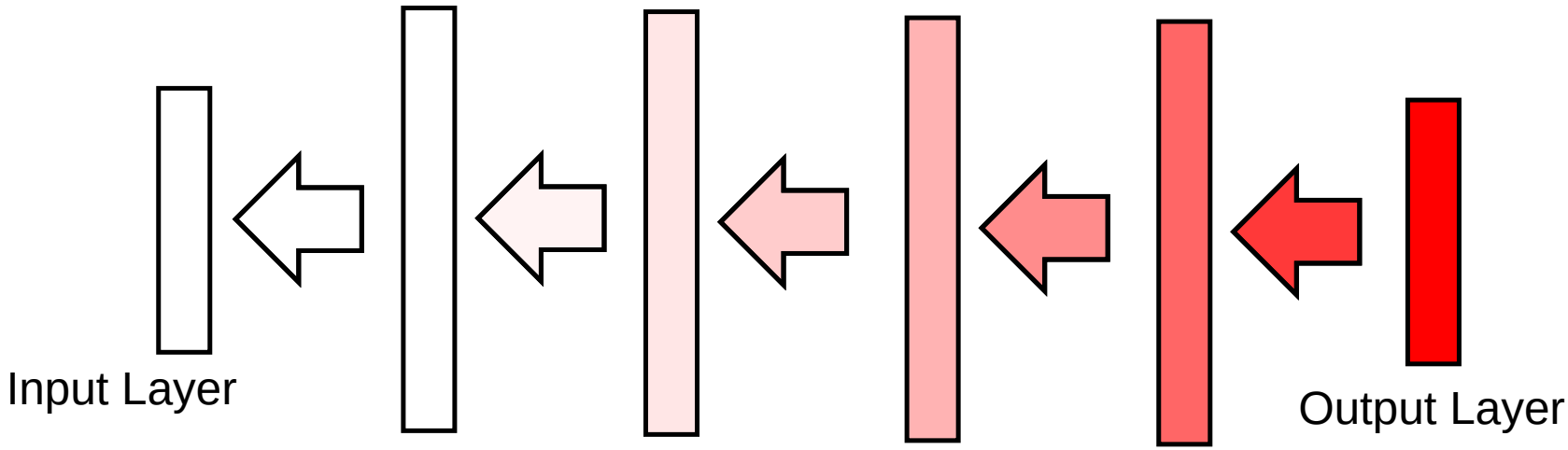
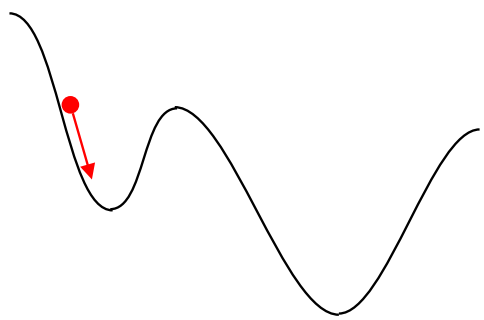



- the gradient is tiny for weights in early layers

# 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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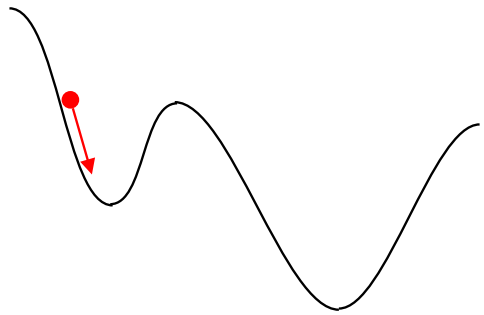
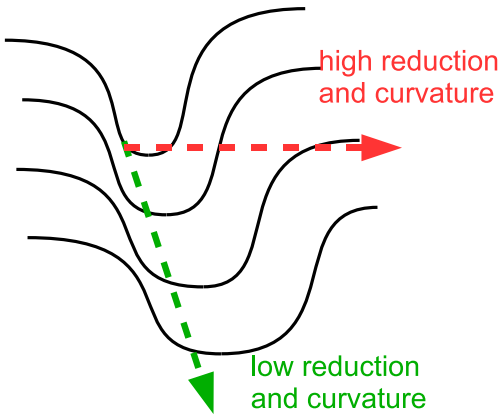
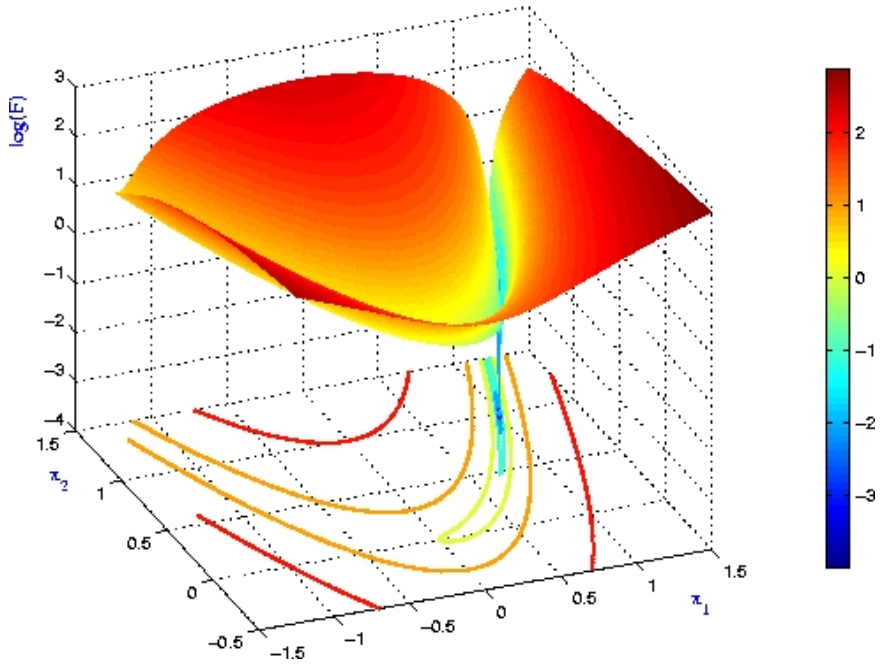


- pathological curvature, like the type seen in the well-known Rosenbrock function:

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



# Attempted solutions for deep learning problem

**Some early attempts address the vanishing gradients/pathological curvature issue**:

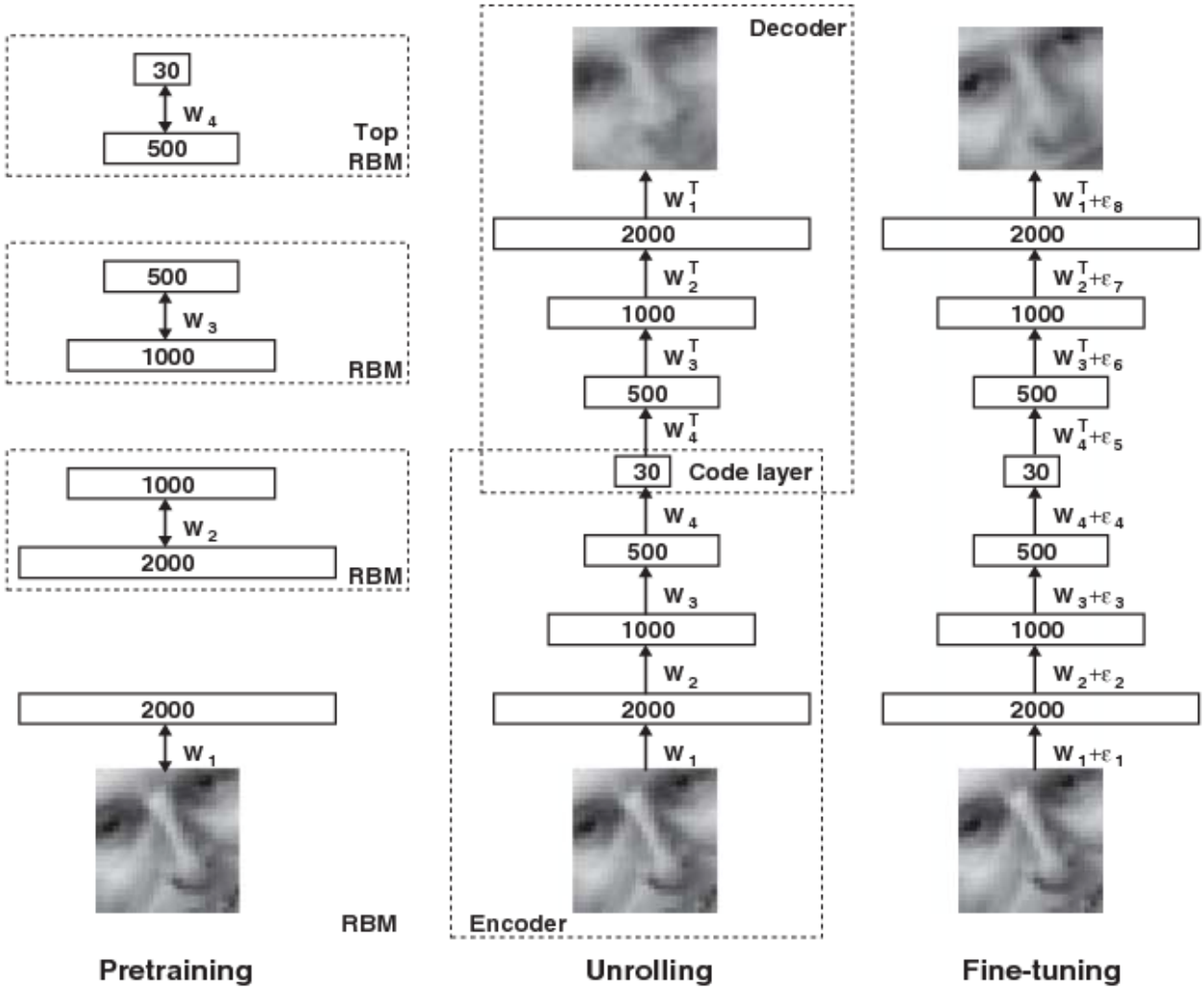
## Momentum

- average of the previous gradients with exponential decay
- physical analogy: builds "momentum" while descending down narrow valleys

## Adaptive learning rates ("R-prop")

- attempts to address the "vanishing gradients" problem directly
- individual parameters have learning rates that are adapted dynamically
- like a heuristically computed diagonal Hessian approximation

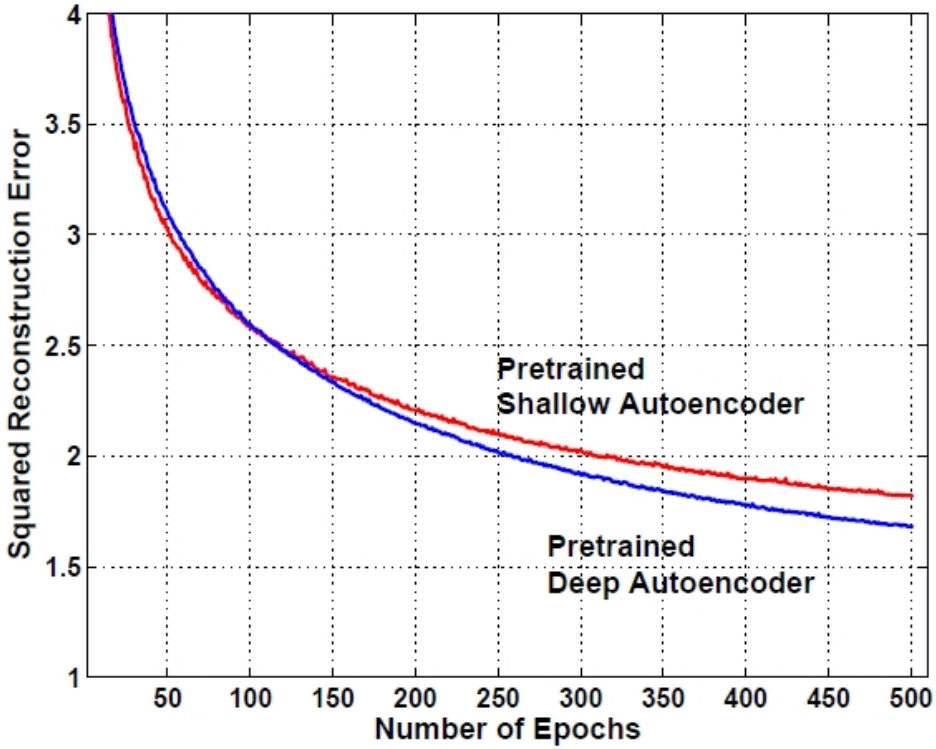
# Pre-training for deep auto-encoders




(from Hinton and Salakhutdinov, 2006)

# Pre-training (cont.)

- doesn't generalize to all the sorts of deep-architectures we might wish to train
- still requires a classical optimization algorithm to "fine-tune" the parameters
- does it get full power out of deep auto-encoders?

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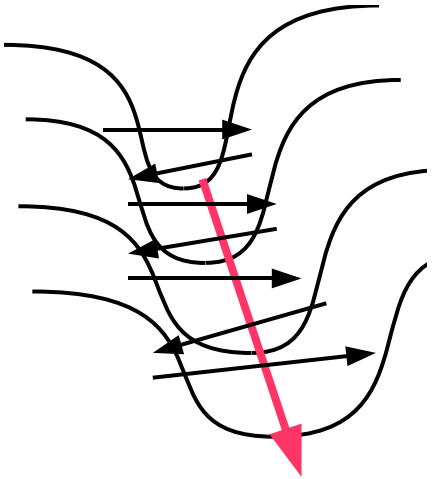
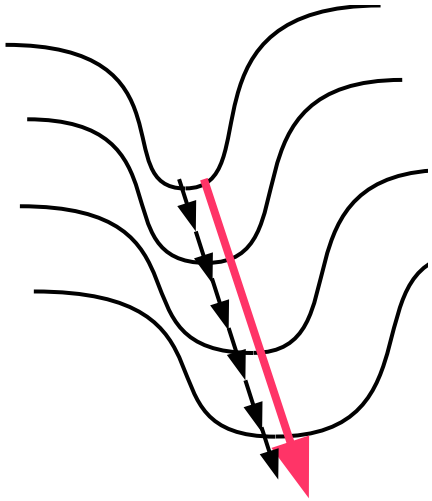
- in Newton's method, $\mathrm{B} = \mathrm{H}$ or $\mathrm{H} + \lambda \mathrm{I}$
- fully optimizing $q_\theta(p)$ this w.r.t. $p$ gives: $p = -\mathrm{B}^{-1} \nabla f(\theta)$
- update is: $\theta \leftarrow \theta + \alpha p$ for some $\alpha \leq 1$ determined by a line search

# The importance of curvature (cont.)

**Cartoon example of pathological curvature: the long narrow valley**

- consider the following example where low and high-curvature directions co-occur. Using gradient descent gives one of the following 2 undesirable behaviors:



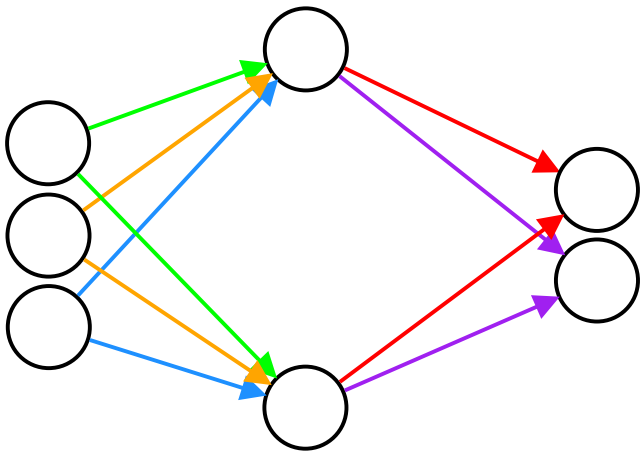


**large learning rate:** high curvature directions pursued too far, undesirable "bouncing" behavior

**small learning rate:** progress along low curvature directions is far too slow

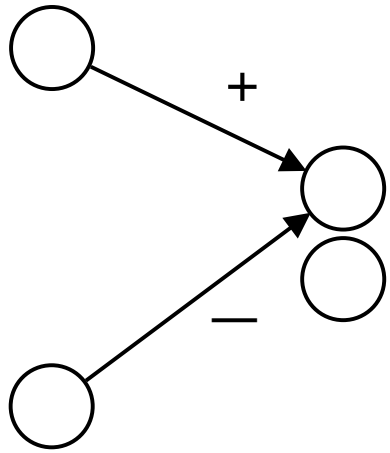
# Pathological curvature in deep-nets

- Suppose we have 2 *nearly* identical units (i.e. nearly identical weights and biases). Let $i$ and $j$ be the two red weights. Let $d$ direction with $d_k = \delta_{ik} - \delta_{jk}$. $d$ is a direction which differentiates these weights.
- Then the reduction is low: $-\nabla f^\top d = (\nabla f)_j - (\nabla f)_i \approx 0$
- But so is the curvature: $d^\top \mathrm{H} d = (\mathrm{H}_{ii} - \mathrm{H}_{ij}) + (\mathrm{H}_{jj} - \mathrm{H}_{ji}) \approx 0 + 0 = 0$



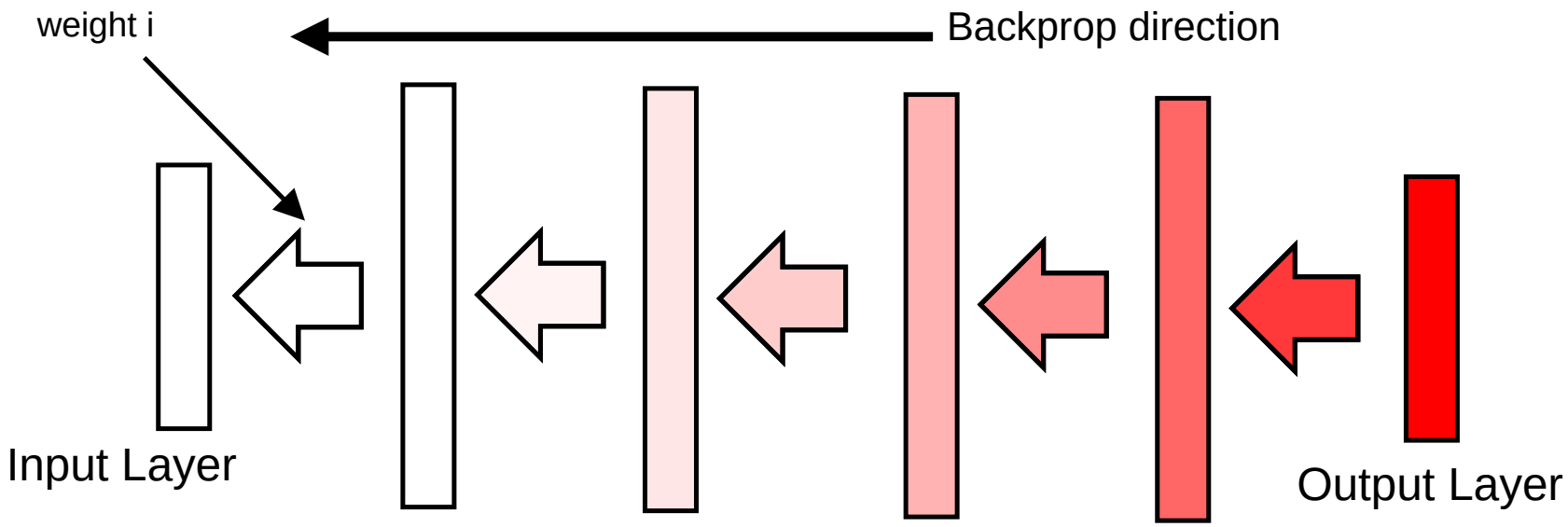
**Left:** Neural net with nearly identical units (in the middle layer). Two weights with the same color have *nearly* identical values.

**Right:** Graphical representation of $d$



# 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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$$\mathrm{H}v = \lim_{\epsilon \to 0} \frac{\nabla f(\theta + \epsilon v) - \nabla f(\theta)}{\epsilon}$$

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- $\mathrm{H}v$ is computed for the *exact* value of $\mathrm{H}$, 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:

---

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

---

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

# Common variants of the HF approach

## Basic/naive

- $\lambda_n = 0$, CG iterations stopped when residual $\|\mathrm{B}p + g\|$ reaches some error tolerance or when negative curvature is detected

## CG-Steihaug

- $\lambda_n = 0$ and instead maintain a heuristically adjusted trust region
- when the iterates produced by the inner CG loop leave the trust region the loops terminates

## Trust-region Newton-Lanczos Method

- $\lambda_n$ is (very expensively) computed to give match a given trust region radius
- robust even when the Hessian is indefinite

# A new variant is required

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- **the bad news**: common variants of HF (e.g. Steihaug) don't work particular well for neural networks

- 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 $\lambda$?
  - 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)

# Forwards and backwards pass to compute the gradient

$\theta = (W_1, b_1, W_2, b_2, ..., W_L, b_L)$

---

1: $y_1 = \vec{in}$
2: **for** $i = 1$ to $L$ **do**
3: $\quad x_i = W_i y_i + b_i$
4: $\quad y_i = \sigma(x_i)$
5: **end for**
6: **for** $i = L$ down to $1$ **do**
7: $\quad$ **if** $i < L$ **then**
8: $\quad\quad \frac{dE}{dx_i} = \frac{dE}{dx_{i+1}} \odot y_{i+1} \odot (1 - y_{i+1})$
9: $\quad$ **else**
10: $\quad\quad \frac{dE}{dx_i} = \vec{out} - y_{i+1}$
11: $\quad$ **end if**
12: $\quad \frac{dE}{dy_i} = W_i^T \frac{dE}{dx_i}$
13: $\quad \frac{dE}{dW_i} = \frac{dE}{dx_i} y_i^T$
14: $\quad \frac{dE}{db_i} = \frac{dE}{dx_i}$
15: **end for**

---

# The same code with the R-operator applied computes $\mathrm{H}v$

$v = (V_1, c_1, ..., V_L, c_L),\ Hv = (R\{\frac{dE}{dW_1}\}, R\{\frac{dE}{db_1}\}, ..., R\{\frac{dE}{dW_L}\}, R\{\frac{dE}{db_L}\})$

---

$R\{y_1\} = 0$
**for** $i = 1$ to $L$ **do**
  $R\{x_i\} = W_i R\{y_i\} + V_i y_i + c_i$
  $R\{y_i\} = R\{x_i\} \odot y_{i+1} \odot (1 - y_{i+1})$
**end for**
**for** $i = L$ down to 1 **do**
  **if** $i < L$ **then**
    $R\{\frac{dE}{dx_i}\} = R\{\frac{dE}{dx_{i+1}}\} \odot y_{i+1} \odot (1 - y_{i+1}) + \frac{dE}{dx_{i+1}} \odot R\{y_{i+1}\} \odot (1 - 2y_{i+1})$
  **else**
    $R\{\frac{dE}{dx_i}\} = -R\{y_{i+1}\}$
  **end if**
  $R\{\frac{dE}{dy_i}\} = V_i^T \frac{dE}{dx_i} + W_i^T R\{\frac{dE}{dx_i}\}$
  $R\{\frac{dE}{dW_i}\} = R\{\frac{dE}{dx_i}\} y_i^T + \frac{dE}{dx_i} R\{y_i\}^T$
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- can be generalized beyond just least squares to neural nets with "matching" loss functions and output non-linearities (Schraudolph 2002)
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  - e.g. logistic units with cross-entropy error
- works *much* better in practice than Hessian or other curvature matrices (e.g. empirical Fisher)
- and we can compute $\mathrm{G}v$ using an algorithm similar to the one for $\mathrm{H}v$

# CG stopping conditions

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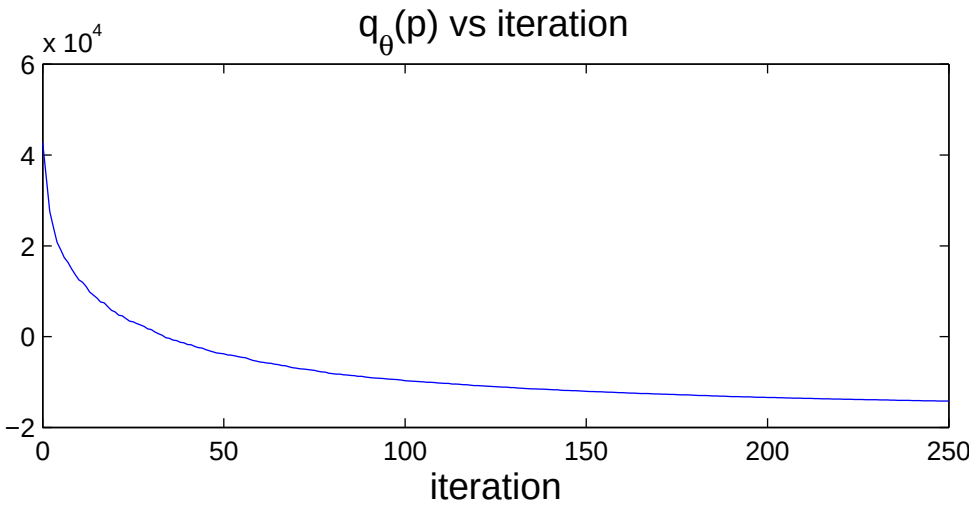
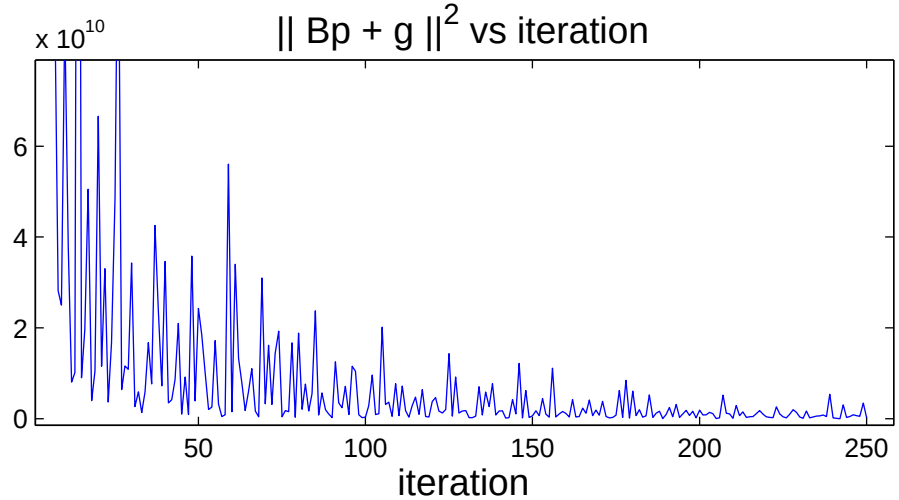
- strictly speaking $\|r\|$ is *not* the quantity that CG minimizes, nor is it the one we really care about



# CG stopping conditions (cont.)

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

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

($\Delta q$ 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

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$$\rho \leftarrow \frac{f(\theta+p)-f(\theta)}{q_\theta(p)-q_\theta(0)}$$

**if** $\rho < \frac{1}{4}$ **then**
  $\lambda \leftarrow \frac{3}{2}\lambda$
**else if** $\rho > \frac{3}{4}$ **then**
  $\lambda \leftarrow \frac{2}{3}\lambda$
**end if**

# Structural damping

- the normal damping term can be interpreted as putting an $\ell_2$ prior on the parameters that says "don't change":

$$f(\theta + p) \approx q_\theta(p) \equiv f(\theta) + \nabla f(\theta)^\top p + \frac{1}{2} p^\top (\mathrm{G} + \lambda \mathrm{I}) p$$
$$= f(\theta) + \nabla f(\theta)^\top p + \frac{1}{2} p^\top G p + \frac{\lambda}{2} \|p\|^2$$

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- for extremely non-linear models like Recurrent Neural Nets (RNNs) we expect this effect to be pronounced and so we would prefer to "damp" directions in a more intelligent way

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- fortunately $J_h v$ occurs as an intermediate quantity in the algorithm for computing $Jv$
- so it is a trivial matter to modify the algorithm include the term $\frac{\gamma}{2} p J_h^\top J_h p$

# Other enhancements

- using M-preconditioned CG with the diagonal preconditioner:

$$M = \left[ \text{diag} \left( \sum_i \nabla f_i \odot \nabla f_i \right) + \lambda \mathrm{I} \right]^{\alpha}$$

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- (see the paper for further details)

Thank you for your attention