UNIVERSITY OF COPENHAGEN

Variations on Stochastic Gradient Descent

Computational Statistics

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Errata

- There is rationale for step size differences in least squared loss and log-likelihood loss: gradients are larger in former.

Last Time

SGD
Introduced stochastic gradient descent (SGD) and mini-batch version thereof.

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Problems

We indicated that there were problems with vanilla SGD: poor convergence, erratic behavior.

Algorithm 1: Mini-Batch SGD

Data: $\gamma_0 > 0$

for $k \leftarrow 1, 2, \dots$ **do**

  $A_k \leftarrow$ random mini-batch of m samples;

  $x_k \leftarrow x_{k-1} - \frac{\gamma_k}{|A_k|} \sum_{i \in A_k} \nabla f_i(x_{k-1})$;

Today

How can we improve stochastic gradient descent?

Momentum
Base update on combination of gradient step and previous point.

Two versions: Polyak and Nesterov momentum

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Base update on combination of gradient step and previous point.

Two versions: Polyak and Nesterov momentum

Adaptive Gradients

Adapt learning rate to particular feature.

Momentum

Basic Idea
Give the particle **momentum**: like a heavy ball

Not specific to stochastic GD!

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Polyak Momentum

Classical version

$\mu \in [0, 1)$ decides strength of momentum; $\mu = 0$ gives standard gradient descent

Typically let $x_{-1} = x_0$.

Guaranteed convergence for quadratic functions

Algorithm 2: GD with Polyak Momentum

Data: $\gamma > 0$, $\mu \in [0, 1)$

for $k \leftarrow 1, 2, \ldots$ **do**

  $x_k \leftarrow x_{k-1} - \gamma \nabla f(x_{k-1}) + \mu(x_{k-2} - x_{k-2})$;

Polyak Momentum in Practice

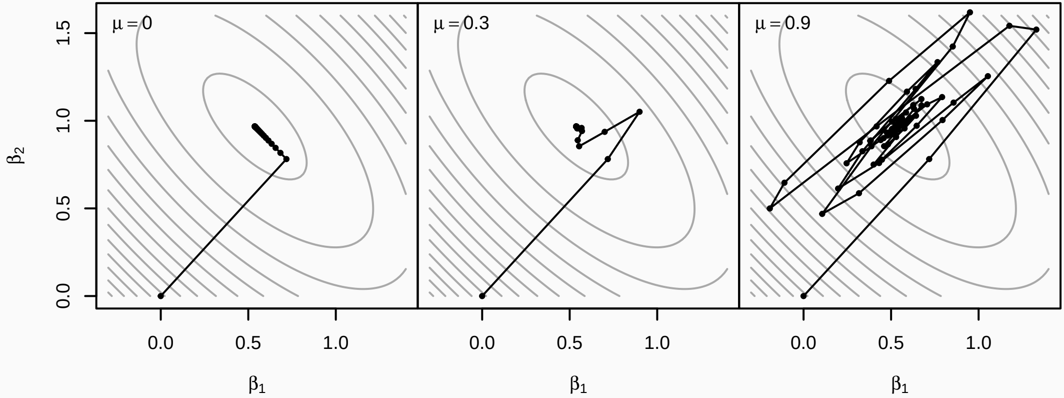

Figure 1: Trajectories of GD for different momentum values for a least-squares problem

Local Minima

For nonconvex f, gradient descent may get stuck at a local minimum.

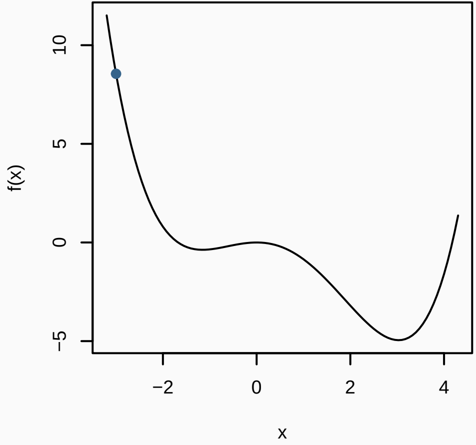

Figure 2: $\mu = 0$

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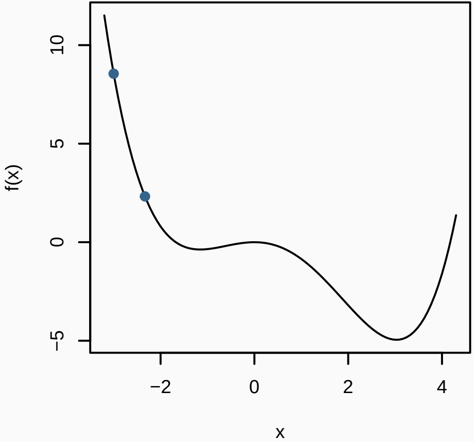

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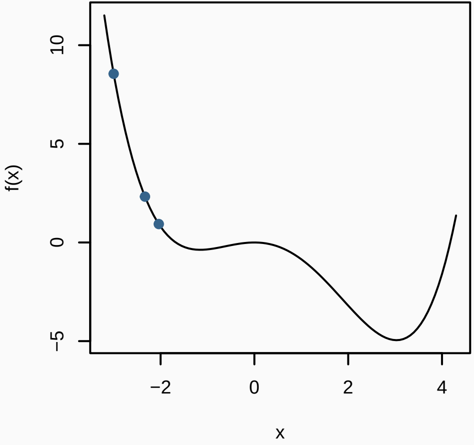

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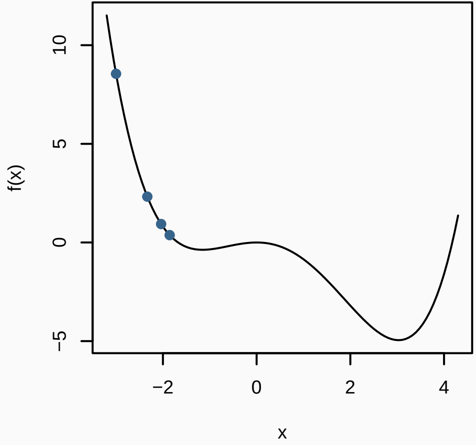

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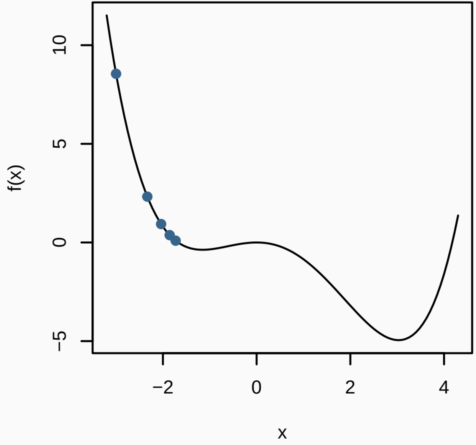

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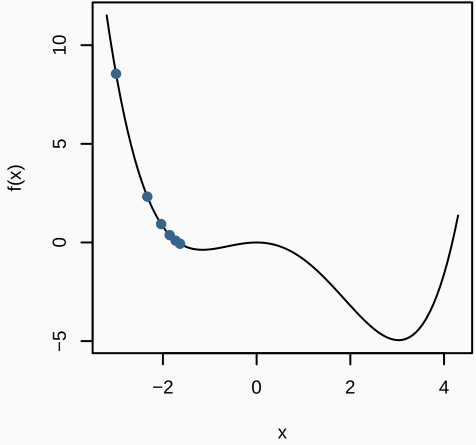

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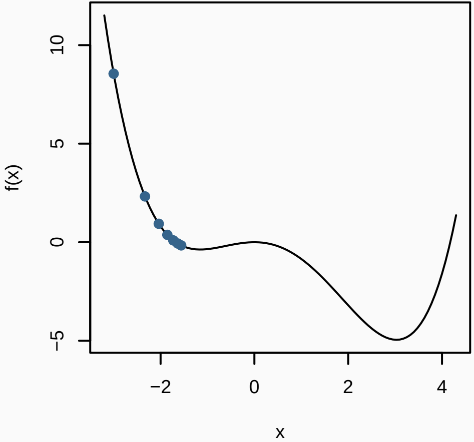

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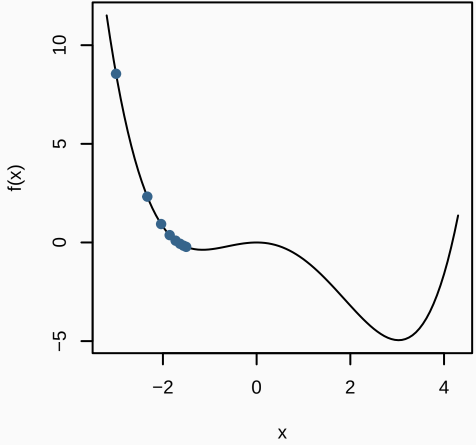

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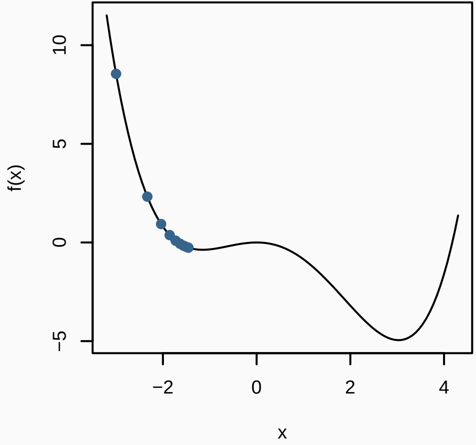

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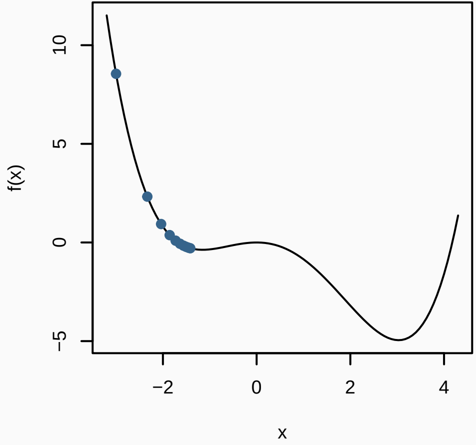

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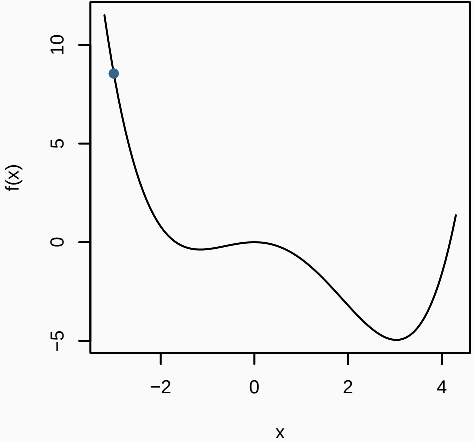
Escaping Local Minima

With momentum, we can (sometimes) remedy this problem.



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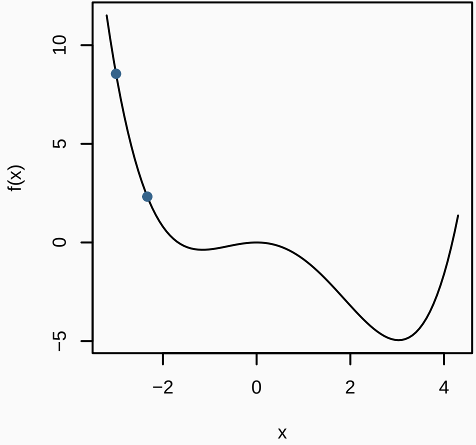

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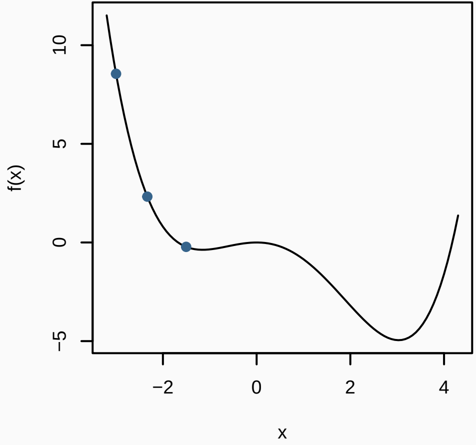

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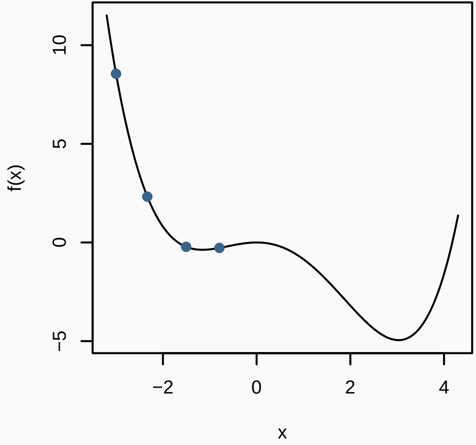

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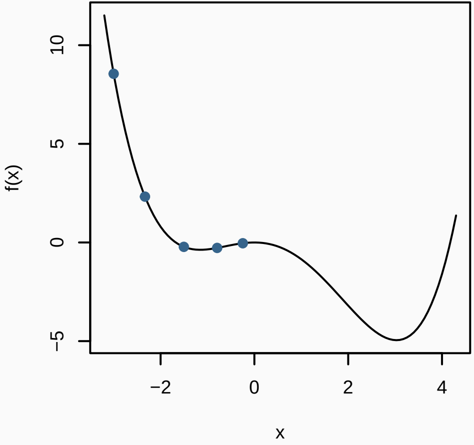

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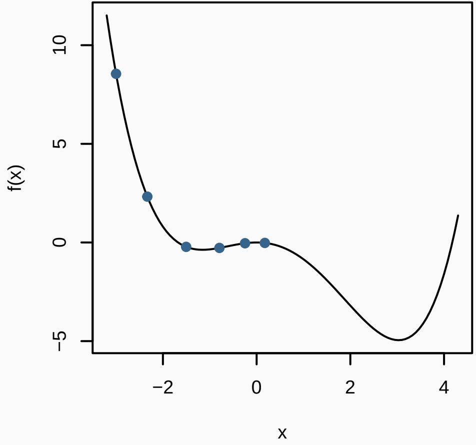

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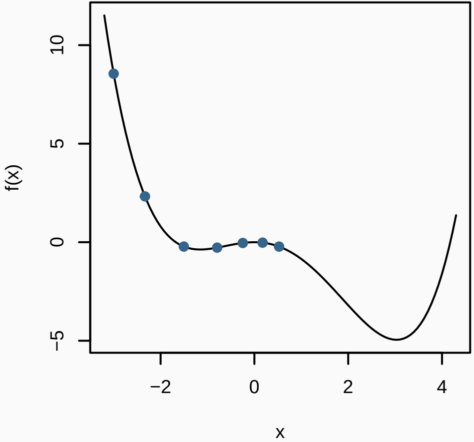

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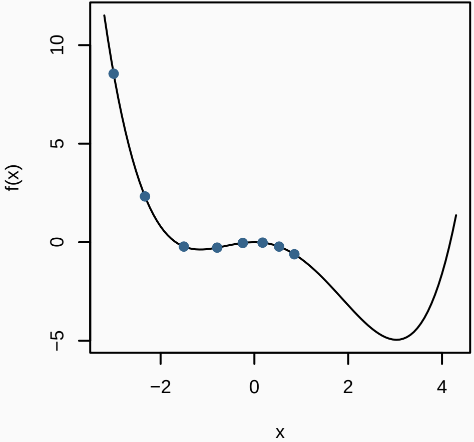

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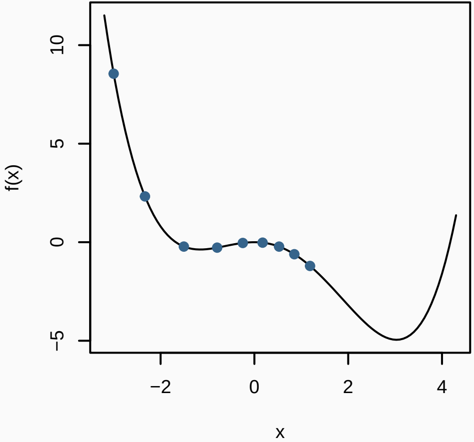

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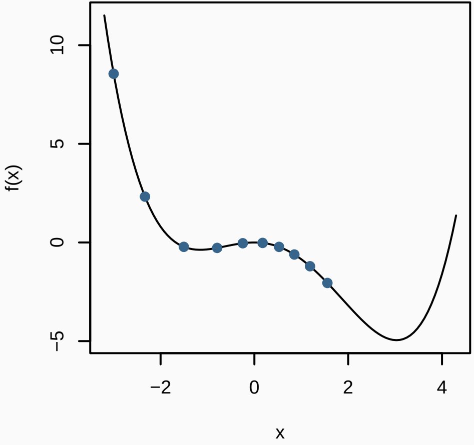

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Motivation for Momentum

- Escape local minima
- Accelerate

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Problems

No longer a descent method!

More problematic: might not converge any more

Convergence Failure

For some problems, the momentum method may instead lead to a failure to converge.

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Consider

$$f(x) = \begin{cases} \frac{25x^2}{2} & \text{if } x < 1, \\ \frac{x^2}{2} + 24x - 12 & \text{if } 1 \leq x < 2, \\ \frac{25x^2}{2} - 24x + 36 & \text{if } x \geq 2. \end{cases}$$

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For an "optimal" step size $1 = 1/L$ with $L = 25$, GD momentum steps converge to three limit points.

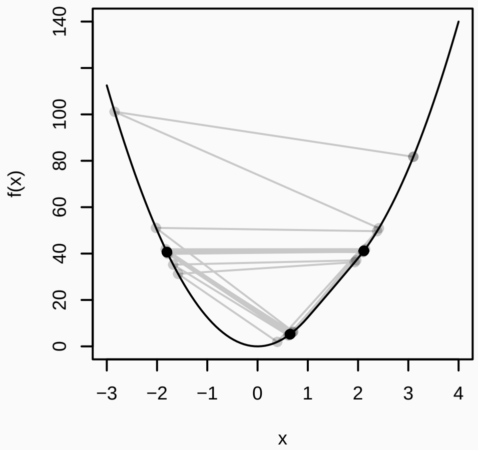

Figure 4: Initialized at $x_0 = 3.2$, the algorithm fails to converge.

Nesterov Momentum

Algorithm 3: GD with Nesterov Momentum

Data: $\gamma > 0$, $\mu \in [0, 1)$

for $i \leftarrow 1, 2, \dots$ **do**

$$v_k \leftarrow x_{k-1} - \gamma \nabla f(x_{k-1});$$

$$x_k \leftarrow v_k + \mu(v_k - v_{k-1});$$

Overcomes problem classical (Polyak) momentum has.

Nesterov: Sutskever Perspective

Consider two iterations of Nesterov algorithm:

$$
\begin{aligned}
v_t &= x_{t-1} - \gamma \nabla f\left(x_{t-1}\right) \\
x_t &= v_t + \mu\left(v_t - v_{t-1}\right) \\
v_{t+1} &= x_t - \gamma \nabla f\left(x_t\right) \\
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But since $x_k = v_k$ for $k = 1$ by construction, we can swap x_k for v_k and get the update

$$
x_k = x_{k-1} + \mu(x_{k-1} - x_{k-2}) - \gamma \nabla f(x_k + \mu(x_{k-1} - x_{k-2})).
$$

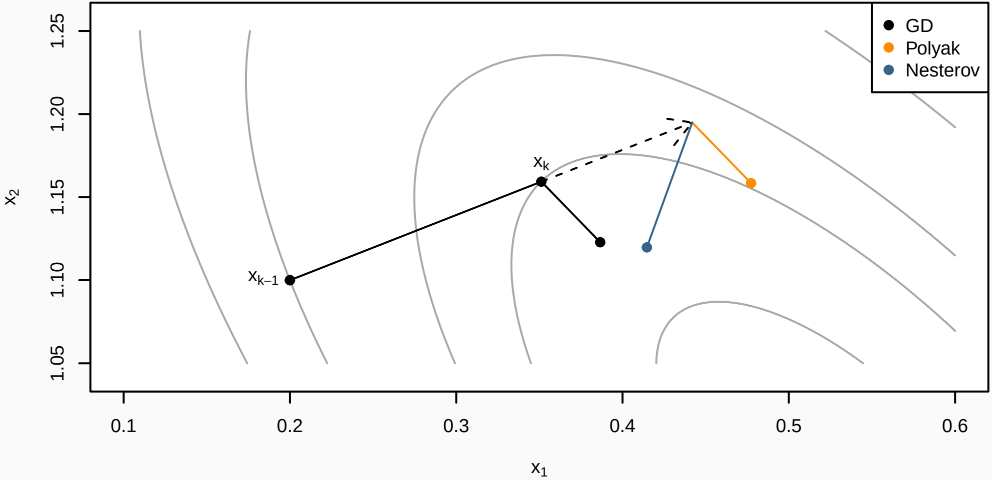

Figure 5: Illustration of Nesterov and Polyak momentum

Optimal Momentum

For gradient descent with $\gamma = 1/L$, the optimal choice of μ_k for general convex and smooth f is

$$\mu_k = \frac{a_{k-1} - 1}{a_k}$$

for a series of

$$a_k = \frac{1 + \sqrt{4a_{k-1}^2 + 1}}{2}$$

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First step ($k = 1$) is just standard gradient descent

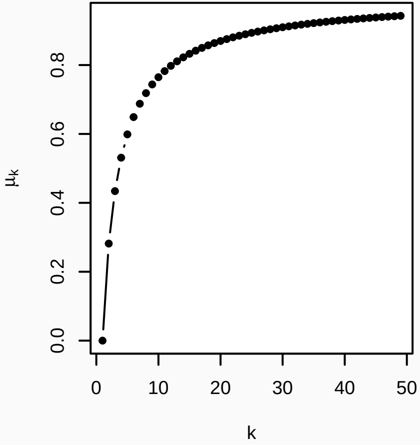

Figure 6: Optimal momentum for Nesterov acceleration (for GD).

Convergence

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Even better for quadratic and strongly convex!

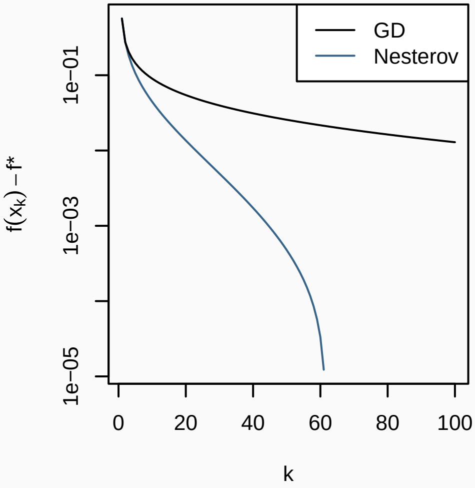

Figure 7: Practical suboptimality plot for logistic regression with $n = 1\,000$, $p = 100$.

Exercise: Rosenbrock's Banana

Steps

1. Minimize
$$f(x_1, x_2) = (a - x_1)^2 + b(x_2 - x_1^2)^2$$
with $a = 1$ and $b = 100$ using GD with Polyak momentum. Optimum is (a, a^2).
2. Implement gradient descent.
3. Add Polyak momentum.

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Plot Contours

```r
x1 <- seq(-2, 2, length.out =
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x2 <- seq(-1, 3, length.out =
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z <- outer(x1, x2, f)
contour(x1, x2, z, nlevels =
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What About SGD?

So far, we have mostly talked about standard GD, but we can use momentum (Polyak or Nesterov) for SGD as well.

For standard GD, Nesterov is the dominating method for achieving acceleration; for SGD, Polyak momentum is actually quite common.

In term of convergence, all bets are now off.

No optimal rates anymore, just heuristics.

Adaptive Gradients

General Idea

Some directions may be important, but feature information is sparse.

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AdaGrad
Store matrix of gradient history,

$$G_k = \sum_{i=1}^{k} \nabla f(x_k) \nabla f(x_k)^\intercal,$$

and update by multiplying gradient with $G_k^{-1/2}$.

Algorithm 5: AdaGrad

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for $k \leftarrow 1, 2, \ldots$ **do**
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Effects

Larger learning rates for sparse features

Step-sizes adapt to curvature.

AdaGrad In Practice

Simplified Version

Computing $\nabla f \nabla f^\intercal$ is $O(p^2)$; expensive!

Replace $G_k^{-1/2}$ with $\mathrm{diag}(G_k)^{-1/2}$

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Algorithm 6: Simplified AdaGrad

Data: $\gamma > 0$, $\epsilon > 0$

for $k \leftarrow 1, 2, \ldots$ **do**

$\quad G_k \leftarrow G_{k-1} + \mathrm{diag}\left(\nabla f(x_{k-1})^2\right)$;

$\quad x_k \leftarrow x_{k-1} - \gamma\, \mathrm{diag}\left(\epsilon I_p + G_k\right)^{-1/2} \nabla f(x_{k-1})$;

RMSProp

Acronym for **R**oot **M**ean **S**quare **Prop**agation.

Idea
Divide learning rate by running average of magnitude of recent gradients:

$$v(x,k) = \xi v(x,k-1) + (1-\xi)\nabla f(x_k)^2$$

where ξ is the forgetting factor.

Similar to AdaGrad, but uses forgetting to gradually decrease influence of old data.

Algorithm 7: RMSProp

Data: $\gamma > 0$, $\xi > 0$
for $k \leftarrow 1, 2, \dots, \xi \in [0,1)$ **do**
  $v_k = \xi v_{k-1} + (1-\xi)\nabla f(x_{k-1})$;
  $x_k \leftarrow x_{k-1} - \frac{\gamma}{\sqrt{v_k}} \odot \nabla f(x_{k-1})$;

ADAM

Acronym for **Ada**ptive **m**oment estimation

Basically RMSProp + *momentum* (for both gradients and second moments theorof)

Popular and still in much use today.

Implementation Aspects of SGD

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Any language (e.g. R) that imposes overhead for loops, will have a difficult time with SGDS

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Storage Order

In a regression setting, when indexing a single obervation at a time, slicing rows is not efficient n is large.

We can either transpose first or use a row-major storage order (not possible in R).

Example: Nonlinear Least Squares

Let's assume we're trying to solve a least-squares type of problem:

$$f(\theta) = \frac{1}{2n} \sum_{i=1}^{n} (y_i - g(\theta; x_i, y_i))^2$$

with $\theta = (\alpha, \beta)$ and

$$g(\theta; x, y) = \alpha \cos(\beta x).$$

Example: Nonlinear Least Squares

Let's assume we're trying to solve a least-squares type of problem:

$$f(\theta) = \frac{1}{2n}\sum_{i=1}^{n}(y_i - g(\theta; x_i, y_i))^2$$

with $\theta = (\alpha, \beta)$ and

$$g(\theta; x, y) = \alpha \cos(\beta x).$$

Then

$$\nabla_\theta f(x, \theta) = \begin{bmatrix} \cos(\beta x) \\ -\alpha x \sin(\beta x) \end{bmatrix}.$$

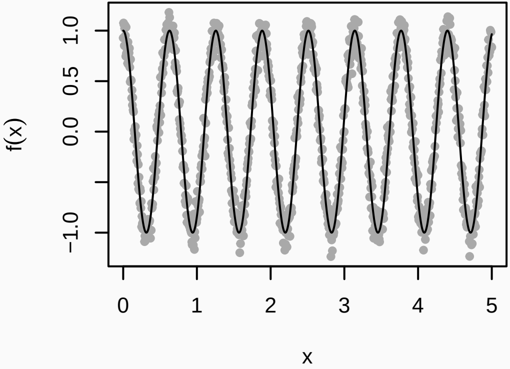

Figure 8: Simulation from problem

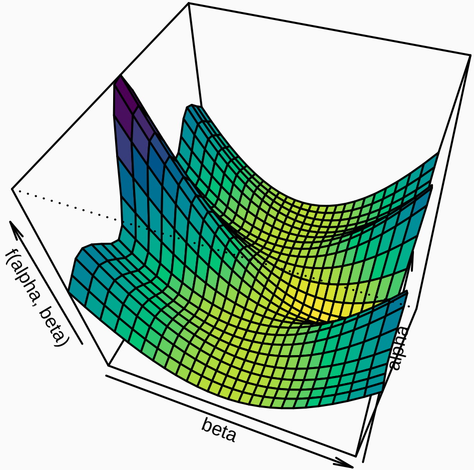

Figure 9: Perspective plot of function

Surfaces

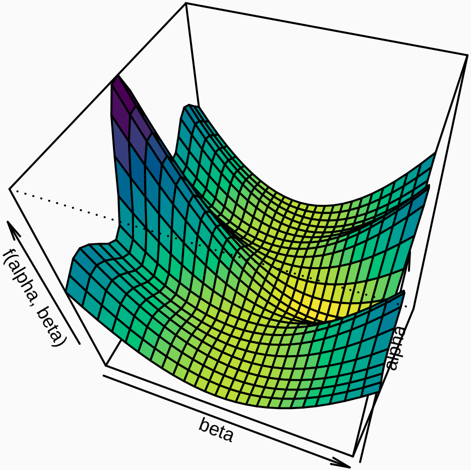

Figure 9: Perspective plot of function

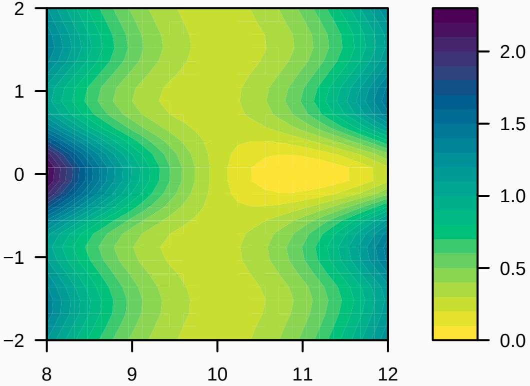

Figure 10: Contour plot of f

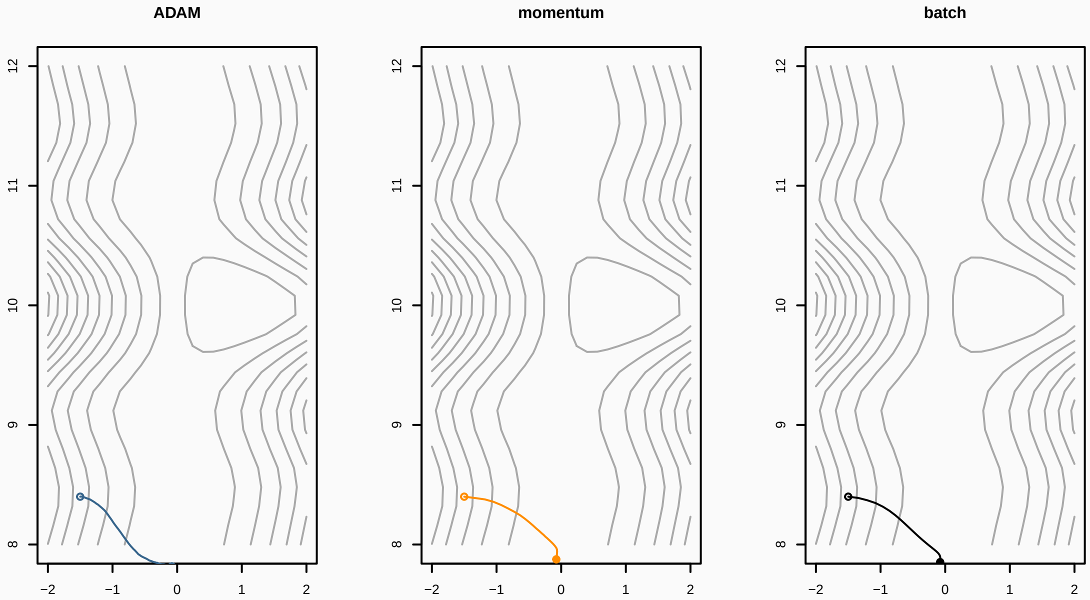

Figure 11:

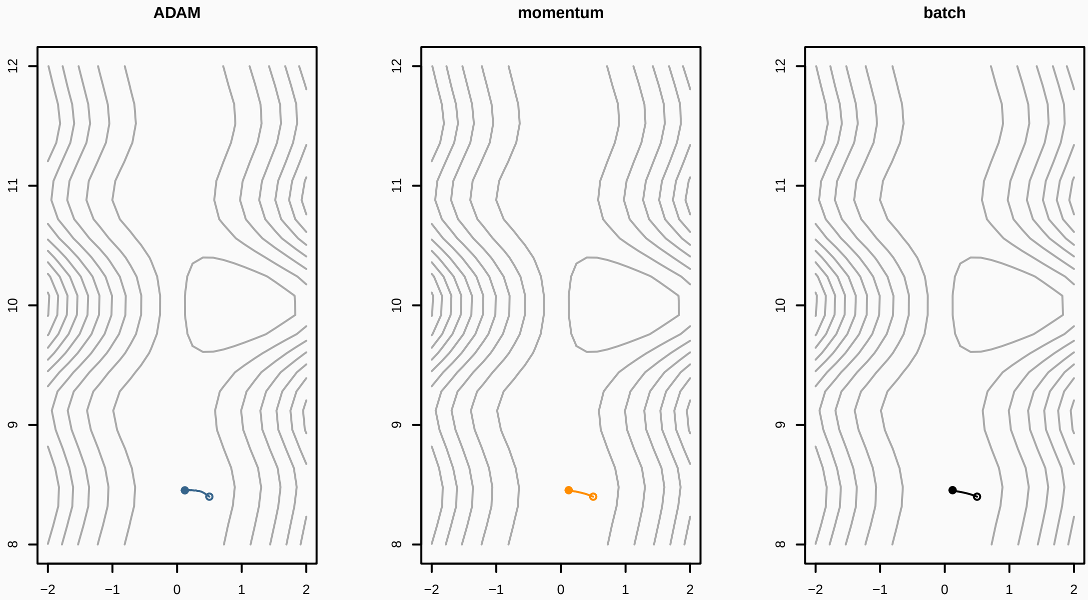

Figure 11:

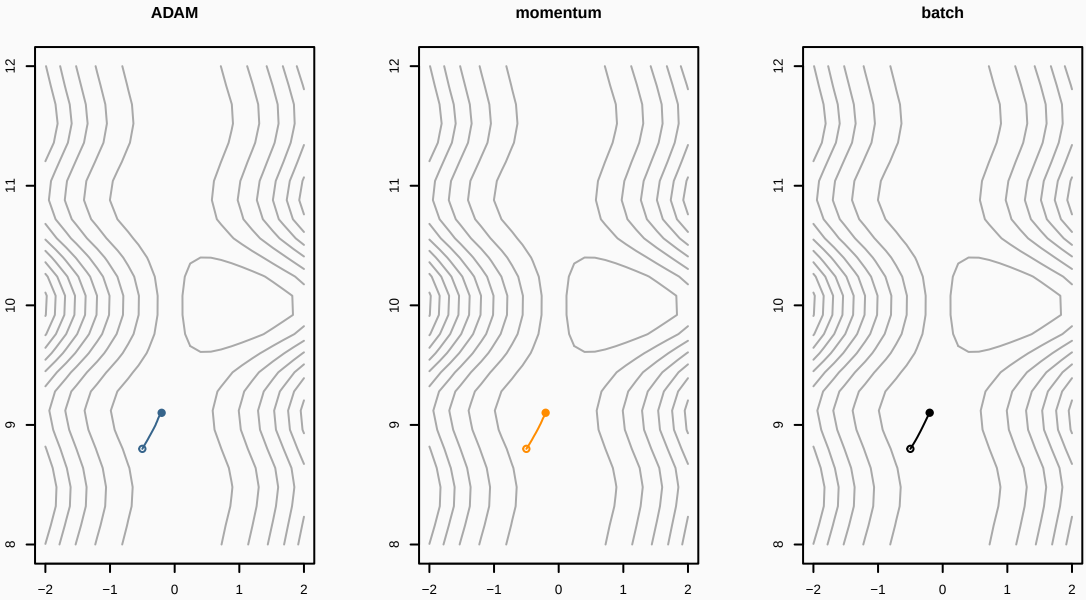

Figure 11:

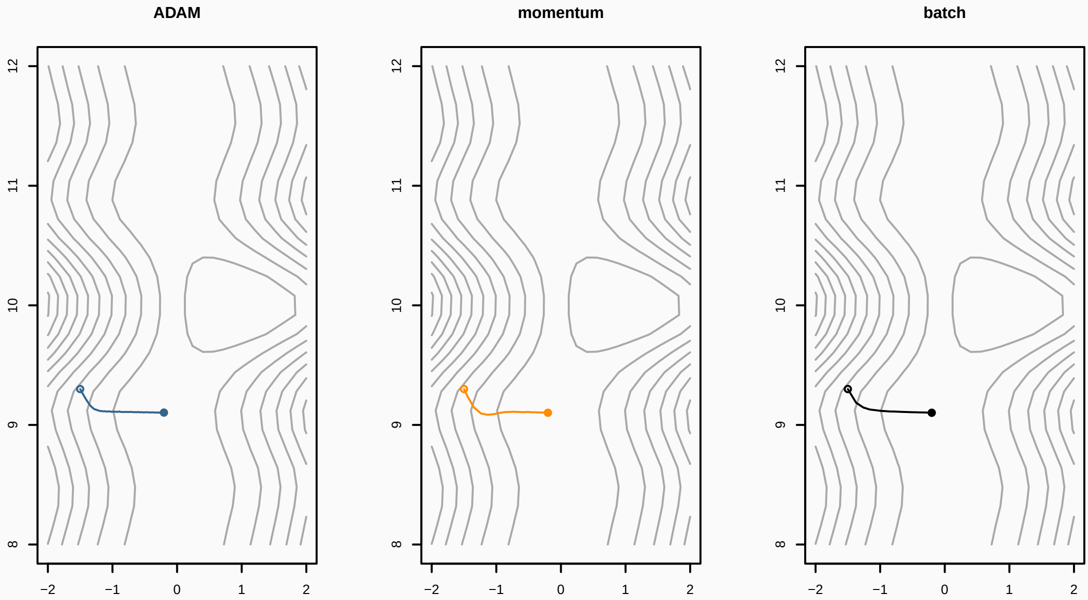

Figure 11:

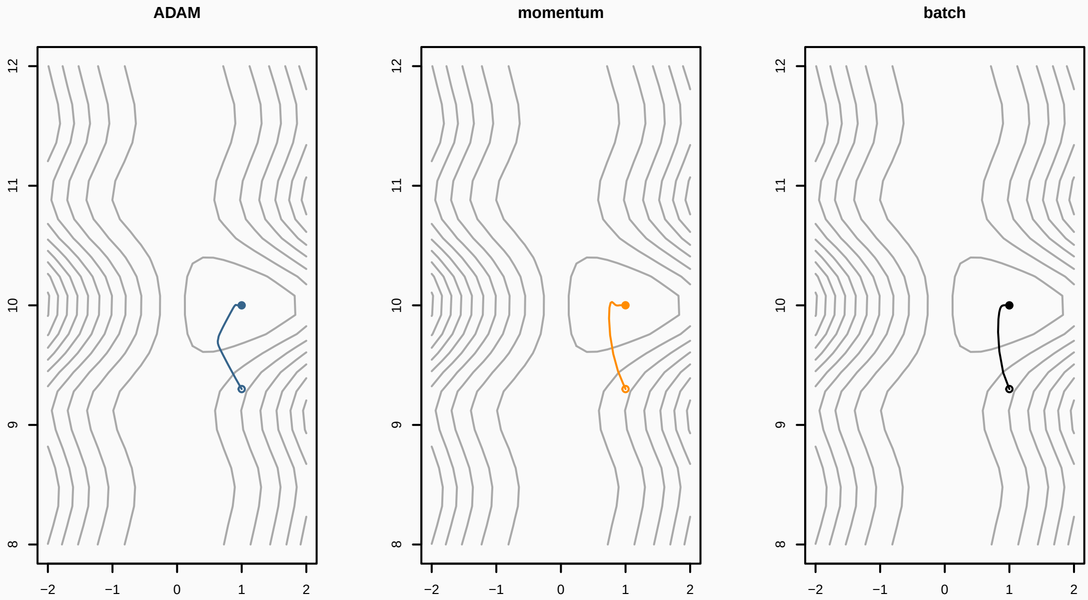

Figure 11:

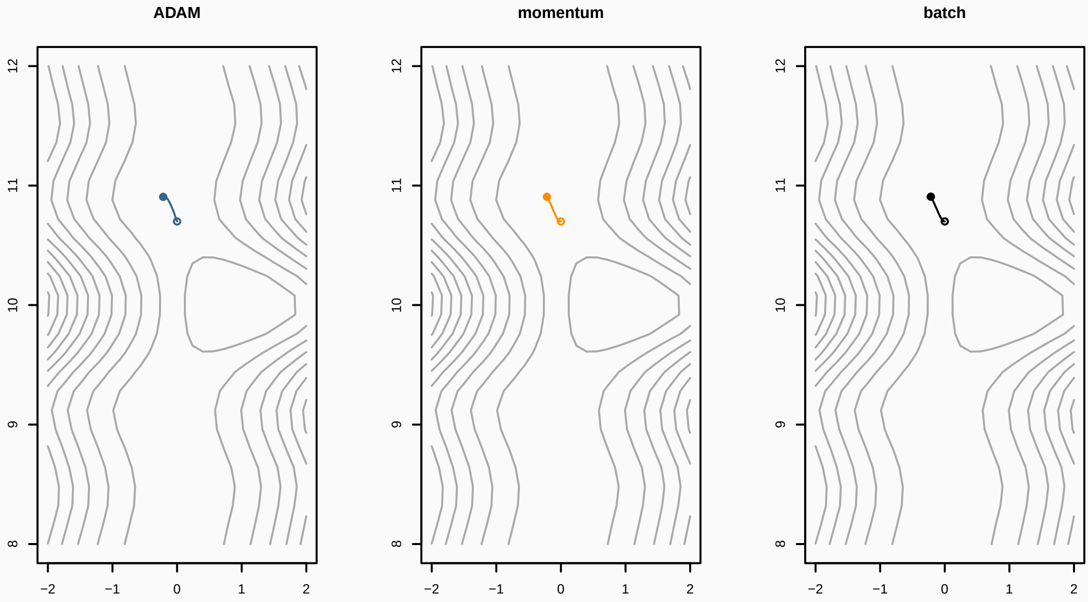

Figure 11:

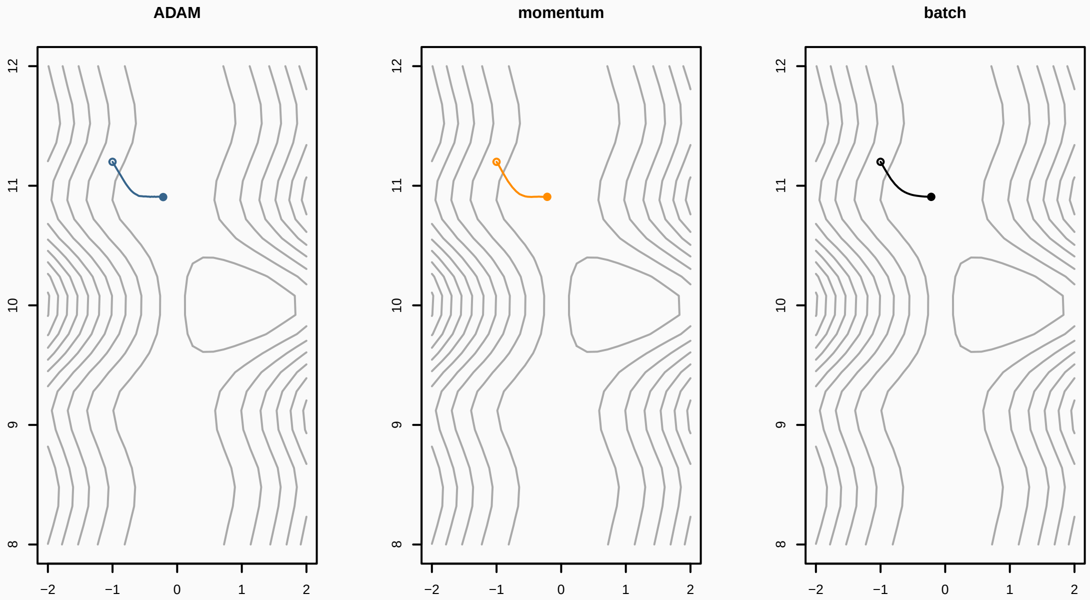

Figure 11:

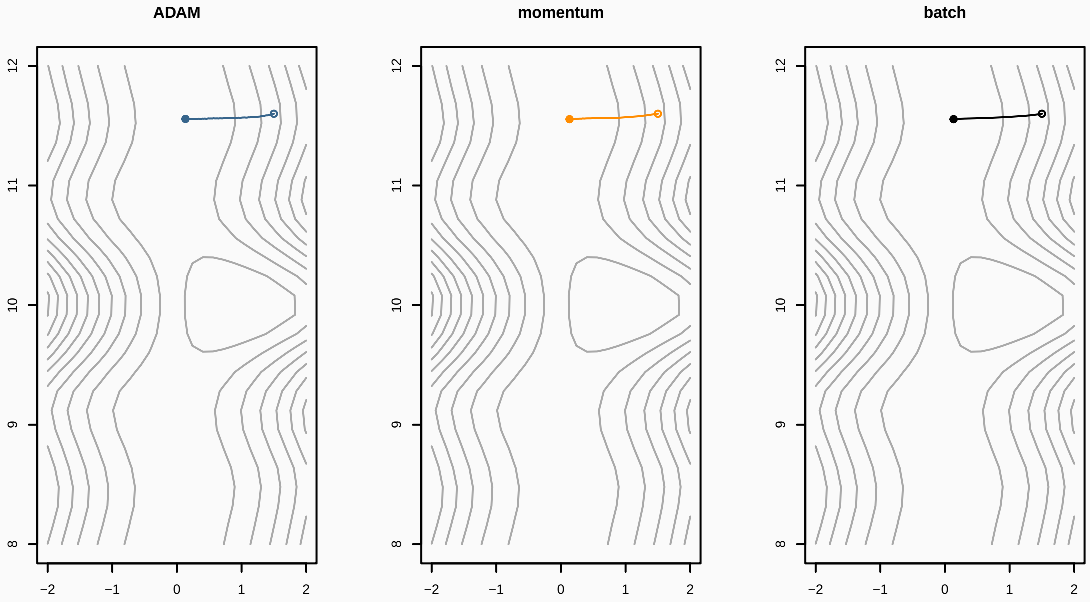

Figure 11:

Rcpp

Very attractive for stochastic methods due to all the loop constructs and slicing.

However, Rcpp lacks linear algebra functions.

Approaches

- Still use only Rcpp (but then you need to write your own linear algebra functions[1]
- Use RcppEigen or RcppArmadillo.

[1] Not recommended!

Gradient Descent in RcppArmadillo

```
arma::vec gradient_descent(
  arma::vec x0,
  double alpha,
  int max_iter,
  double tol
) {
  int n = x0.n_elem;
  arma::vec x = x0;
  arma::vec grad(n);

  for (int iter = 0; iter < max_iter; ++iter) {
    grad = grad_f(x);
    x = x - alpha * grad;

    if (arma::norm(grad, 2) < tol) {
        break;
    }
  }
  return x;
}
```

Exercise: SGD with Rcpp

1. Use Rcpp to write a stochastic gradient descent algorithm. Don't bother with the batch version: stick to standard one-sample version.
2. Introduce momentum.

Additional Resources

- Goh (2017) is a great treatise on momentum in gradient descent; lots of interactive visualizations

Next Time

Reproducibility

How to make your code reproducible

We build an R package.

Next Time

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How to make your code reproducible

We build an R package.

Summary

We summarize the course.

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Summary

We summarize the course.

Exam Advice

We talk about the upcoming oral examinations.

Thank you!