Lecture 5 - Training & Regularizing Neural Networks

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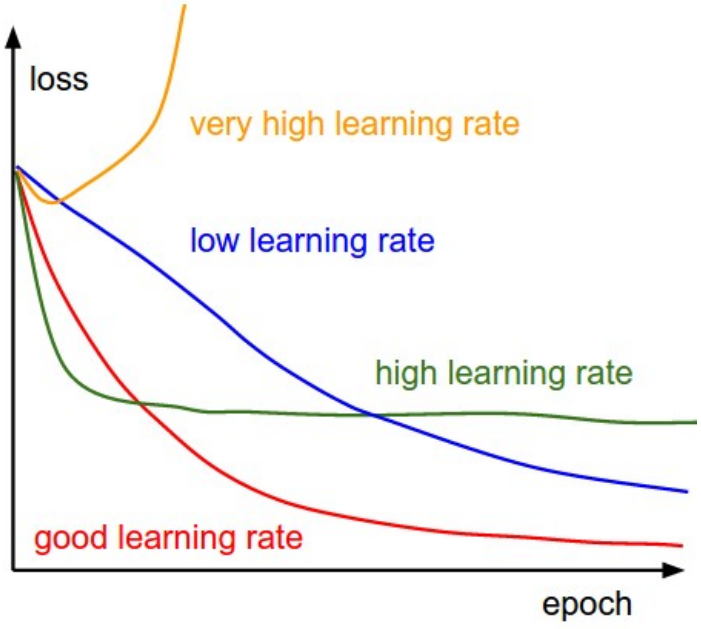
Baby sitting the training process

Training neural networks not completely trivial!

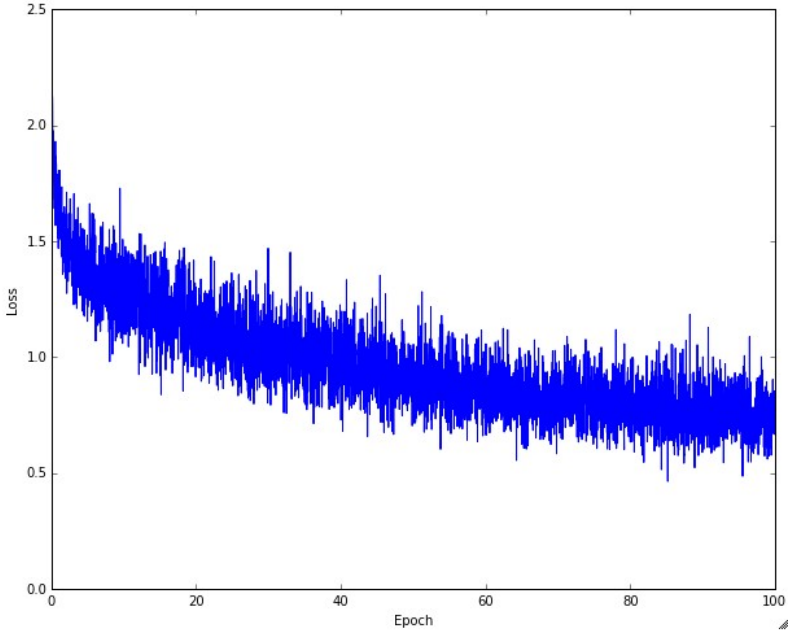
- Several **hyper-parameters** affect the quality of your training.
- These include
  - learning rate
  - degree of regularization
  - network architecture
  - hyper-parameters controlling weight initialization
- If these (potentially correlated) hyper-parameters are not appropriately set $\Longrightarrow$ you will not learn an **effective** network.
- Multiple quantities you should monitor during training.
- These quantities indicate
  - a reasonable hyper-parameter setting and/or
  - how hyper-parameters setting could be changed for the better.

What to monitor during training

Monitor & Visualize the loss/cost curve

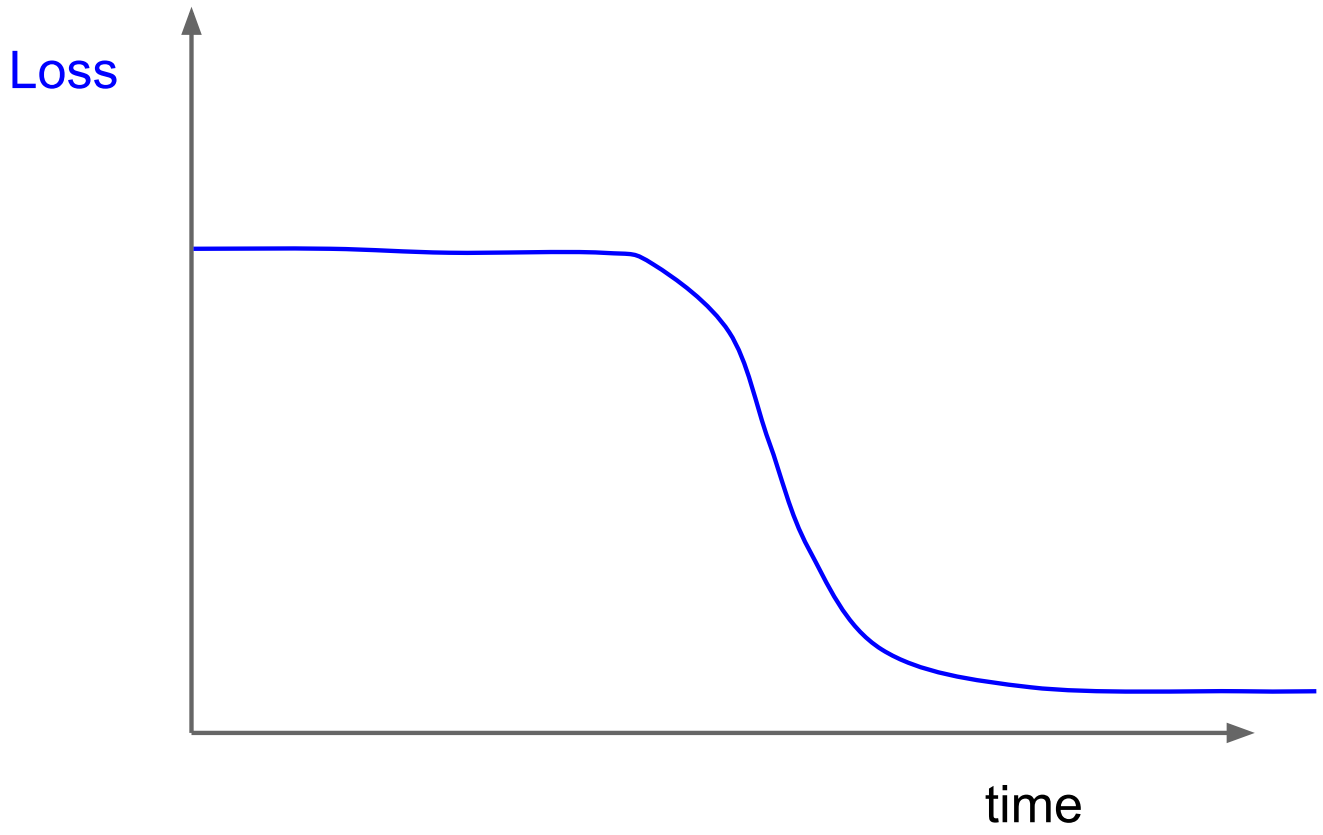


Evolution of your training loss is telling you something!

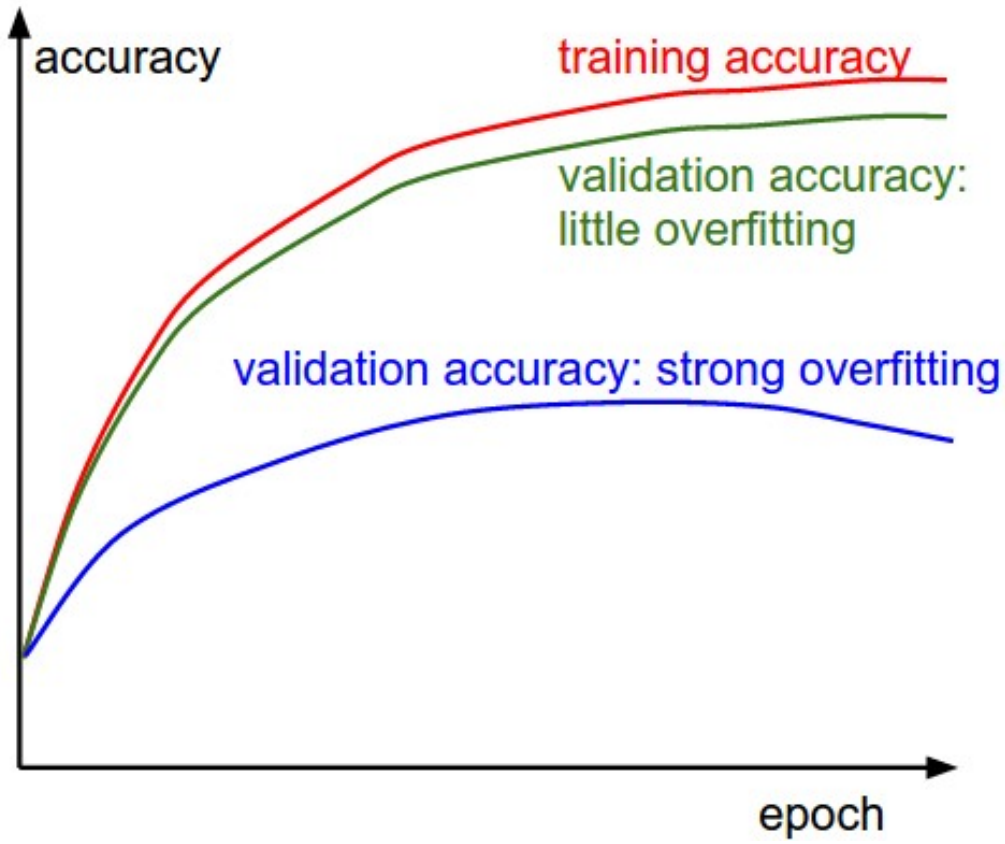


Typical training loss over time

Telltale sign of a bad initialization



Monitor & visualize the accuracy

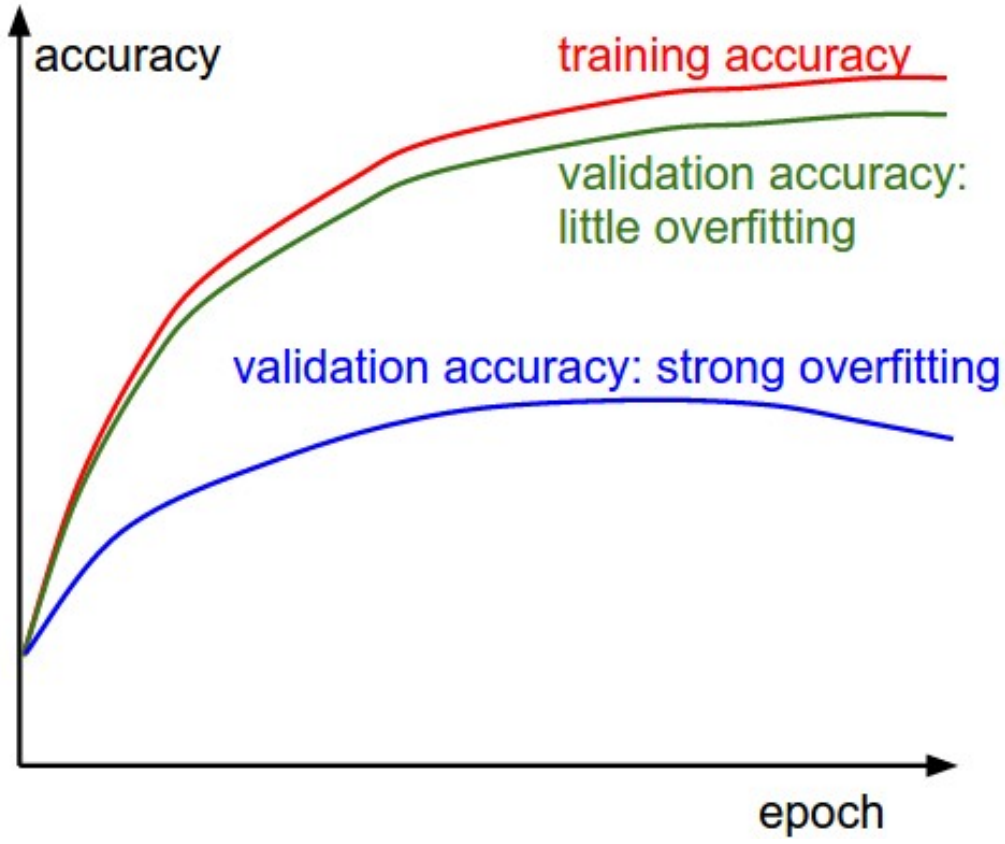


Gap between training and validation accuracy indicates amount of over-fitting.

Over-fitting $\Longrightarrow$ should increase regularization during training:

- Increase the degree of L_2 regularization.
- More dropout.
- Use more training data.

Monitor & visualize the accuracy



Gap between training and validation accuracy indicates amount of over-fitting.

Under-fitting $\Longrightarrow$ model capacity not high enough:

- Increase the size of the network.

Track the ratio of weight updates to weight magnitudes

- Track the **ratio** of the magnitude of the update vector to the magnitude of the parameter vector.
- So for a weight matrix, W, and vanilla SGD updates:

$$r = \frac{\| -\eta \nabla_W J \|}{\|W\|}$$

- A rough heuristic is that $r \sim .001$.
- If $r \ll .001 \implies$ learning rate might be too low.
- If $r \gg .001 \implies$ learning rate might be too high.

Parameter Updates: Variations of Stochastic Gradient Descent/Gradient Descent

Remember Gradient Descent optimization

- Want to minimize the function $f : \mathbb{R}^d \to \mathbb{R}$
- Gradient descent update step at time t

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \eta_t \nabla f(\mathbf{x}^{(t)})$$

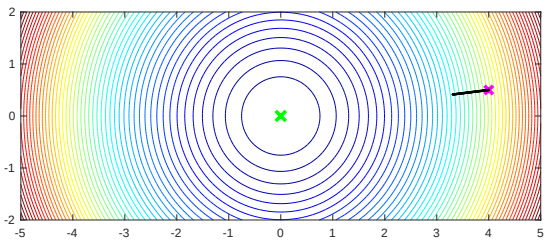
- How to choose η_t ?
- Depends on
  - the shape of f and
  - how fast a convergence you want.
- **Important property**:
  Gradient vector $\nabla f(\mathbf{x}^{(t)})$ is always orthogonal to the iso-contour curve of f at $\mathbf{x}^{(t)}$.

Example behaviour on the ideal f for gradient descent

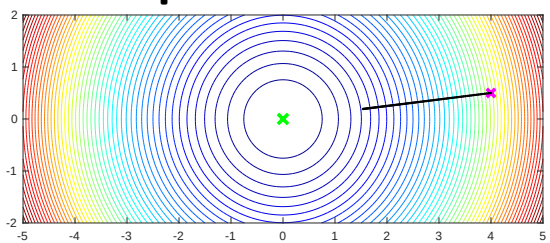
Use **gradient descent** to minimize $f(\mathbf{x}) = x_1^2 + x_2^2$ with

- $\mathbf{x}_0 = (4, .5)^T$,
- η_t constant at each iteration and
- a fixed number of update steps.

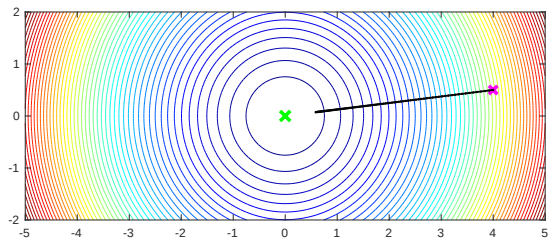
Gradient descent paths for different η_t's



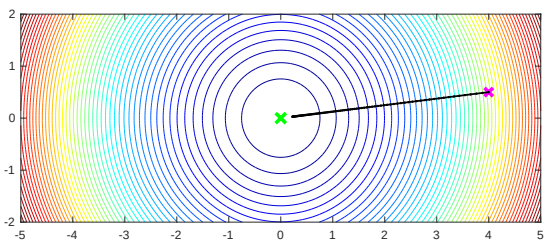
$\eta_t = .001$



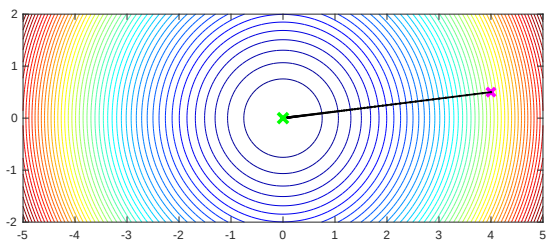
$\eta_t = .005$



$\eta_t = .01$



$\eta_t = .015$



$\eta_t = .02$

Note in this example the update step always points directly to the optimum point

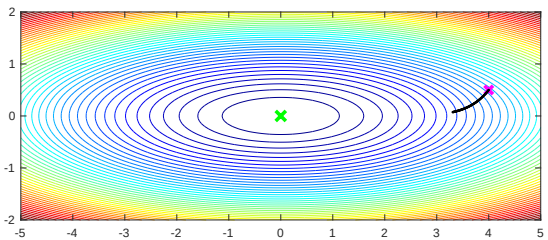
$\Longrightarrow$ can increase η_t liberally (without worrying about divergence) to speed up convergence.

Example behaviour on a suitable f for gradient descent

Use gradient descent to minimize $f(\mathbf{x}) = x_1^2 + 10x_2^2$ with

- $\mathbf{x}_0 = (4, .5)^T$,
- η_t constant at each iteration and
- a fixed number of update steps.

Gradient descent paths for different η_t's



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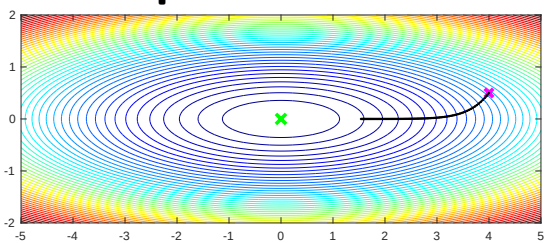

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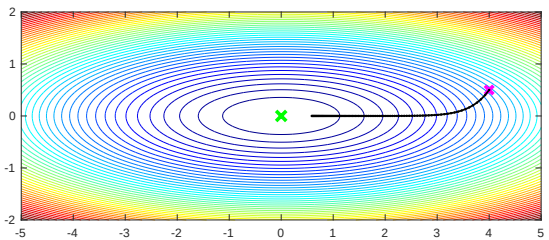

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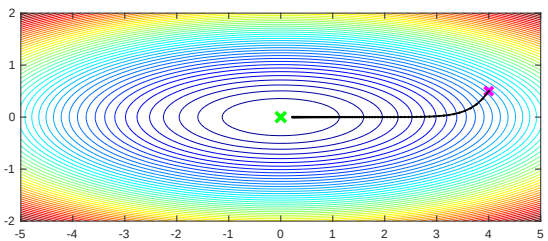

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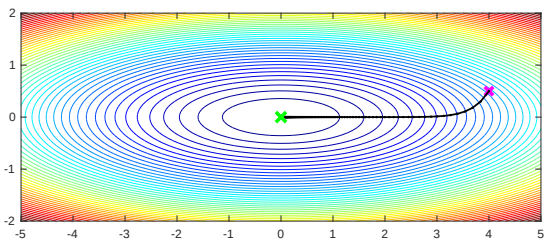

$\eta_t = .02$

Note in this example the update direction points directly to the optimum when $x_{t,2} = 0$.

Example behaviour on a less suitable f for gradient descent

Use gradient descent to minimize $f(\mathbf{x}) = x_1^2 + 50x_2^2$ with

- $\mathbf{x}_0 = (4, .5)^T$,
- η_t constant at each iteration and
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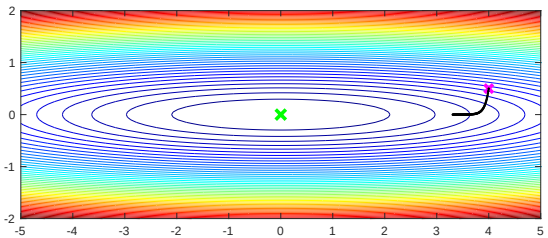
Gradient descent path for different η_t's



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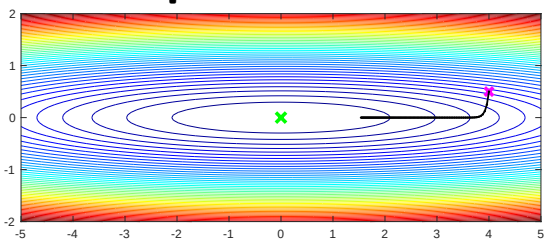

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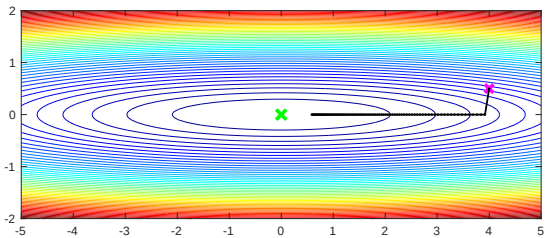

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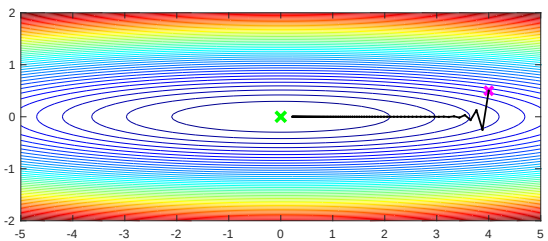

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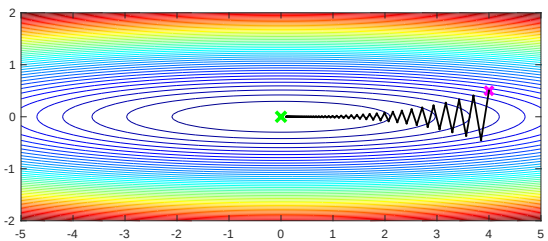
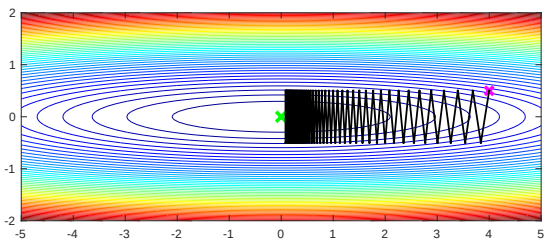


$\eta_t = .019$



$\eta_t = .02$

Note as η_t increases GD path increasingly zig-zags across the valley. In this case GD diverges for $\eta_t > .02$. To begin all paths move $\approx$ orthogonal to *optimum* direction.

Focus on GD and simple quadratic cost function

The set-up

Want to minimize w.r.t. $\mathbf{x}$:

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T A\mathbf{x} \quad \text{where } A = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

and $\lambda_1 > 0$ and $\lambda_2 > 0$.
(The optimum value is at $\mathbf{x}^* = \mathbf{0}$.)

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How does GD work on this problem?

- Apply GD with fixed η and initial guess $\mathbf{x}^{(0)}$ for $\mathbf{x}^*$
- Questions:
  - For what values of η will GD converge?
  - What is the rate of convergence?

The GD estimate at update t

Quadratic function we want to minimize:

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T A\mathbf{x} \quad \text{where } A = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

and $\lambda_1 > 0$ and $\lambda_2 > 0$.

- The gradient $\nabla_{\mathbf{x}} f(\mathbf{x})$ is

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = A\mathbf{x}$$

- At update t have

$$\begin{aligned} \mathbf{x}^{(t)} &= (I - \eta A)^t \, \mathbf{x}^{(0)} \\ &= \begin{pmatrix} (1-\eta\lambda_1)^t & 0 \\ 0 & (1-\eta\lambda_2)^t \end{pmatrix} \mathbf{x}^{(0)} \end{aligned}$$

Convergence when?

- At update t have

$$\mathbf{x}^{(t)} = \begin{pmatrix} (1-\eta\lambda_1)^t & 0 \\ 0 & (1-\eta\lambda_2)^t \end{pmatrix} \mathbf{x}^{(0)}$$

- For convergence ($\mathbf{x}^{(t)} \to \mathbf{x}^*$ at $t \to \infty$) need

$$|1-\eta\lambda_1| < 1 \quad \text{and} \quad |1-\eta\lambda_2| < 1$$

$$\Longrightarrow$$

$$0 < \eta < \frac{2}{\max(\lambda_1, \lambda_2)}$$

η that gives fastest convergence?

- Difference between function evaluated at $\mathbf{x}^{(t)}$ and $\mathbf{x}^*$:

$$f(\mathbf{x}^{(t)}) - f(\mathbf{x}^*) = \sum_{i=1}^{2} (1 - \eta\lambda_i)^{2t} \lambda_i \, {x_i^{(0)}}^2$$

- The **rate of convergence** of above to zero is determined by

$$\max(|1 - \eta\lambda_1|, |1 - \eta\lambda_2|)$$

- Want to find the $0 < \eta < 2/\max(\lambda_1, \lambda_2)$ that maximizes the rate of convergence $\implies$

$$\min_{\eta} \max(|1 - \eta\lambda_1|, |1 - \eta\lambda_2|)$$

- Solution is

$$\eta^* = \frac{2}{\lambda_1 + \lambda_2}$$

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- Solution is

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Rate of convergence at η^*

- Difference between function evaluated at $\mathbf{x}^{(t)}$ and $\mathbf{x}^*$:

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- For the optimal learning rate have

$$|1 - \eta^*\lambda_1| = |1 - \eta^*\lambda_2| = \frac{\lambda_2/\lambda_1 - 1}{\lambda_2/\lambda_1 + 1}$$

- Let $\kappa = \lambda_2/\lambda_1$ then rate of convergence is defined by

$$\frac{\kappa - 1}{\kappa + 1}$$

- Larger κ (assuming $\lambda_2 > \lambda_1$) $\implies$ closer $(\kappa - 1)/(\kappa + 1)$ is to 1 $\implies$ slower the convergence of the GD estimate.

Rate of convergence at η^*

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- Larger κ (assuming $\lambda_2 > \lambda_1$) $\implies$ closer $(\kappa - 1)/(\kappa + 1)$ is to 1 $\implies$ slower the convergence of the GD estimate.

Rate of convergence depends on ratio - λ_2/λ_1

$$f(\mathbf{x}^{(t)}) - f(\mathbf{x}^*) = \sum_{i=1}^{2} \left(\frac{\kappa - 1}{\kappa + 1} \right)^{2t} \lambda_i \, {x_i^{(0)}}^2$$

where

$$\kappa = \frac{\lambda_2}{\lambda_1}$$

- κ is known as the condition number (indicating how close a matrix is to singular)
- When $\kappa = 1$ for η^* have convergence in one update step
- When $\kappa \gg 1$ for η^* (and all other valid η) have poor convergence rate for GD.

Can extend result to d dimensions

Have

$$A = \text{diag}(\lambda_1, \ldots, \lambda_d)$$

- GD converges when

$$0 < \eta < \frac{2}{\lambda_{\max}}$$

- Have fastest convergence when

$$\eta^* = \frac{2}{\lambda_{\max} + \lambda_{\min}}$$

- Then for optimal η^*

$$f(\mathbf{x}^{(t)}) - f(\mathbf{x}^*) = \sum_{i=1}^{d} \left(\frac{\kappa - 1}{\kappa + 1} \right)^{2t} \lambda_i \, {x_i^{(0)}}^2$$

  where $\kappa = \lambda_{\max}/\lambda_{\min}$.

- When κ increases convergence rate of GD decreases.

Back to our discussion...

Pathological case for GD optimization

- The curvature in different directions is very different for f.
- Optimization results in a zig-zagging path across the ravine $\Longrightarrow$ slow convergence.

Unfortunately, in neural network cost functions

ravines are common around local optima.

Gradient descent and the problem of choosing η_t

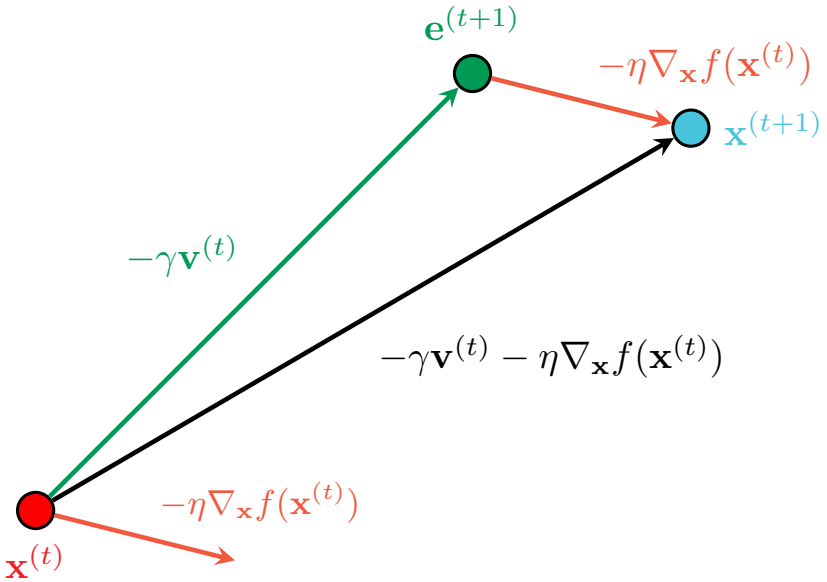
- η_t too small $\implies$ slow convergence speed but smooth update path.
- η_t too large $\implies$ optimization can potentially diverge and potentially have an inefficient zig-zag update path.

Solution 1: SGD with momentum

- Introduce **momentum** vector as well as the gradient vector.
- Let $\gamma \in [0, 1]$ and $\mathbf{v}$ is the momentum vector

$$\mathbf{v}^{(t+1)} = \gamma\, \mathbf{v}^{(t)} + \eta\, \nabla_{\mathbf{x}} f(\mathbf{x}^{(t)}) \quad \leftarrow \text{update vector}$$
$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \mathbf{v}^{(t+1)}$$

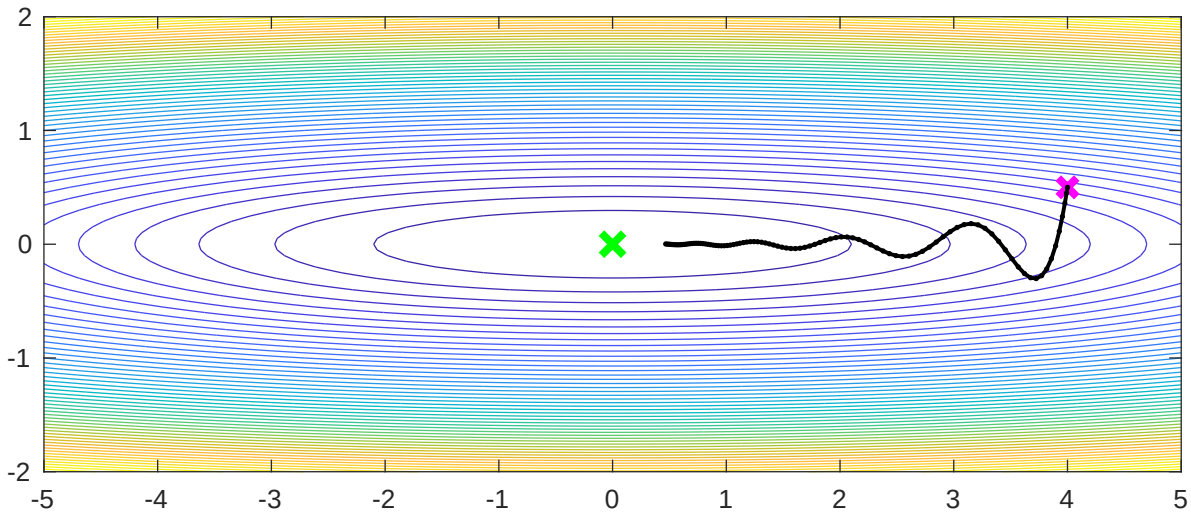
Typically γ set to .9.



How and why momentum helps

How?

- Momentum helps accelerate SGD in the appropriate direction.
- Momentum dampens the oscillations of default SGD.
  $\implies$ **Faster convergence**.



($\gamma = .9$, $\eta = .001$, 95 update steps)

Why?

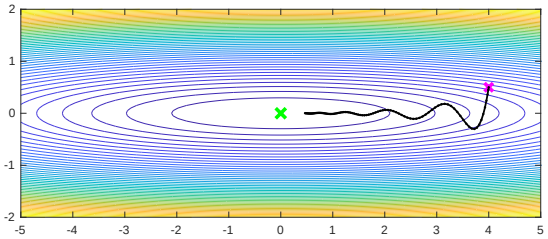
- For dimensions whose gradient is constantly changing then their entries in the update vector are damped.

Example behaviour of "GD + mom" for a ravine

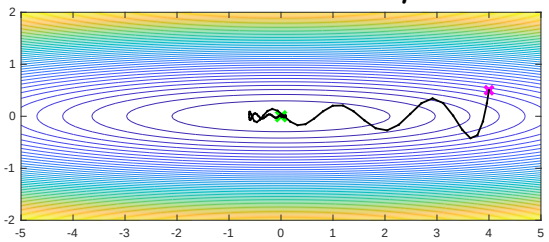
Use gradient descent to minimize $f(\mathbf{x}) = x_1^2 + 50x_2^2$ with

- $\mathbf{x}_0 = (4, .5)^T$,
- η_t constant at each iteration and
- a fixed number of update steps.

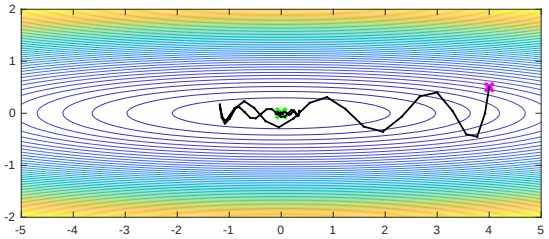
GD + mom path for different η_t's and $\gamma = .9$



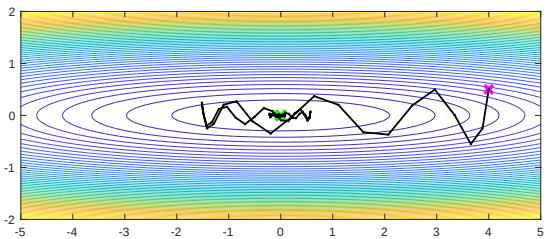
$\eta_t = .001$



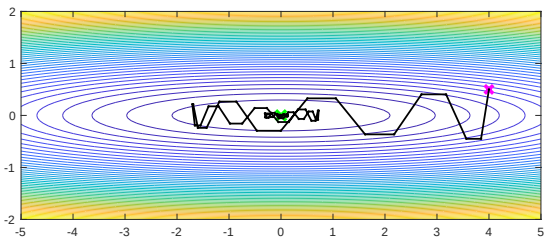
$\eta_t = .005$



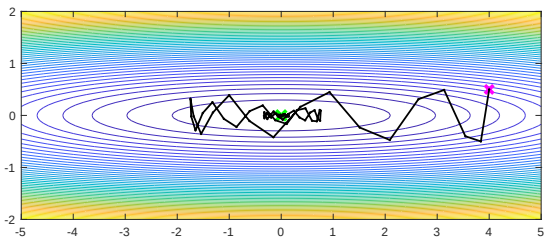
$\eta_t = .01$



$\eta_t = .015$



$\eta_t = .019$



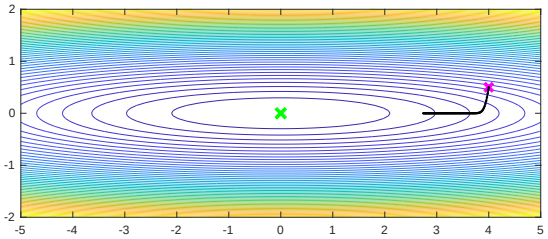
$\eta_t = .02$

Example behaviour of "GD + mom" for a ravine

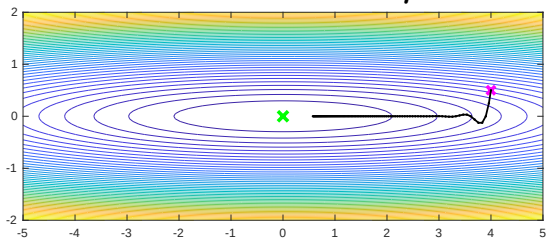
Use gradient descent to minimize $f(\mathbf{x}) = x_1^2 + 50x_2^2$ with

- $\mathbf{x}_0 = (4, .5)^T$,
- η_t constant at each iteration and
- a fixed number of update steps.

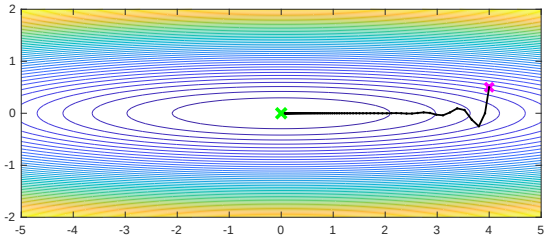
GD + mom path for different η_t's and $\gamma = .5$



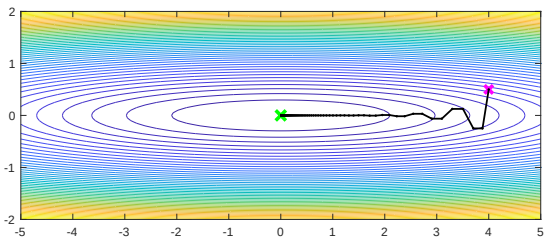
$\eta_t = .001$



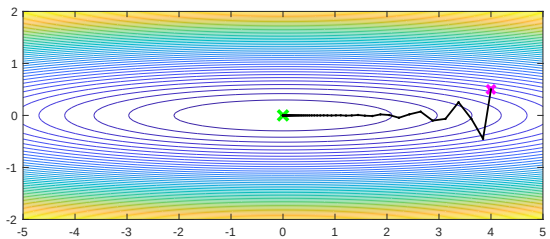
$\eta_t = .005$



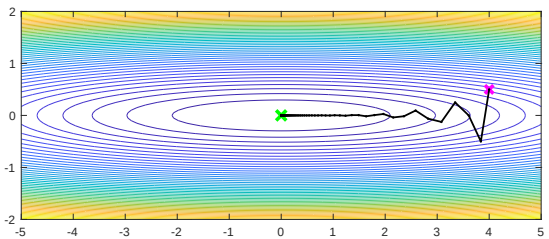
$\eta_t = .01$



$\eta_t = .015$



$\eta_t = .019$



$\eta_t = .02$

Can view momentum as GD with a variable learning rate

- The gradient descent at update t can be written as

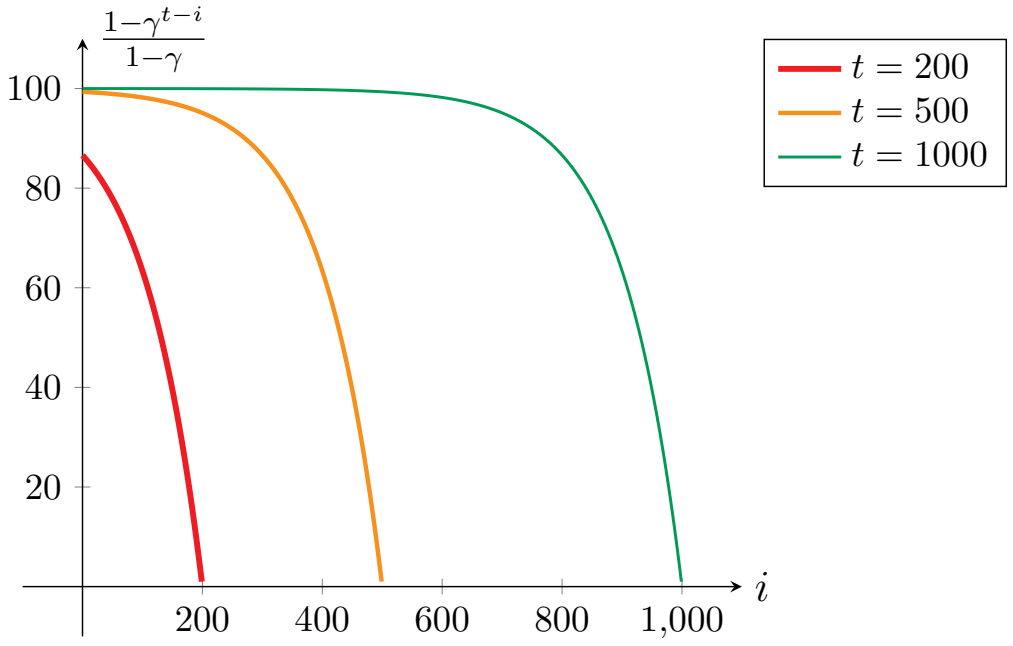
$$\mathbf{x}^{(t)} = \mathbf{x}^{(0)} - \eta \sum_{i=0}^{t-1} \nabla_{\mathbf{x}} f(\mathbf{x}^{(i)})$$

- The gradient descent + momentum at update t can be written as

$$\mathbf{x}^{(t)} = \mathbf{x}^{(0)} - \eta \sum_{i=0}^{t-1} \left(\frac{1-\gamma^{t-i}}{1-\gamma} \right) \nabla_{\mathbf{x}} f(\mathbf{x}^{(i)})$$

Effective learning rate for SGD + momentum

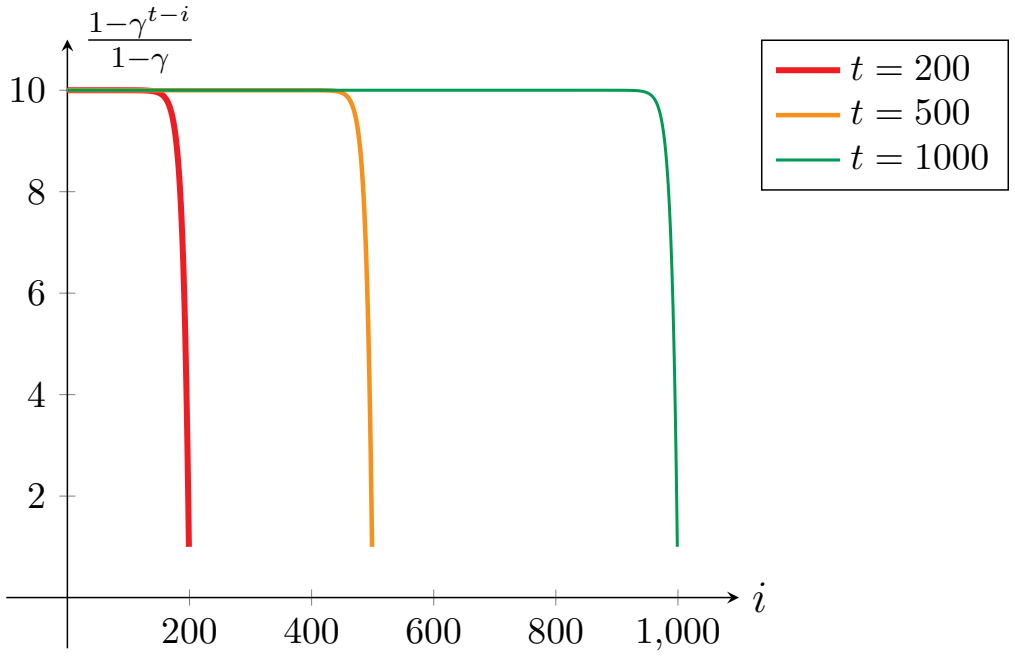
$$\gamma = .99$$



$$\mathbf{x}^{(t)} = \mathbf{x}^{(0)} - \eta \sum_{i=0}^{t-1} \left(\frac{1-\gamma^{t-i}}{1-\gamma} \right) \nabla_{\mathbf{x}} f(\mathbf{x}^{(i)})$$

Effective learning rate for SGD + momentum

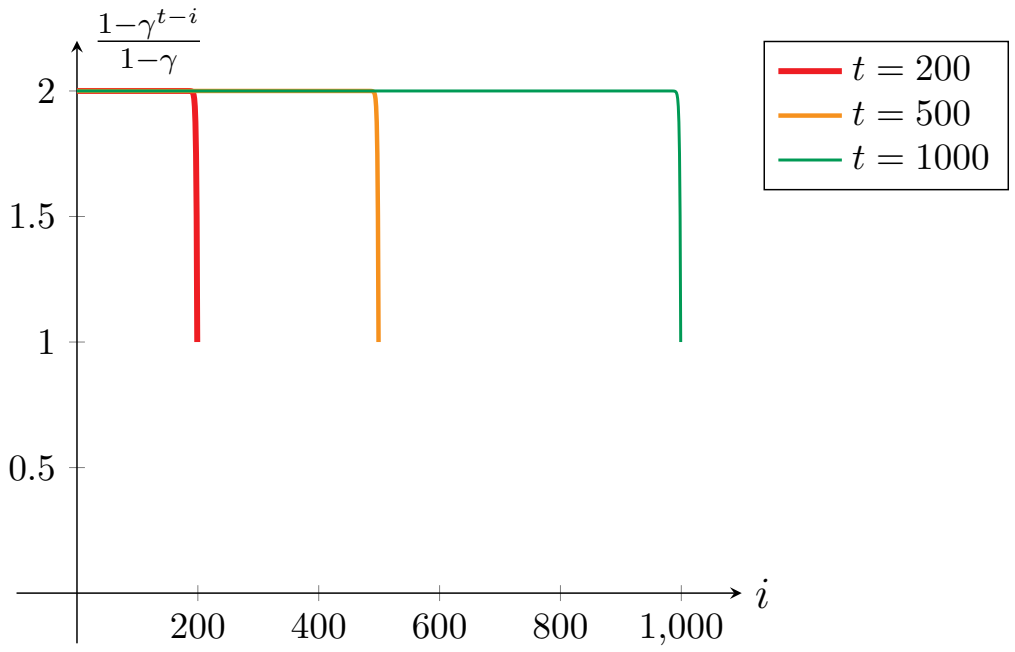
$$\gamma = .9$$



$$\mathbf{x}^{(t)} = \mathbf{x}^{(0)} - \eta \sum_{i=0}^{t-1} \left(\frac{1-\gamma^{t-i}}{1-\gamma} \right) \nabla_{\mathbf{x}} f(\mathbf{x}^{(i)})$$

Effective learning rate for SGD + momentum

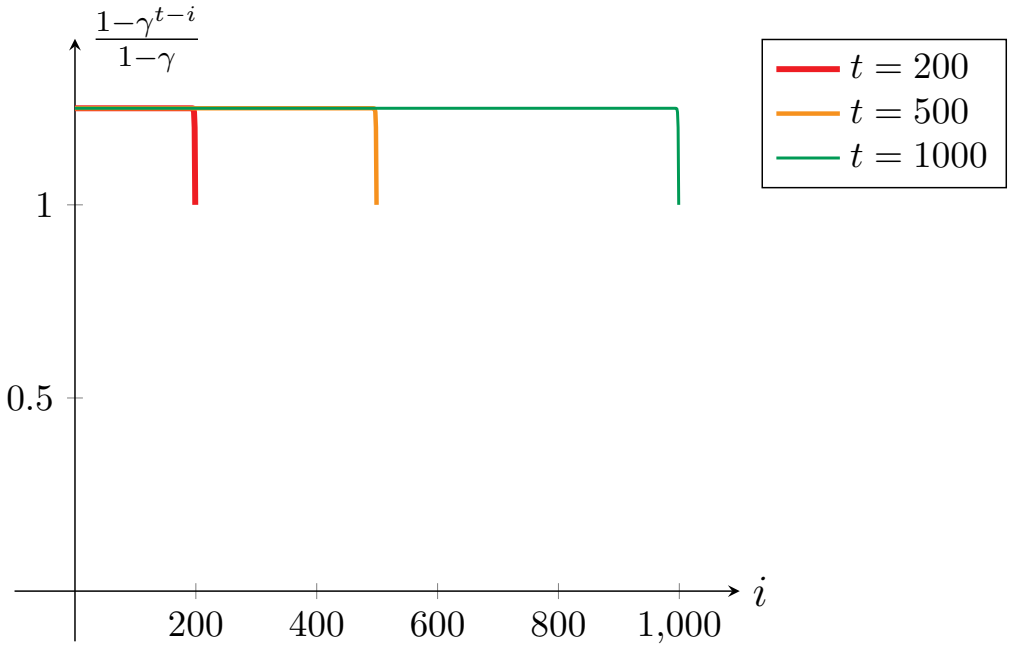
$$\gamma = .5$$



$$\mathbf{x}^{(t)} = \mathbf{x}^{(0)} - \eta \sum_{i=0}^{t-1} \left(\frac{1-\gamma^{t-i}}{1-\gamma} \right) \nabla_{\mathbf{x}} f(\mathbf{x}^{(i)})$$

Effective learning rate for SGD + momentum

$$\gamma = .2$$



$$\mathbf{x}^{(t)} = \mathbf{x}^{(0)} - \eta \sum_{i=0}^{t-1} \left(\frac{1-\gamma^{t-i}}{1-\gamma} \right) \nabla_{\mathbf{x}} f(\mathbf{x}^{(i)})$$

Have only scratched the surface here...

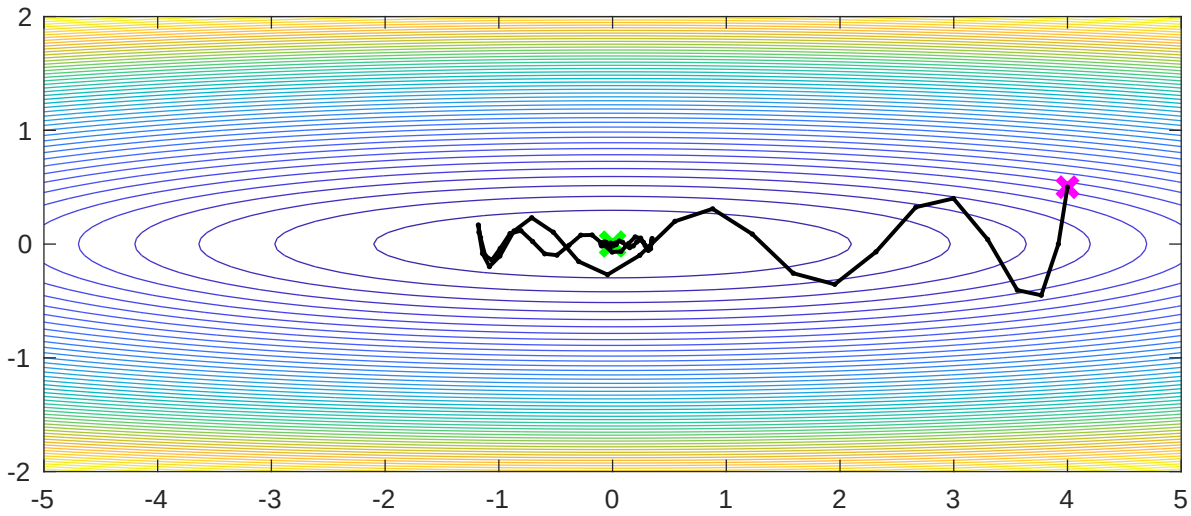
For a more sophisticated analysis and clear exposition of momentum please check out: Why Momentum Really Works

Momentum not the complete answer

- When using momentum

  $\Longrightarrow$ can pick up too much speed in one direction.

  $\Longrightarrow$ can overshoot the local optimum.



($\gamma = .9$, $\eta = .01$, 95 update steps)

Solution: Nesterov accelerated gradient (NAG)

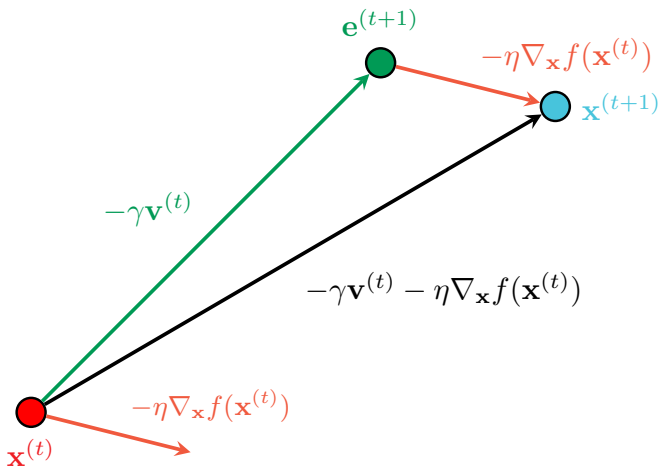
- Look and measure ahead.
- Use gradient at an estimate of the parameters at the next iteration.
- Let $\gamma \in [0, 1]$ then

$$\mathbf{e}^{(t+1)} = \mathbf{x}^{(t)} - \gamma \mathbf{v}^{(t)} \quad \leftarrow \text{estimate of } \mathbf{x}^{(t+1)}$$

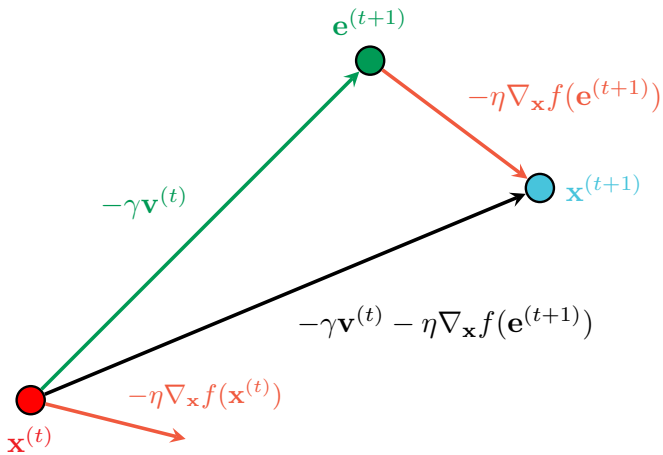
$$\mathbf{v}^{(t+1)} = \gamma\, \mathbf{v}^{(t)} + \eta\, \nabla_{\mathbf{x}} f(\mathbf{e}^{(t+1)}) \quad \leftarrow \text{update vector}$$

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \mathbf{v}^{(t+1)}$$

Typically γ set to .9.



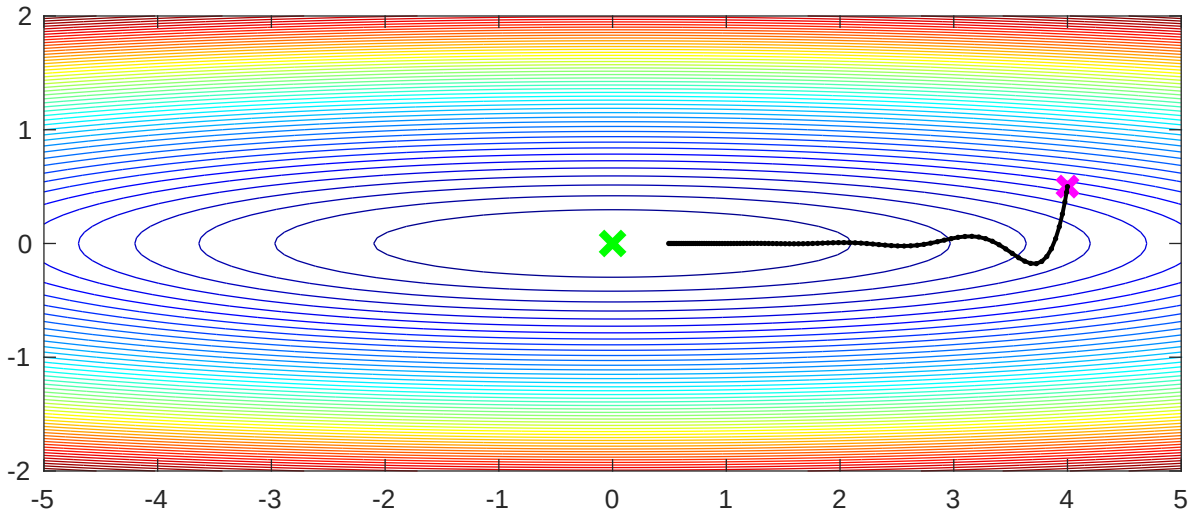
Momentum update



NAG update

How and why NAG helps

- The anticipatory update prevents the algorithm having too large updates and overshooting.
- Algorithm has increased responsiveness to the landscape of f.



($\gamma = .9$, $\eta = .001$, 95 update steps)

Note:
NAG shown to greatly increase the ability to train RNNs:

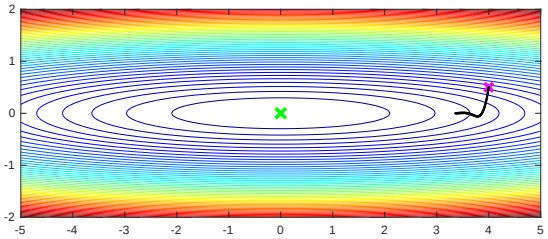
Bengio, Y., Boulanger-Lewandowski, N. & Pascanu, R. *Advances in Optimizing Recurrent Networks, (2012).*

Example behaviour of "NAG" for a ravine

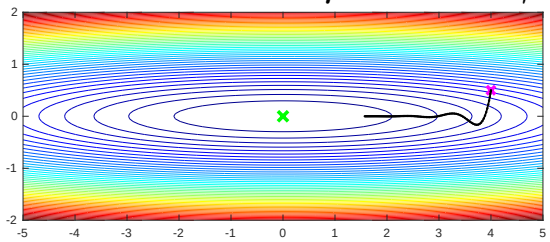
Use gradient descent to minimize $f(\mathbf{x}) = x_1^2 + 50x_2^2$ with

- $\mathbf{x}_0 = (4, .5)^T$,
- η_t constant at each iteration and
- a fixed number of update steps.

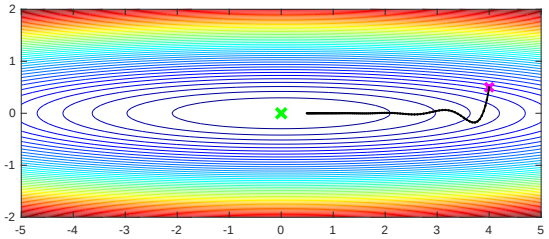
NAG path for different η_t's and $\gamma = .9$



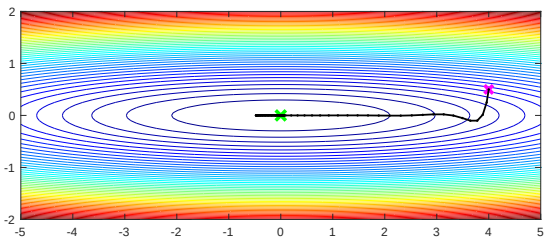
$\eta_t = .0001$



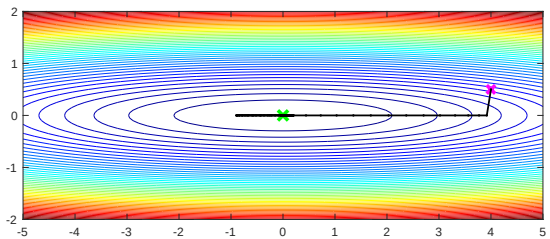
$\eta_t = .0005$



$\eta_t = .001$



$\eta_t = .005$



$\eta_t = .01$

More convenient form of NAG update

- Let $\gamma \in [0, 1]$ then

$$\mathbf{e}^{(t+1)} = \mathbf{x}^{(t)} - \gamma \mathbf{v}^{(t)} \quad \leftarrow \text{estimate of } \mathbf{x}^{(t+1)}$$

$$\mathbf{v}^{(t+1)} = \gamma\, \mathbf{v}^{(t)} + \eta\, \nabla_{\mathbf{x}} f(\mathbf{e}^{(t+1)}) \quad \leftarrow \text{update vector}$$

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \mathbf{v}^{(t+1)}$$

- Form of update inconvenient as usually have $\mathbf{x}^{(t)}, \nabla_{\mathbf{x}} f(\mathbf{x}^{(t)})$.
  - Can make a variable transformation

$$\mathbf{m}^{(t)} = \mathbf{x}^{(t)} - \gamma \mathbf{v}^{(t)} \quad \left(\equiv \mathbf{e}^{(t+1)}\right)$$

  - Can write $\mathbf{x}^{(t+1)}$ as

$$\mathbf{x}^{(t+1)} = \mathbf{m}^{(t+1)} + \gamma \mathbf{v}^{(t+1)} = \mathbf{x}^{(t)} - \mathbf{v}^{(t+1)}$$

$$\Longrightarrow$$

$$\begin{aligned} \mathbf{m}^{(t+1)} &= \mathbf{x}^{(t)} - (1+\gamma)\mathbf{v}^{(t+1)} \\ &= \mathbf{m}^{(t)} + \gamma \mathbf{v}^{(t)} - (1+\gamma)\mathbf{v}^{(t+1)} \end{aligned}$$

where

$$\mathbf{v}^{(t+1)} = \gamma\, \mathbf{v}^{(t)} + \eta\, \nabla_{\mathbf{x}} f(\mathbf{m}^{(t)})$$

Improvements to NAG

- Want to adapt the updates to each individual parameter.
- Perform larger or smaller updates depending on the landscape of the cost function.
- Family of algorithms with **adaptive learning rates**
  - AdaGrad
  - AdaDelta
  - RMSProp
  - Adam

AdaGrad

- For a cleaner statement introduce some notation:

$$\mathbf{g}_t = \nabla_{\mathbf{x}} f(\mathbf{x}^{(t)}) \quad \text{and } \mathbf{g}_t = (g_{t,1}, \ldots, g_{t,d})^T.$$

- Keep a record of the sum of the squares of the gradients w.r.t. each x_i up to time t:

$$G_{t,i} = \sum_{j=1}^{t} g_{j,i}^2$$

- The AdaGrad update step for each dimension is

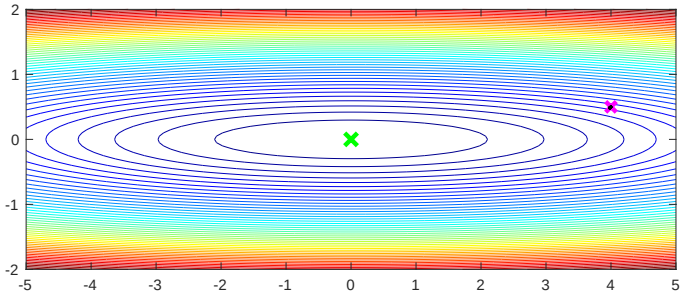
$$x_i^{(t+1)} = x_i^{(t)} - \frac{\eta}{\sqrt{G_{t,i} + \epsilon}} g_{t,i}$$

- Usually set $\epsilon = 1e-8$ and $\eta = .01$.

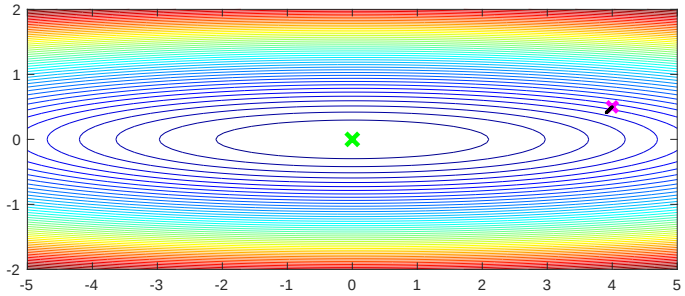
J. Duchi, E. Hazan & Y. Singer, *Adaptive Subgradient Methods for Online Learning and Stochastic Optimization*, Journal of Machine Learning Research, 2011.

Adagrad's performance on the ravine

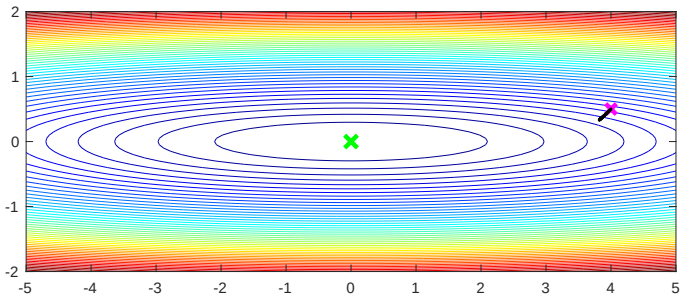
Adagrad's paths for different η_t's



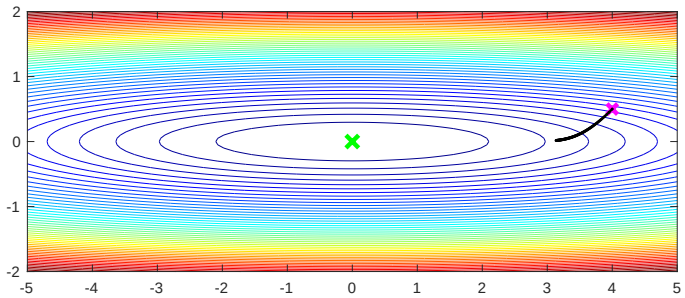
$\eta_t = .001$



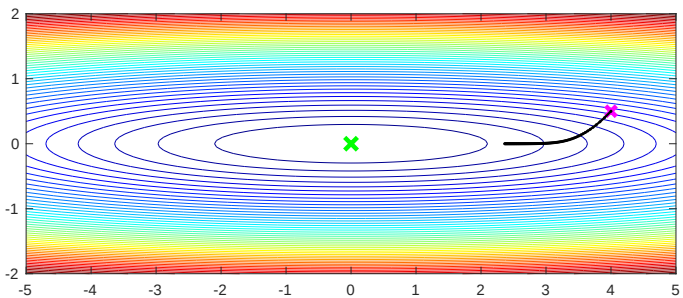
$\eta_t = .005$



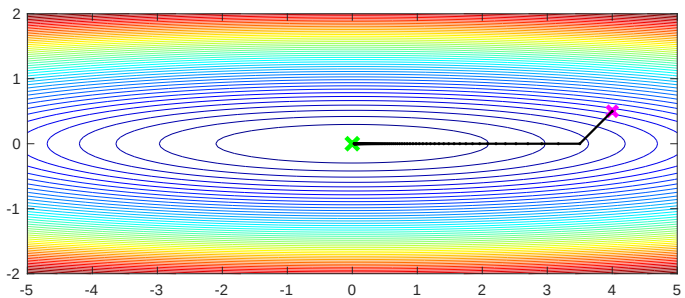
$\eta_t = .01$



$\eta_t = .05$



$\eta_t = .1$



$\eta_t = .5$

Big weakness of AdaGrad

- Each $g_{t,i}^2$ is positive.

  $\Longrightarrow$ Each $G_{t,i} = \sum_{j=1}^{t} g_{j,i}^2$ keeps growing during training.

  $\Longrightarrow$ the effective learning rate $\eta/(\sqrt{G_{t,i} + \epsilon})$ shrinks and eventually $\longrightarrow 0$.

  $\Longrightarrow$ updates of $\mathbf{x}^{(t)}$ stop.

AdaDelta

- Devised as an improvement to AdaGrad.
- Tackles AdaGrad's convergence to zero of the learning rate as t increases.
- AdaDelta's two central ideas
  - scale learning rate based on the previous gradient values (like AdaGrad) but only using a recent time window,
  - include an acceleration term (like momentum) by accumulating prior updates.

M. Zeiler, *ADADELTA: An Adaptive Learning Rate Method*, 2012. `http://arxiv.org/abs/1212.5701`

Technical details of AdaDelta

- Compute gradient vector $\mathbf{g}_t$ at current estimate $\mathbf{x}^{(t)}$.
- Update average of previous squared gradients (AdaGrad-like step)

$$\tilde{G}_{t,i} = \rho\, \tilde{G}_{t-1,i} + (1-\rho)\, g_{t,i}^2$$

- Compute the update vector

$$u_{t,i} = \frac{\sqrt{U_{t-1,i} + \epsilon}}{\sqrt{\tilde{G}_{t,i} + \epsilon}}\, g_{t,i}$$

- Compute exponentially decaying average of updates (momentum-like step)

$$U_{t,i} = \rho\, U_{t-1,i} + (1-\rho)\, u_{t,i}^2$$

- The AdaDelta update step:

$$x_i^{(t+1)} = x_i^{(t)} - u_{t,i}$$

RMSProp

Also addresses AdaGrad's radically diminishing learning rate:

- RMSProp an **adaptive learning rate** method proposed by Geoff Hinton in *Lecture 6e of his Coursera Class*.
- Stores an exponentially decaying average of the square of the gradient vector:

$$E\left[\mathbf{g}_{t+1}^2\right] = \gamma\ E\left[\mathbf{g}_t^2\right] + (1-\gamma)\,\mathbf{g}_{t+1}^2$$

- The RMSProp update rule:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \frac{\eta}{\sqrt{E\left[\mathbf{g}_{t+1}^2\right] + \epsilon}}\,\mathbf{g}_{t+1}$$

- Typically set $\gamma = .9$ and $\eta = 0.001$.

Adaptive Moment Estimation (Adam)

- Computes **adaptive learning rates** for each parameter.
- How?
  - Stores an **exponentially decaying average** of
    - ⋆ past gradients $\mathbf{m}^{(t)}$ and
    - ⋆ past squared gradients $\mathbf{v}^{(t)}$
  - $\mathbf{m}^{(t)}$ and $\mathbf{v}^{(t)}$ estimate the mean and variance of the sequence of computed gradients in each dimension.
  - Uses the variance estimate to
    - ⋆ damp the update in dimensions varying alot and
    - ⋆ increase the update in dimensions with low variation.

D. P. Kingma & J. L. Ba, *Adam: a Method for Stochastic Optimization*, International Conference on Learning Representations, 2015.

Update equations for Adam

- Let $\mathbf{g}_t = \nabla_{\mathbf{x}} f(\mathbf{x}^{(t)})$

$$\mathbf{m}^{(t+1)} = \beta_1 \mathbf{m}^{(t)} + (1 - \beta_1)\, \mathbf{g}_t$$
$$\mathbf{v}^{(t+1)} = \beta_2 \mathbf{v}^{(t)} + (1 - \beta_2)\, \mathbf{g}_t \;.*\; \mathbf{g}_t$$

- Set $\mathbf{m}^{(0)} = \mathbf{v}^{(0)} = \mathbf{0} \implies \mathbf{m}^{(t)}$ and $\mathbf{v}^{(t)}$ are biased towards zero (especially during the initial time-steps).
- Counter these biases by setting:

$$\hat{\mathbf{m}}^{(t+1)} = \frac{\mathbf{m}^{(t+1)}}{1 - \beta_1^t}, \qquad \hat{\mathbf{v}}^{(t+1)} = \frac{\mathbf{v}^{(t+1)}}{1 - \beta_2^t}$$

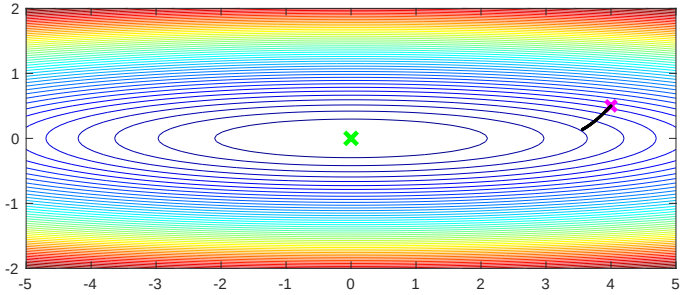
- The Adam update rule:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \frac{\eta}{\sqrt{\hat{\mathbf{v}}^{(t+1)}} + \epsilon}\, \hat{\mathbf{m}}^{(t+1)}$$

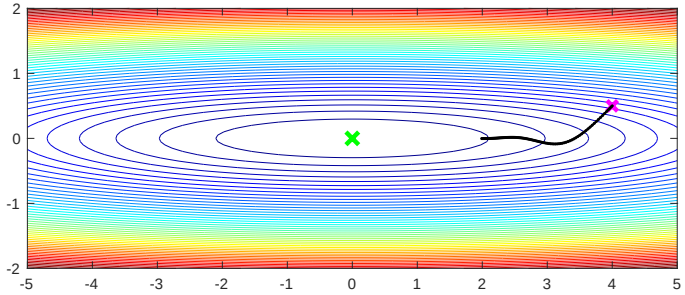
- Suggested default values $\beta_1 = .9, \beta_2 = .999, \epsilon = 10^{-8}$.

Adam's performance on the ravine

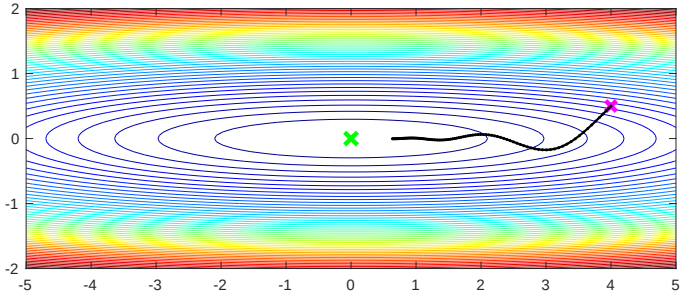
Adam paths for different η_t's



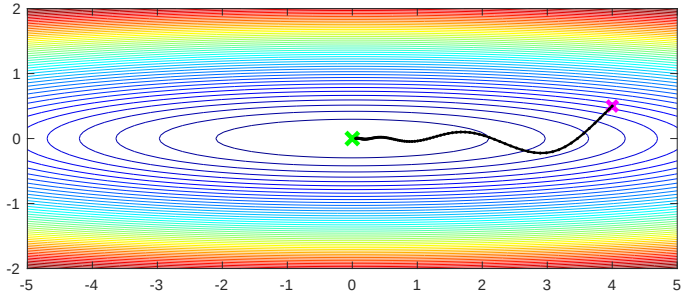
$\eta_t = .001$



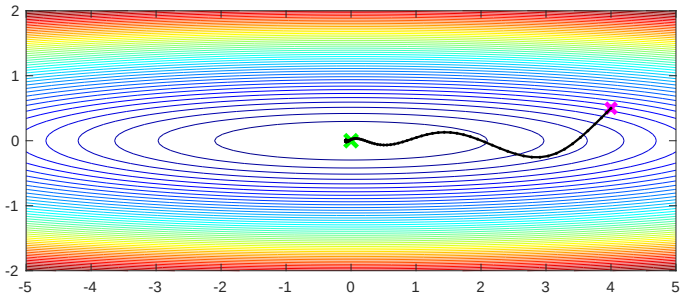
$\eta_t = .005$



$\eta_t = .01$



$\eta_t = .015$



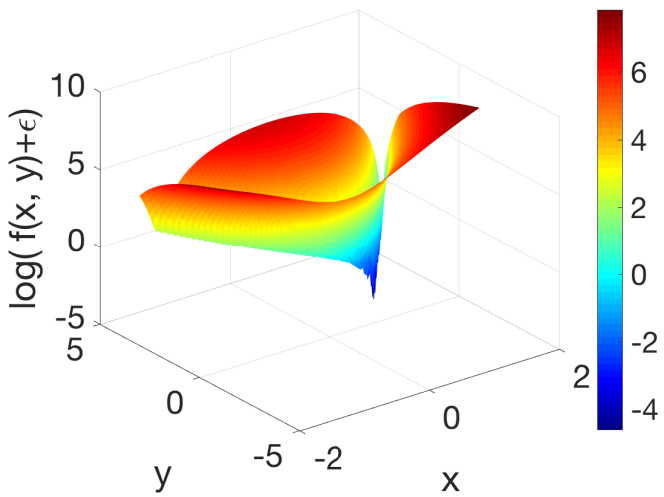
$\eta_t = .02$

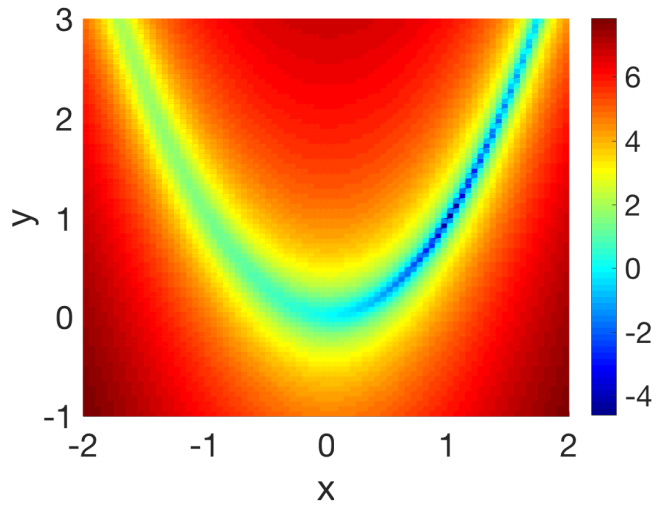
Comparison of performance on the Rosenbrock function

- **2D Rosenbrock function**

$$f(\mathbf{x}) = (x_1 - 1)^2 + 100(x_2 - x_1^2)^2$$

- Visualization of $\log(f(\mathbf{x}) + .01)$

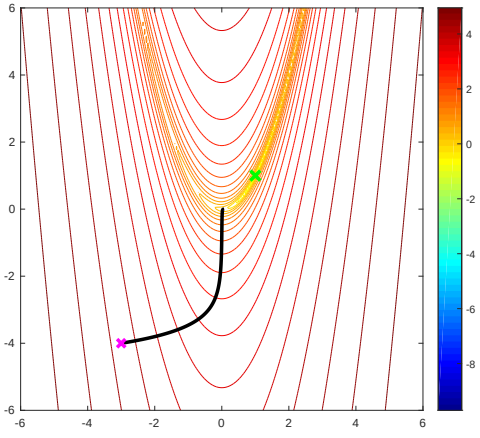




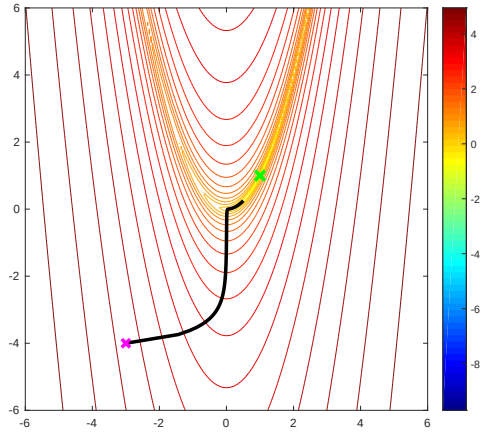
top-down viewpoint

Rosenbrock optimization with GD

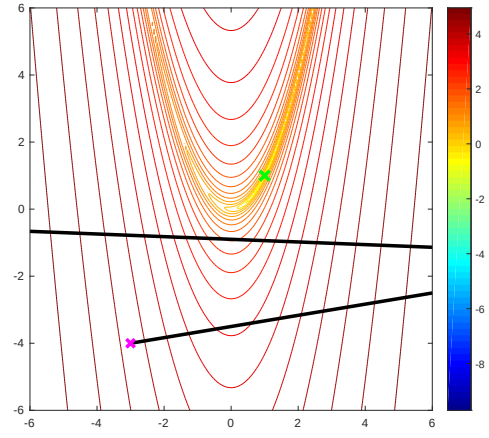
Learning rate: $\eta_0 = .00001$ and # of update steps: $n_{\text{iter}} = 5000$.



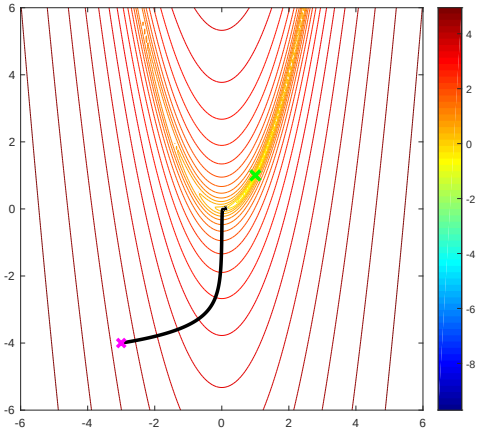
$(\eta_0, n_{\text{iter}})$



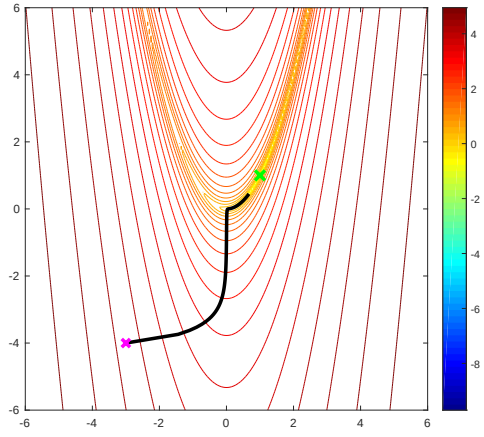
$(10\eta_0, n_{\text{iter}})$



$(100\eta_0, n_{\text{iter}})$



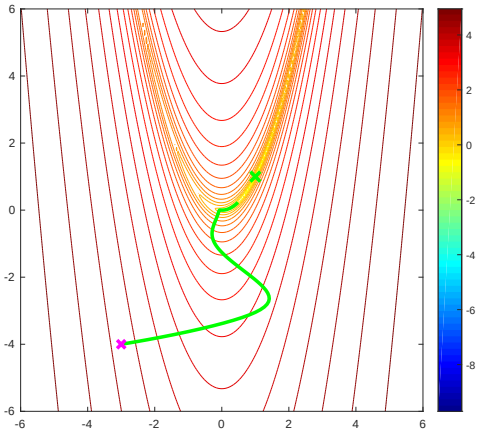
$(\eta_0, 2n_{\text{iter}})$



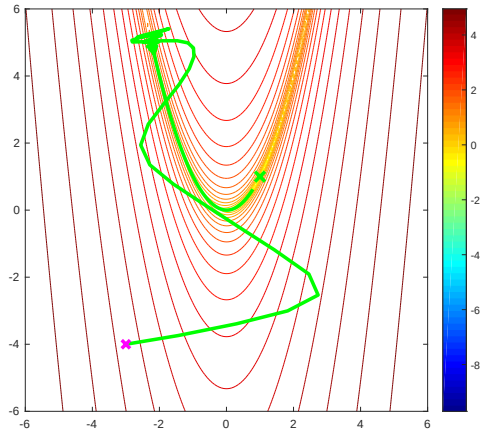
$(10\eta_0, 2n_{\text{iter}})$

Rosenbrock optimization with GD+Momentum

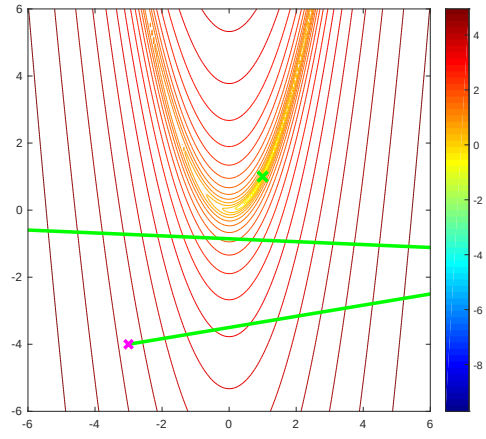
Learning rate: $\eta_0 = .00001$ and # of update steps: $n_{\text{iter}} = 5000$, $\gamma = .9$.



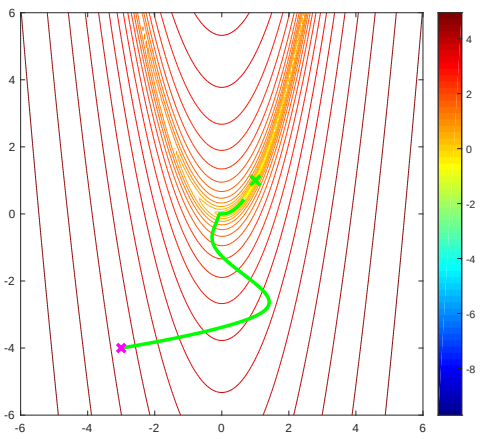
$(\eta_0, n_{\text{iter}})$



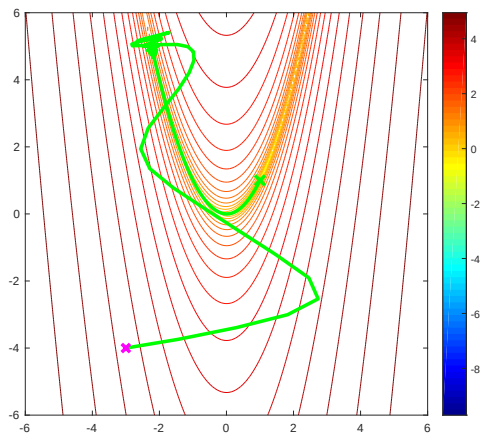
$(10\eta_0, n_{\text{iter}})$



$(100\eta_0, n_{\text{iter}})$



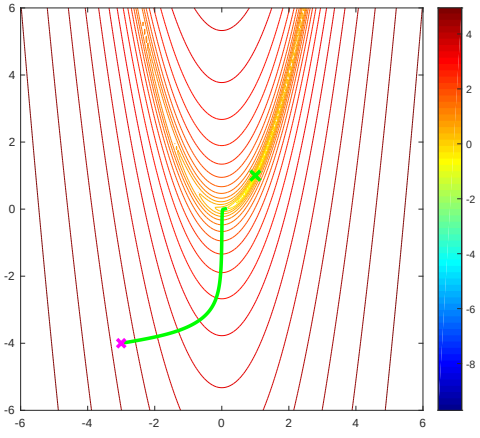
$(\eta_0, 2n_{\text{iter}})$



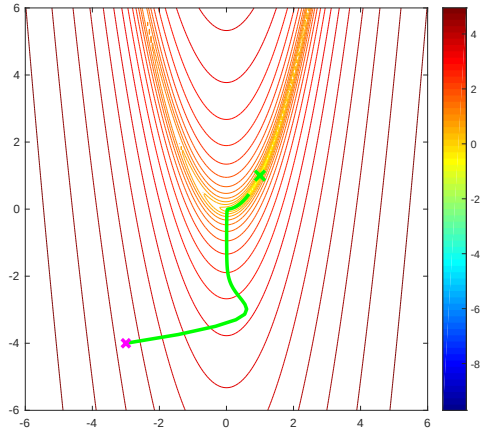
$(10\eta_0, 2n_{\text{iter}})$

Rosenbrock optimization with GD+Momentum

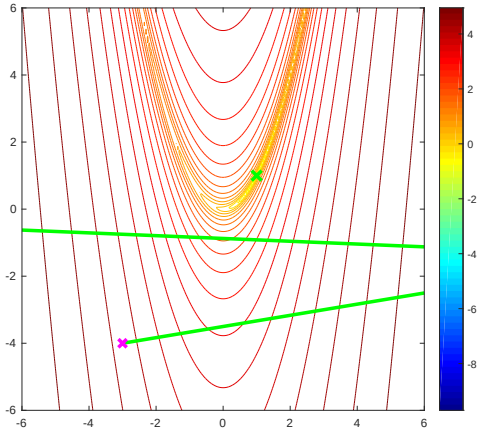
Learning rate: $\eta_0 = .00001$ and # of update steps: $n_{\text{iter}} = 5000$, $\gamma = .5$.



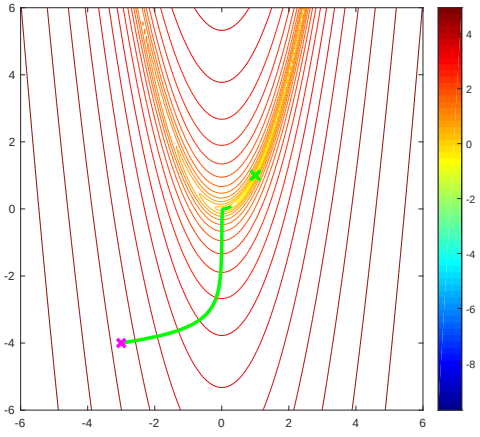
$(\eta_0, n_{\text{iter}})$



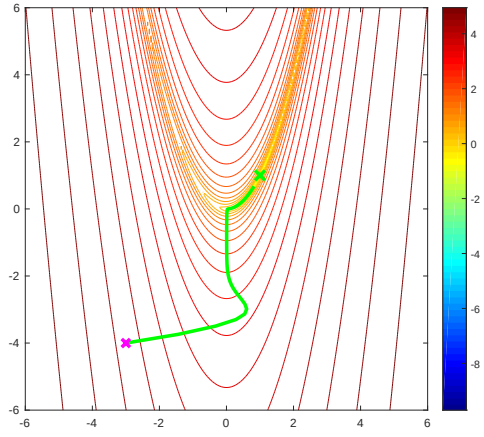
$(10\eta_0, n_{\text{iter}})$



$(100\eta_0, n_{\text{iter}})$



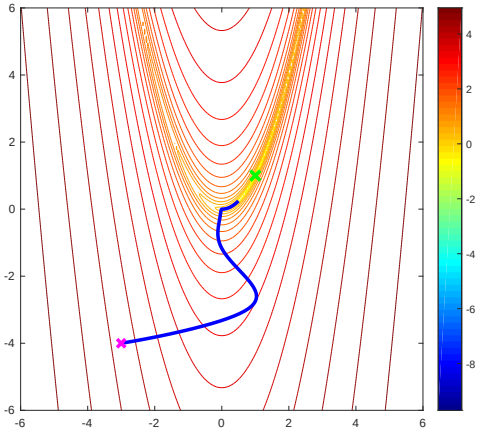
$(\eta_0, 2n_{\text{iter}})$



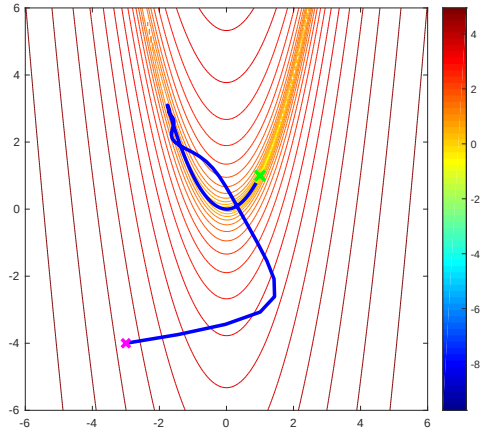
$(10\eta_0, 2n_{\text{iter}})$

Rosenbrock optimization with NAG

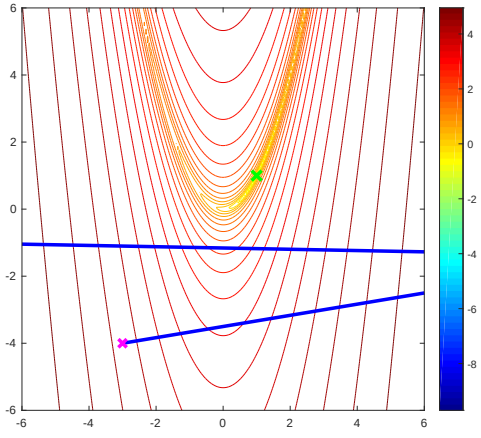
Learning rate: $\eta_0 = .00001$ and # of update steps: $n_{\text{iter}} = 5000$, $\gamma = .9$.



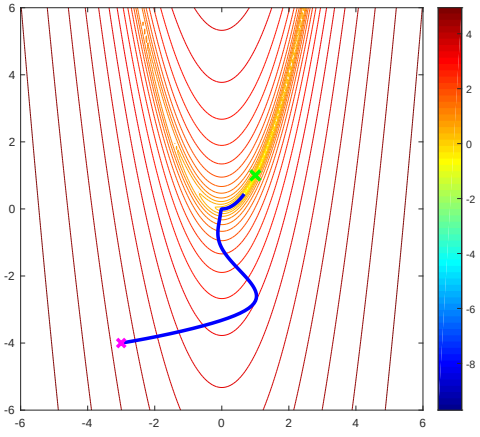
$(\eta_0, n_{\text{iter}})$



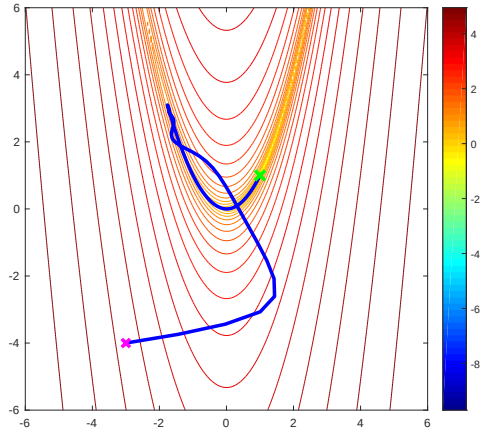
$(10\eta_0, n_{\text{iter}})$



$(100\eta_0, n_{\text{iter}})$



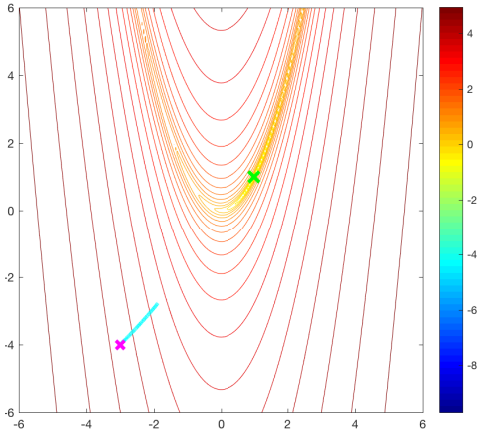
$(\eta_0, 2n_{\text{iter}})$



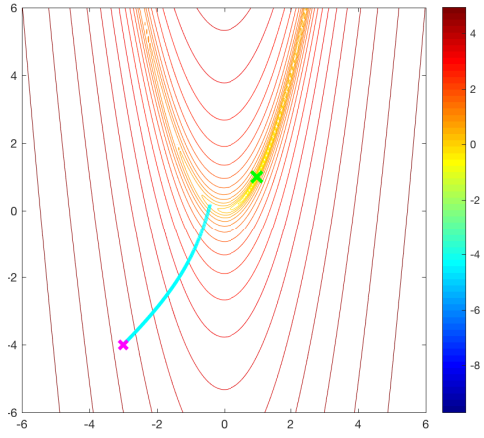
$(10\eta_0, 2n_{\text{iter}})$

Rosenbrock optimization with Adagrad

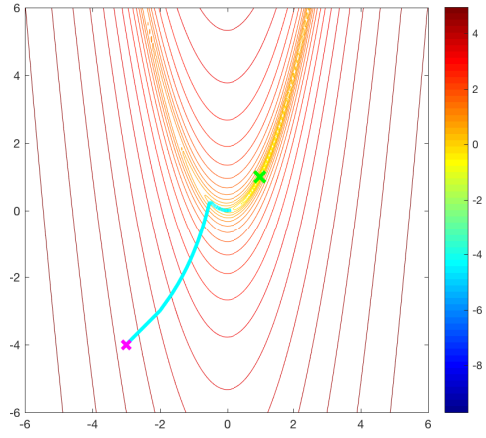
Learning rate: $\eta_0 = .01$ and # of update steps: $n_{\text{iter}} = 5000$.



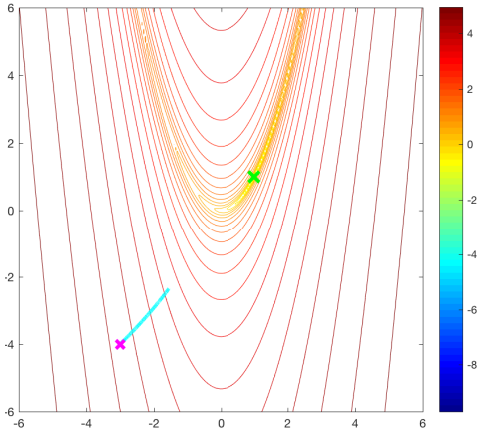
$(\eta_0, n_{\text{iter}})$



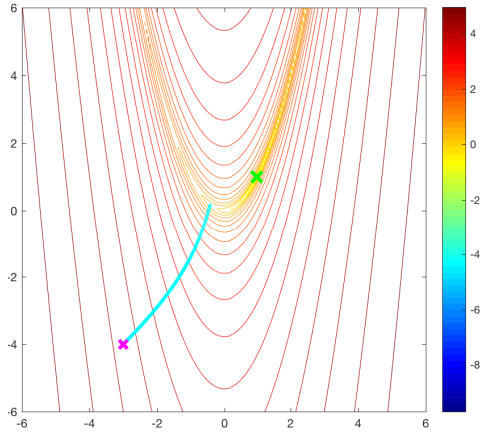
$(10\eta_0, n_{\text{iter}})$



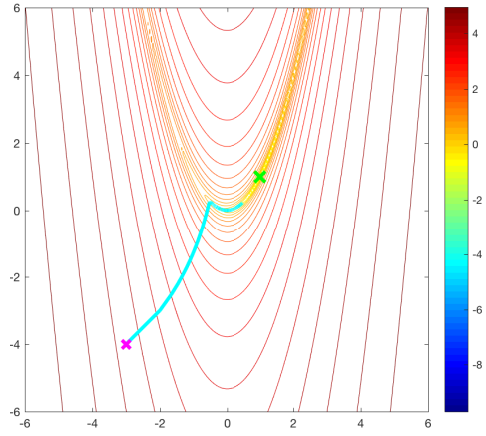
$(100\eta_0, n_{\text{iter}})$



$(\eta_0, 2n_{\text{iter}})$



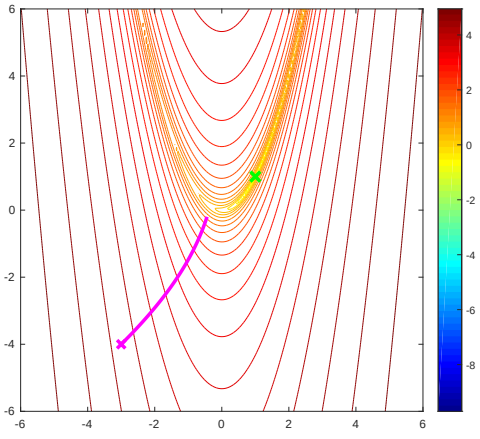
$(10\eta_0, 2n_{\text{iter}})$



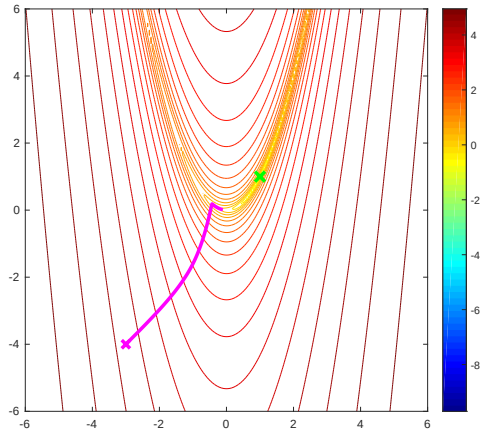
$(100\eta_0, 2n_{\text{iter}})$

Rosenbrock optimization with Adam

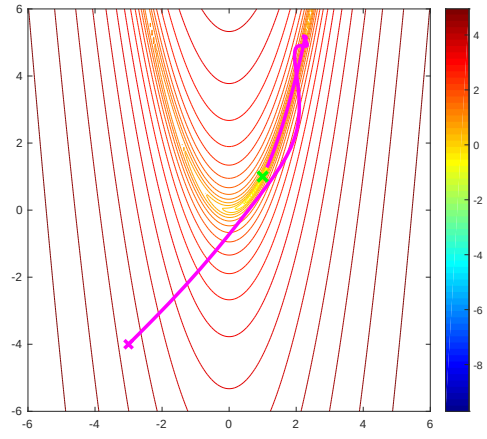
Learning rate: $\eta_0 = .001$ and # of update steps: $n_{\text{iter}} = 5000$.



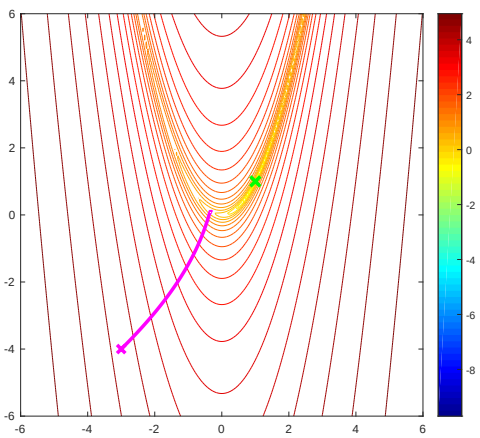
$(\eta_0, n_{\text{iter}})$



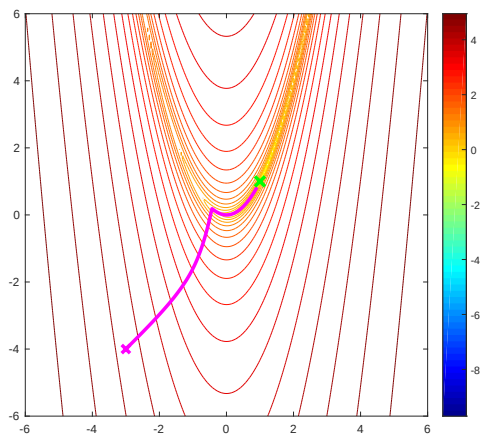
$(10\eta_0, n_{\text{iter}})$



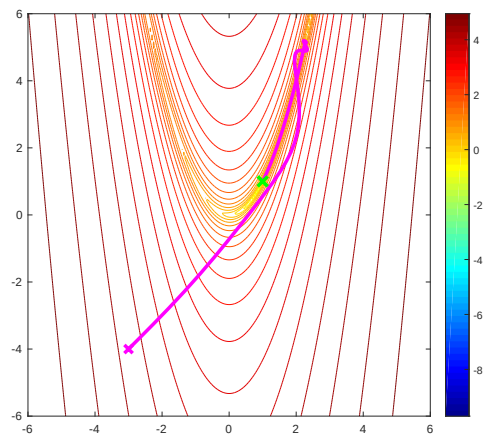
$(100\eta_0, n_{\text{iter}})$



$(\eta_0, 2n_{\text{iter}})$



$(10\eta_0, 2n_{\text{iter}})$



$(100\eta_0, 2n_{\text{iter}})$

Which optimizer to use?

- Data sparse $\implies$ likely to achieve best results using one of the adaptive learning-rate methods.
- Using the adaptive learning-rate methods $\implies$ won't need to tune the learning rate (much!).
- RMSprop, AdaDelta, and Adam are very similar algorithms that do well in similar circumstances.
- Adam slightly outperforms RMSProp near the end of optimization.
- Adam might be the best overall choice.
- But vanilla SGD (without momentum) and a simple learning rate annealing schedule may be sufficient. But time until finding a local minimum may be long....

Annealing the learning rate

Useful to anneal the learning rate

- When training deep networks, usually helpful to anneal the learning rate over time.
- **Why?**
  - Stops the parameter vector from bouncing around too widely.
  - $\Longrightarrow$ can reach into deeper, but narrower parts of the loss function.
- But knowing when to decay the learning rate is tricky!
- Decay too slowly $\Longrightarrow$ waste computations bouncing around chaotically with little improvement.
- Decay too aggressively $\Longrightarrow$ system unable to reach the best position it can.

Common approaches to learning rate decay

- **Step decay**:
  After every nth epoch set

$$\eta = \alpha\eta$$

  where $\alpha \in (0, 1)$. (Instead sometimes people monitor the validation loss and reduce the learning rate when this loss stops improving.)

- **Exponential decay**:

$$\eta = \eta_0 e^{-kt}$$

  where t is iteration number (either w.r.t. number of update steps or epochs). Then η_0 and k are hyper-parameters.

- $1/t$ **decay**:

$$\eta = \frac{\eta_0}{1 + kt}$$

Common approaches to learning rate decay

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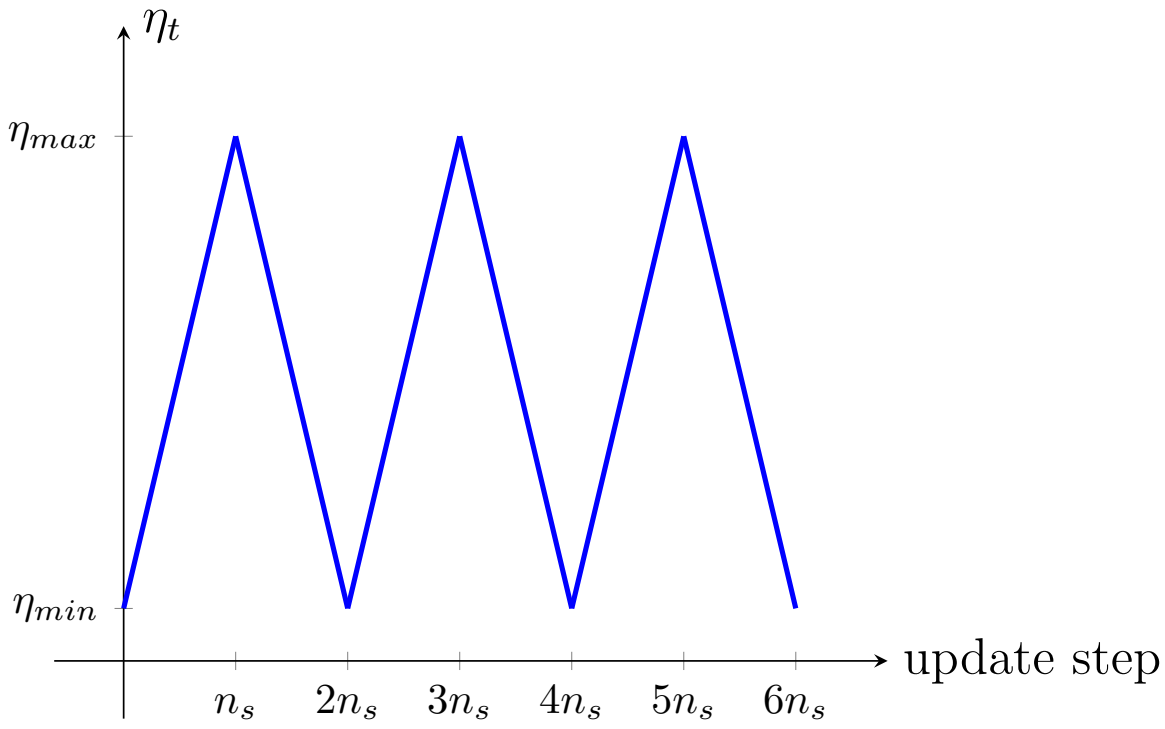
- $1/t$ **decay**:

$$\eta = \frac{\eta_0}{1 + kt}$$

Step decay most common. Better to decay conservatively and train for longer.

Recent idea: Cyclical learning rates

Cyclical learning rates



- Vary learning rate between $\eta_{\min}$ and $\eta_{\max}$ and then back to $\eta_{\min}$. Repeat!
- You will explore this approach in Assignment 2.
- Good blog post describing this Setting the learning rate of your neural network.

Optimization of the training hyper-parameters

Hyperparameters to adjust

- Initial learning rate.
- Learning rate decay schedule.
- Regularization strength
  - L_2 penalty
  - Dropout strength

Cross-validation strategy

- Do a **coarse** $\rightarrow$ **fine** cross-validation in stages.
- **Stage 0**: Identify the range of feasible learning rates & regularization penalties. (usually done interactively and train only for a few updates.)
- **Stage 1**: Broad search. Goal is to narrow the search range. Only run training for a few epochs.
- **Stage 2**: Finer search. Increase training times.
- **Stage ...**: Repeat Stage 2 as necessary.

Use performance on the **validation set** to identify good hyper-parameter settings.

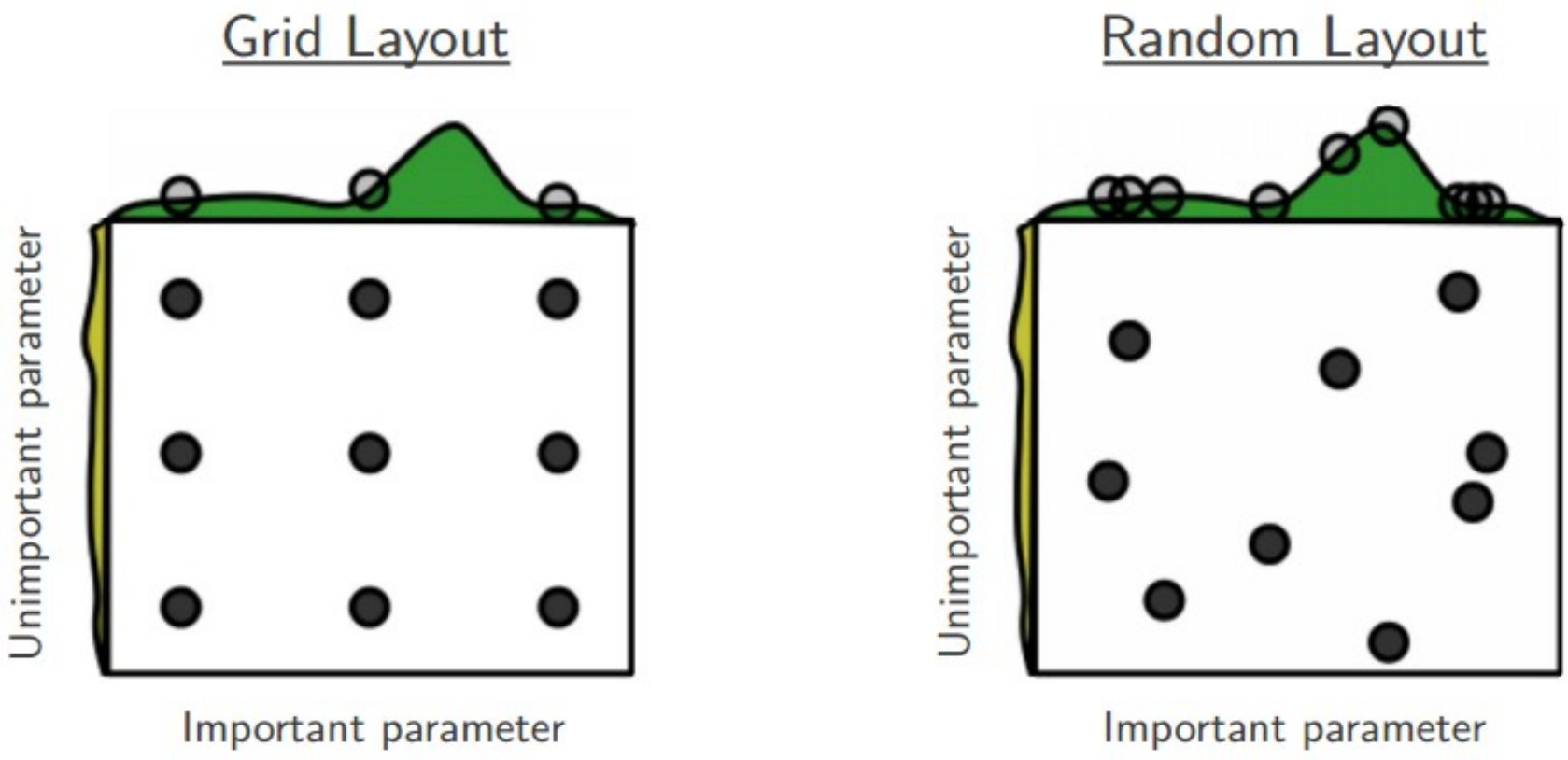
Hyper-parameter ranges

- Search for the **learning-rate** and **regularization** hyperparameters on a log scale.

  Example:
  Generate a potential learning rate with

$$\alpha = \text{uniform}(-6, 1)$$
$$\eta = 10^{\alpha}$$

Prefer random search to grid search



"*randomly chosen trials are more efficient for hyper-parameter optimization than trials on a grid*"

Random Search for Hyper-Parameter Optimization, Bergstra and Bengio, 2012

Evaluation: Model Ensembles

Model Ensembles

- Train multiple independent models (same hyper-parameter settings, different initializations). ($\sim$ 5 models)
- At test time apply each model and average their results.

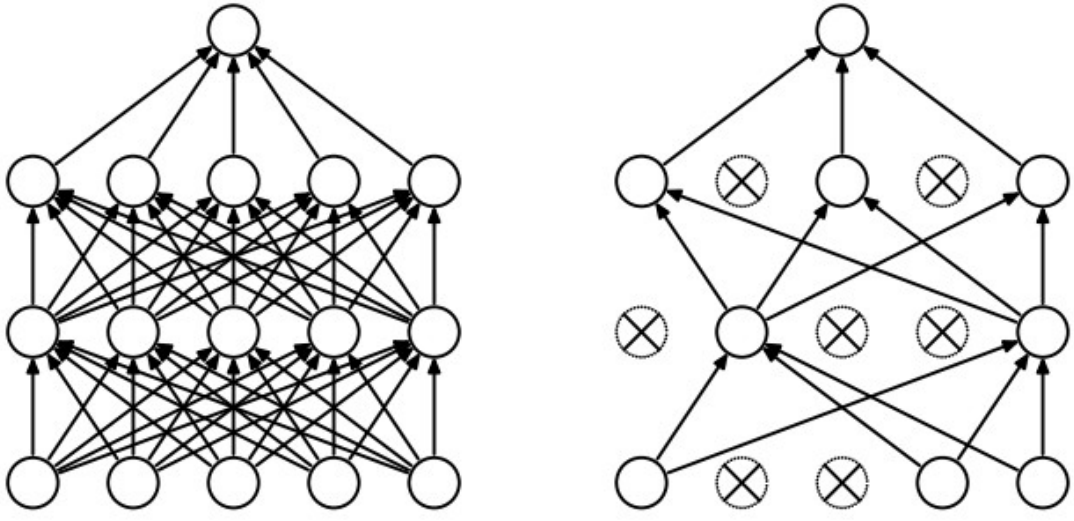
Model Ensemble on the cheap

- Can also get a small boost from averaging multiple model checkpoints of a single model.
- At test time apply each model and average their results.

Regularization Via **Dropout**

Dropout

- **Randomly set some activations to zero in forward pass**



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

[Srivastava et al.]

- Training practice introduced by Hinton.

- **Note**: Each training sample in the mini-batch has its own random dropout mask.

Training with Dropout

Set $p \in (0, 1]$ ← probability of keeping an activation active.

The Forward Pass (for a 2-layer network)

1. Compute the first set of activation values:

$$\mathbf{x}^{(1)} = \max(0, W_1 \mathbf{x}^{(0)} + \mathbf{b}_1)$$

2. Randomly choose which entries of $\mathbf{x}^{(1)}$ to switch off

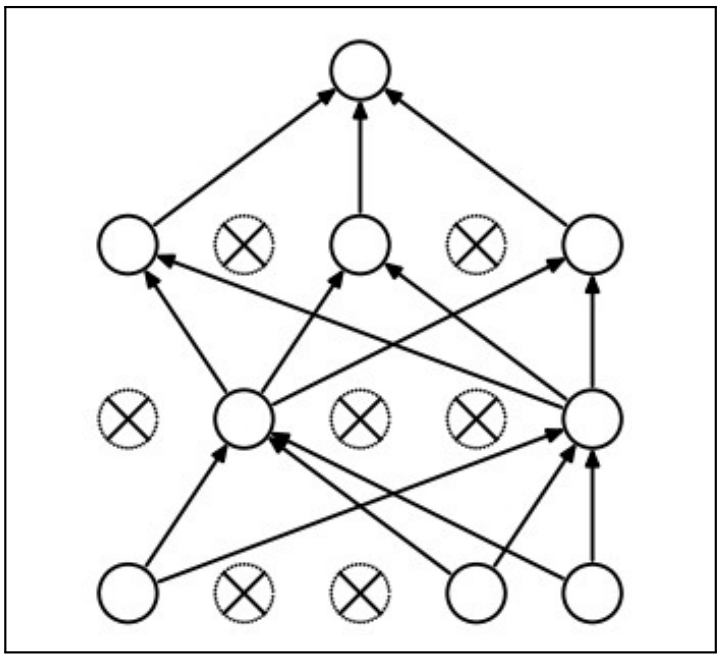
$$\mathbf{u}_1 = \text{rand}(\text{size}(\mathbf{x}^{(1)})) < p \quad \text{(Matlab notation)}$$
$$\mathbf{x}^{(1)} = \mathbf{x}^{(1)} .* \mathbf{u}_1$$

3. Repeat the process for the next layer

$$\mathbf{x}^{(2)} = \max(0, W_2 \mathbf{x}^{(1)} + \mathbf{b}_2)$$
$$\mathbf{u}_2 = \text{rand}(\text{size}(\mathbf{x}^{(2)})) < p \quad \text{(Matlab notation)}$$
$$\mathbf{x}^{(2)} = \mathbf{x}^{(2)} .* \mathbf{u}_2$$

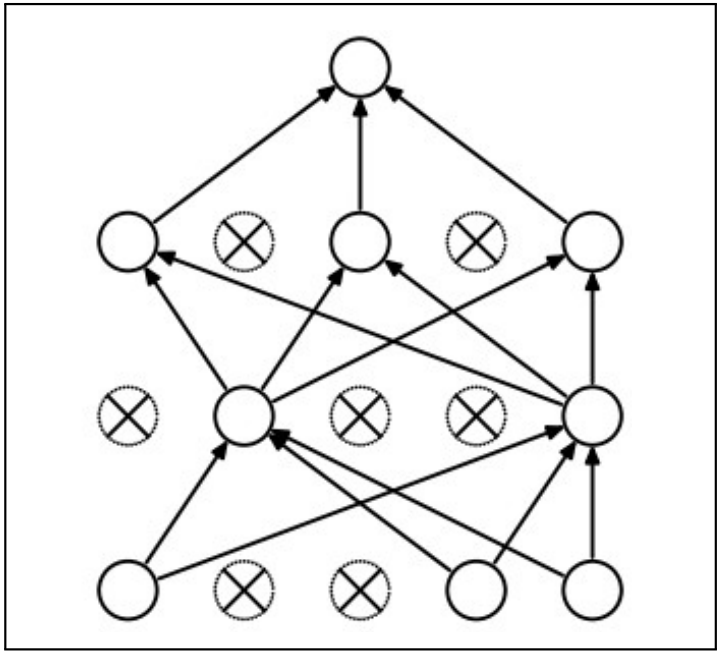
4. Output: $\mathbf{x}^{(3)} = \text{SoftMax}(W_3 \mathbf{x}^{(2)} + \mathbf{b}_3)$

Why is this a good idea?



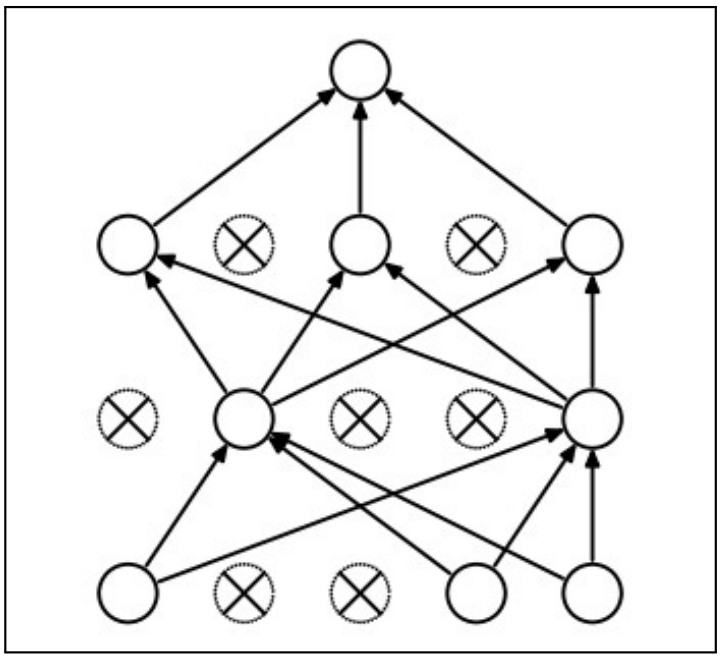
- Forces the network to have a redundant representation.
- **Another interpretation**
  - Dropout is training a large ensemble of models.
  - Each binary mask is one model, gets trained on only ∼one datapoint.

Why is this a good idea?



- Forces the network to have a redundant representation.
- **Another interpretation**
  - Dropout is training a large ensemble of models.
  - Each binary mask is one model, gets trained on only $\sim$one datapoint.

At test time

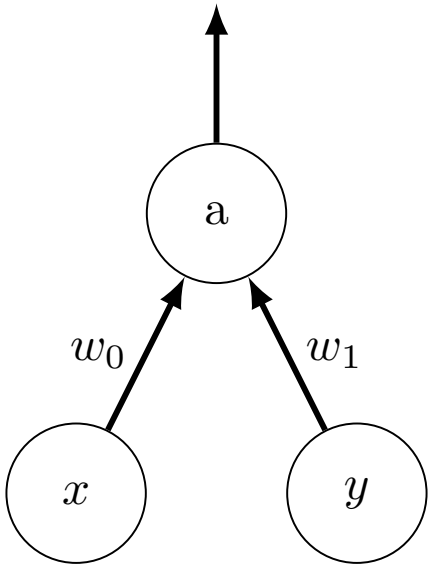


- **Ideally**: Want to integrate out all the noise.
- **Monte Carlo approximation**
  - Do many forward passes with different dropout masks.
  - Average all the predictions.

At test time

- Can do this with a single forward pass (approximately).
- Leave all the activations turned on (no dropout).
- Surely we must compensate?

At test time

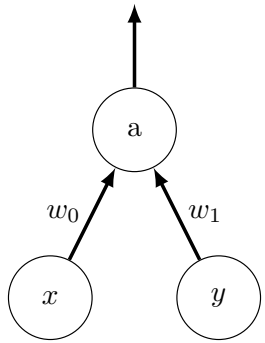


Consider this simple partial network

- During testing if we do not compensate:

$$a_{\text{test}} = w_0 x + w_1 y$$

At test time



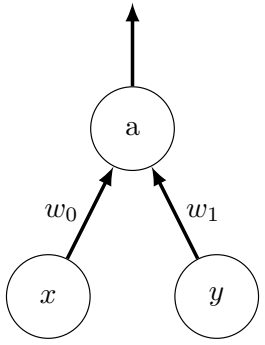
Consider this simple partial network

- During dropout training:
  1. Each input activation x and y is switched off with probability $1 - p$.
  2. The possible input activations are

inputs	probability
$(0, 0)$	$(1-p)^2$
$(x, 0)$	$p(1-p)$
$(0, y)$	$(1-p)p$
(x, y)	p^2

  3. $$\begin{aligned} \mathsf{E}[a_{\text{training}}] &= (1-p)^2(w_0 0 + w_1 0) + p(1-p)(w_0 x + w_1 0) \\ &\quad + p(1-p)(w_0 0 + w_1 y) + p^2(w_0 x + w_1 y) \\ &= p\,(w_0 x + w_1 y) \end{aligned}$$

At test time



Consider this simple partial network

- During **testing** if we do not compensate:

$$a_{\text{test}} = w_0 x + w_1 y$$

- During **dropout training**:

$$\mathsf{E}[a_{\text{training}}] = p\,(w_0 x + w_1 y) = p\,a_{\text{test}}$$

$\Longrightarrow$ have to compensate at test time by scaling the activations by p.

Must compensate at test time

- Must scale the activations so for each neuron:

  output at test time = expected output at training time

- Don't drop activations but have to compensate

$$\mathbf{x}^{(1)} = \max(0, W_1\mathbf{x}^{(0)} + \mathbf{b}_1) * p$$
$$\mathbf{x}^{(2)} = \max(0, W_2\mathbf{x}^{(1)} + \mathbf{b}_2) * p$$
$$\mathbf{x}^{(3)} = \mathrm{SoftMax}(W_3\mathbf{x}^{(2)} + \mathbf{b}_3)$$

More common: Inverted Dropout

- During **training**:

$$\mathbf{x}^{(1)} = \max(0, W_1\mathbf{x}^{(0)} + \mathbf{b}_1)$$
$$\mathbf{u}_2 = (\text{rand}(\text{size}(\mathbf{x}^{(1)})) < p)/p \quad \longleftarrow \text{Note } /p$$
$$\mathbf{x}^{(1)} = \mathbf{x}^{(1)} .* \mathbf{u}_2$$

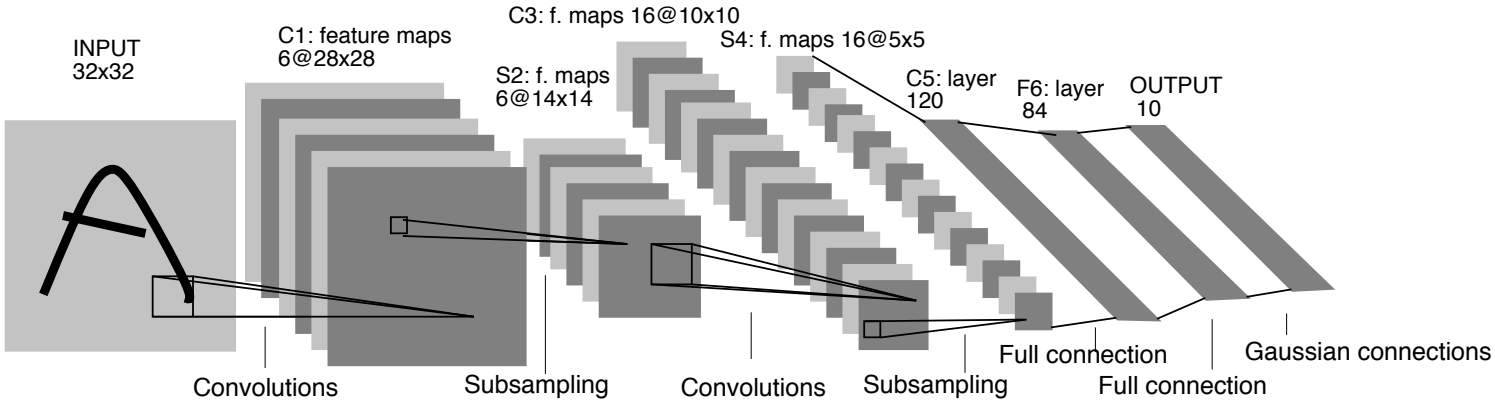
$$\mathbf{x}^{(2)} = \max(0, W_2\mathbf{x}^{(1)} + \mathbf{b}_2)$$
$$\mathbf{u}_2 = (\text{rand}(\text{size}(\mathbf{x}^{(2)})) < p)/p \quad \longleftarrow \text{Note } /p$$
$$\mathbf{x}^{(2)} = \mathbf{x}^{(2)} .* \mathbf{u}_3$$

$$\mathbf{x}^{(3)} = \text{SoftMax}(W_3\mathbf{x}^{(2)} + \mathbf{b}_3)$$

- $\Longrightarrow$ At **test time** no scaling necessary:

$$\mathbf{x}^{(1)} = \max(0, W_1\mathbf{x}^{(0)} + \mathbf{b}_1)$$
$$\mathbf{x}^{(2)} = \max(0, W_2\mathbf{x}^{(1)} + \mathbf{b}_2)$$
$$\mathbf{x}^{(3)} = \text{SoftMax}(W_3\mathbf{x}^{(2)} + \mathbf{b}_3)$$

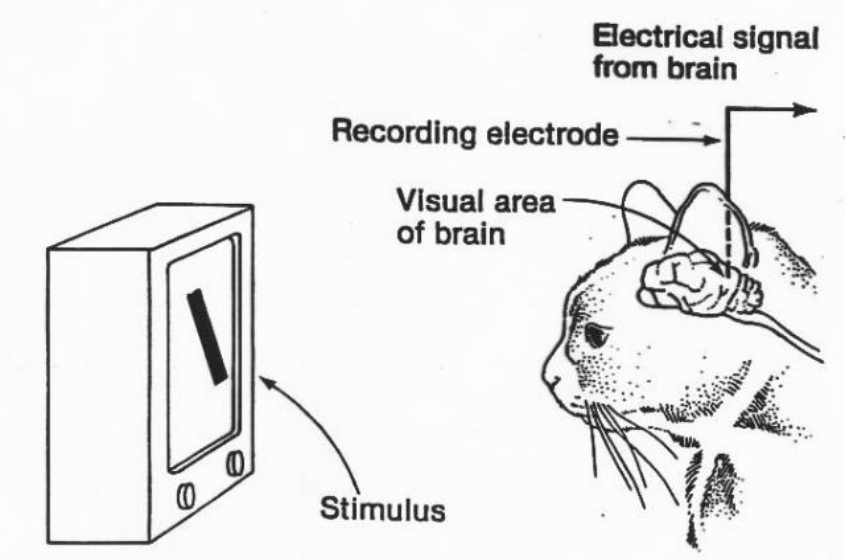
Convolutional Neural Networks (ConvNets)

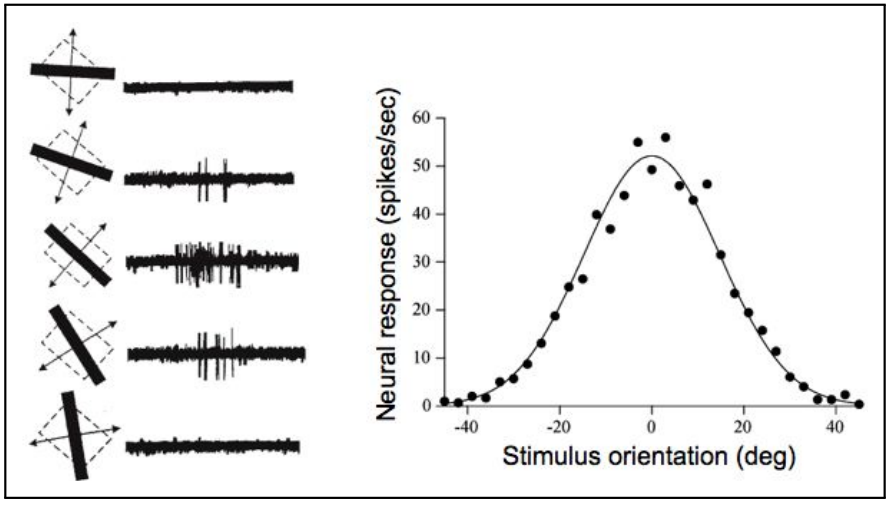


LeNet-5 (LeCun '98)

ConvNets: Some history

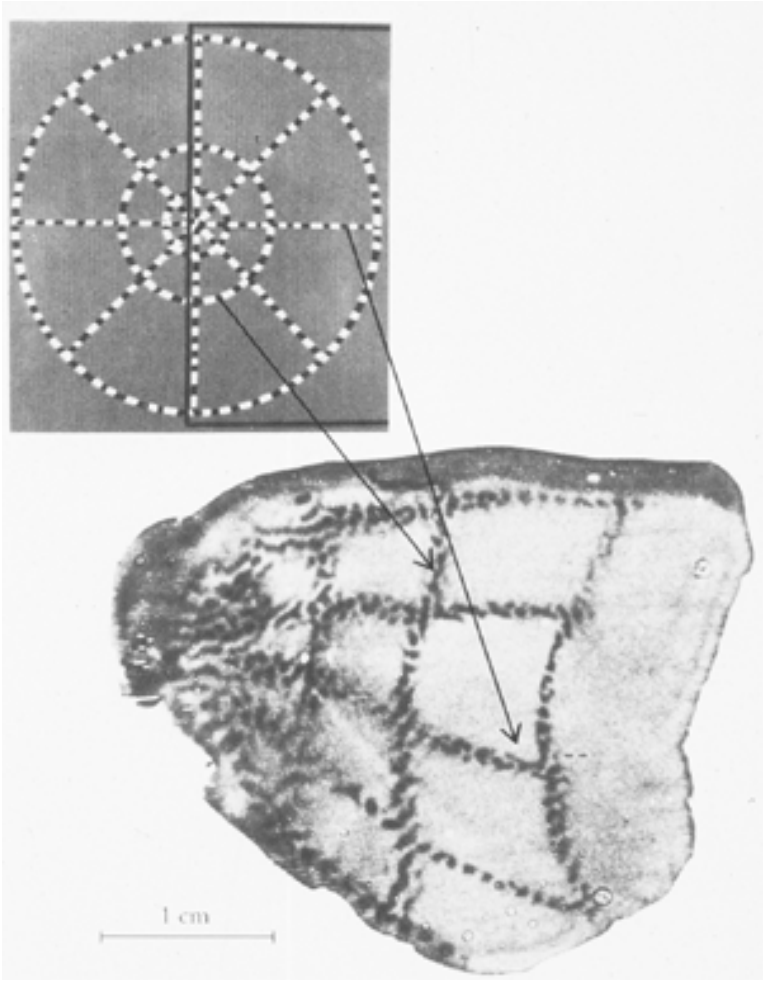
Hubel & Wiesel cat experiments 1968





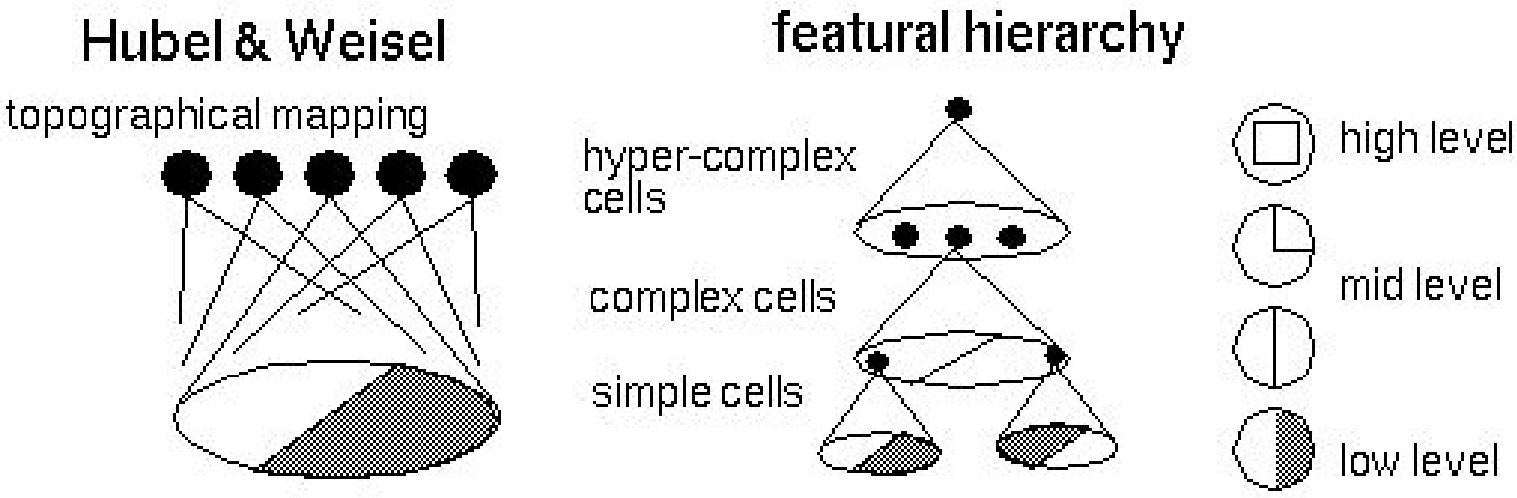
- Discovered *visual cortex* consists of a hierarchy of simple, complex, and hyper-complex cells. (Experiments in 50's & 60's)
- Hubel & Wiesel won the Nobel prize (1981).

Hubel & Wiesel



Topographical mapping in the cortex: nearby cells in cortex represented nearby regions in the visual field.

Hierarchical organization



Neurocognitron

Neocognitron: A Self-organizing Neural Network Model for a Mechanism of Pattern Recognition Unaffected by Shift in Position by Kunihiko Fukushima, 1980.

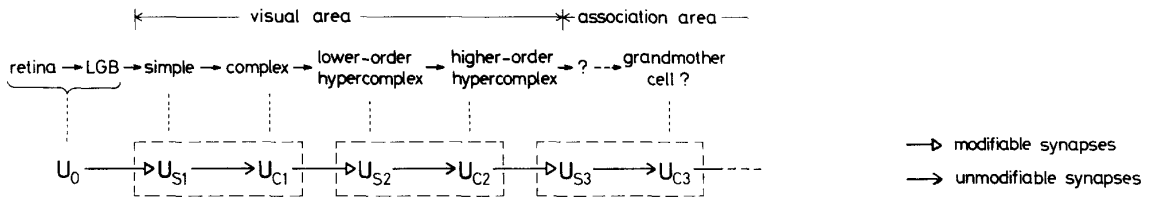
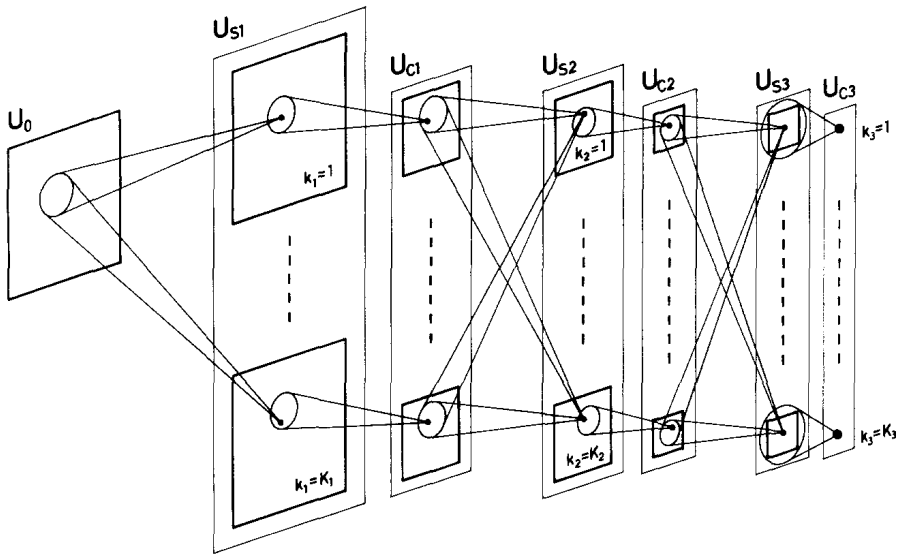
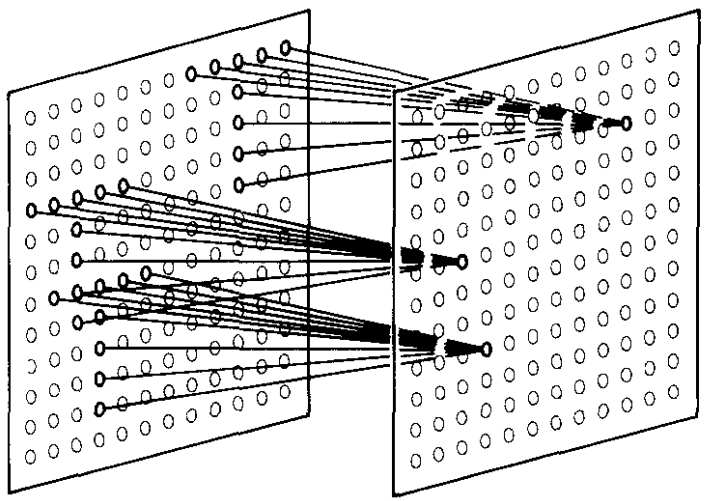


Fig. 1. Correspondence between the hierarchy model by Hubel and Wiesel, and the neural network of the neocognitron

Inspired by Hubel & Wiesel model

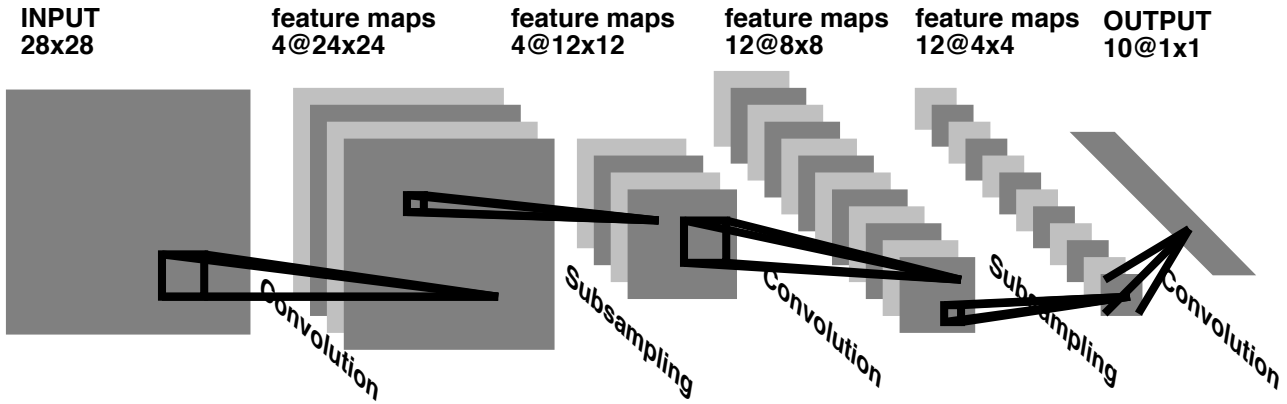




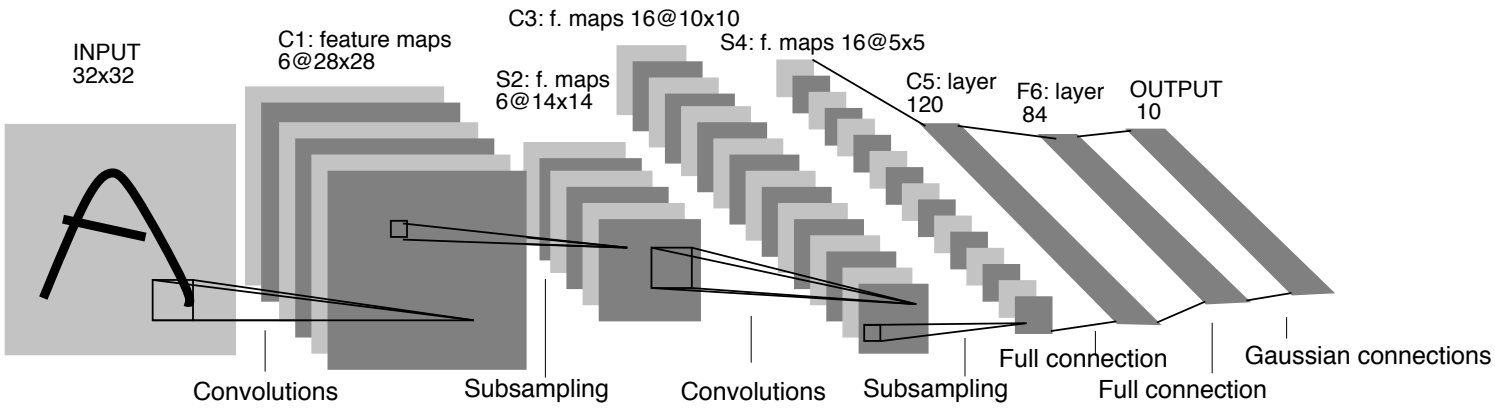
sandwich architecture (SCSCSC...)

simple cells: modifiable parameters, **complex cells**: perform pooling

LeCun's *LeNet* ConvNets

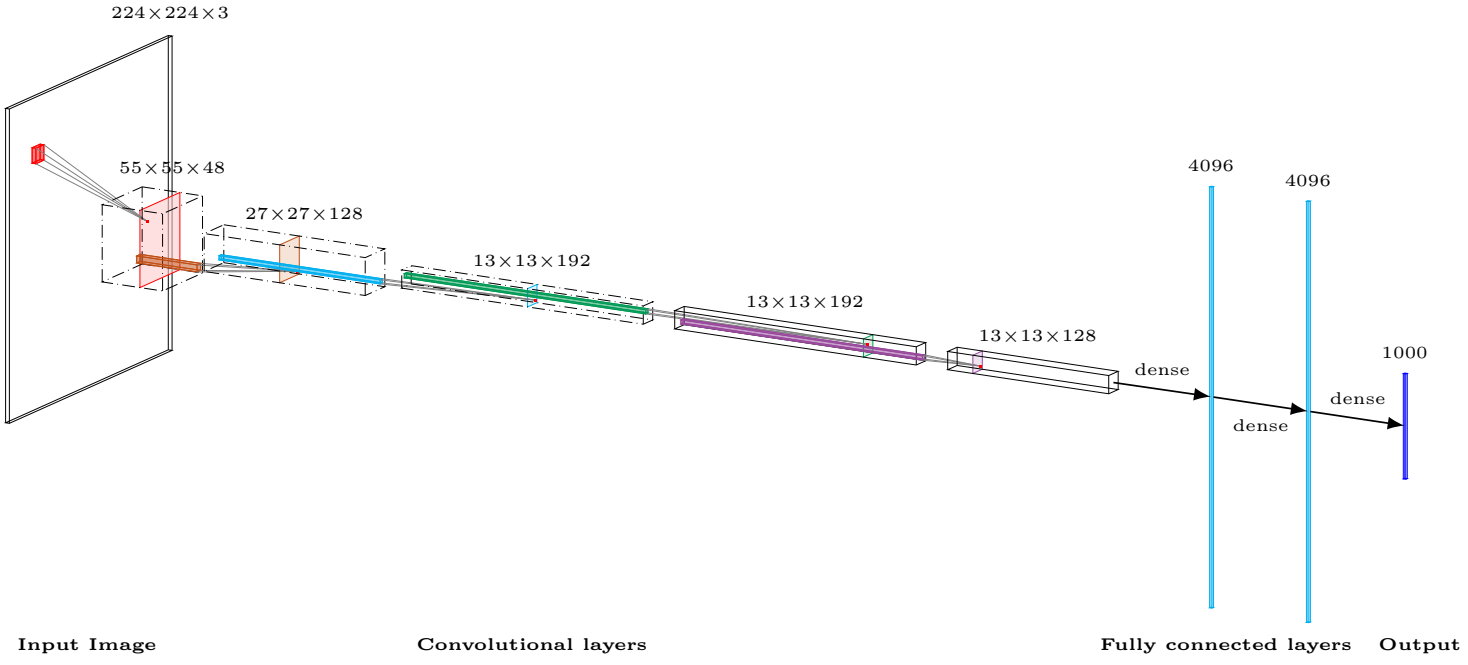


LeNet 1 '90



LeNet 5 '95

AlexNet



ImageNet Classification with Deep Convolutional Neural Networks by Krizhevsky, Sutskever, Hinton, 2012