Solvers and stuff

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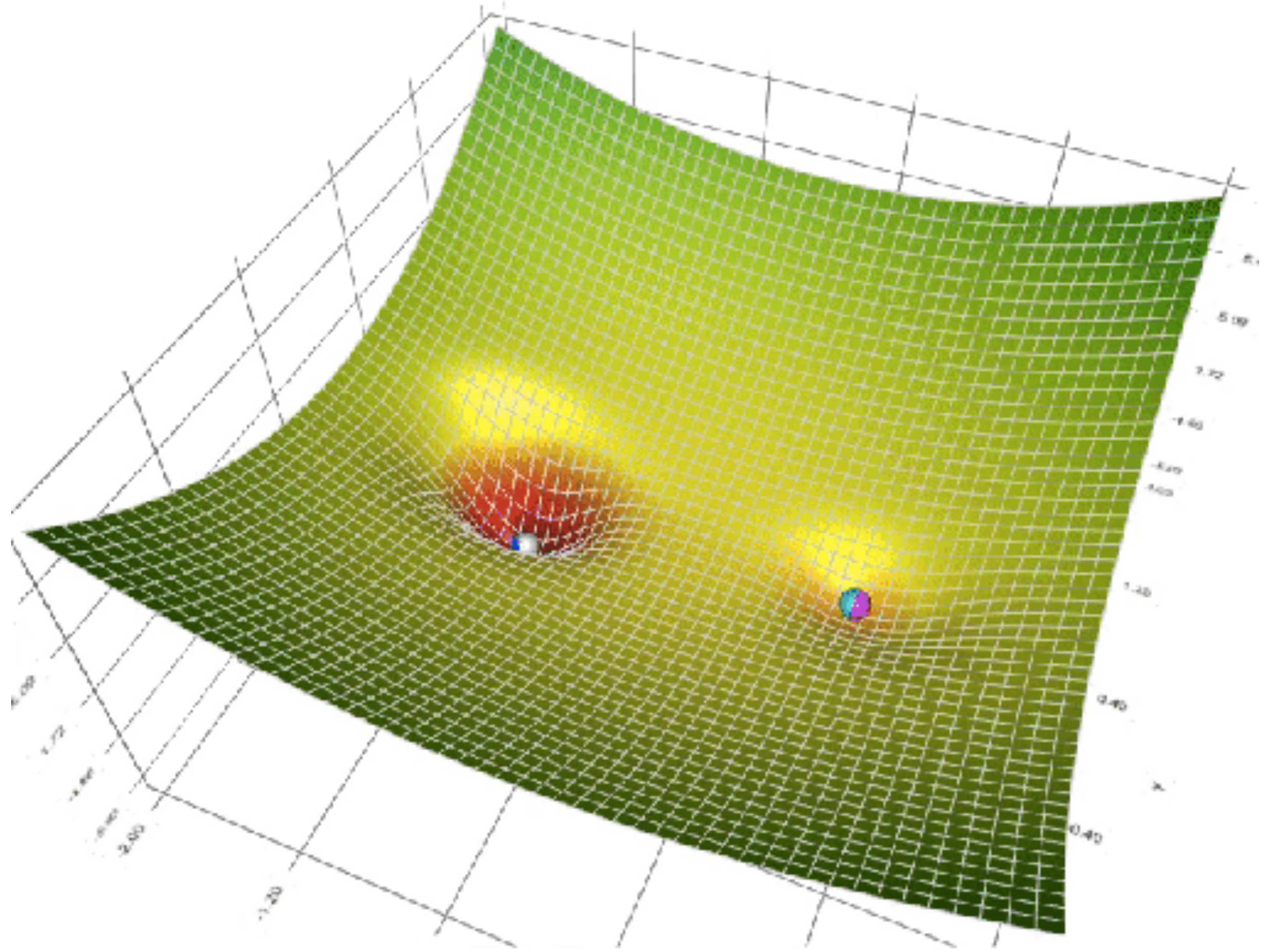
Gradient descent

$$\mathbf{w} = \mathbf{w} - \eta \frac{\partial \mathscr{L}(\mathbf{w})}{\partial \mathbf{w}}$$

$$= \mathbf{w} - \eta \nabla_{\mathbf{w}} \mathscr{L}(\mathbf{w})$$

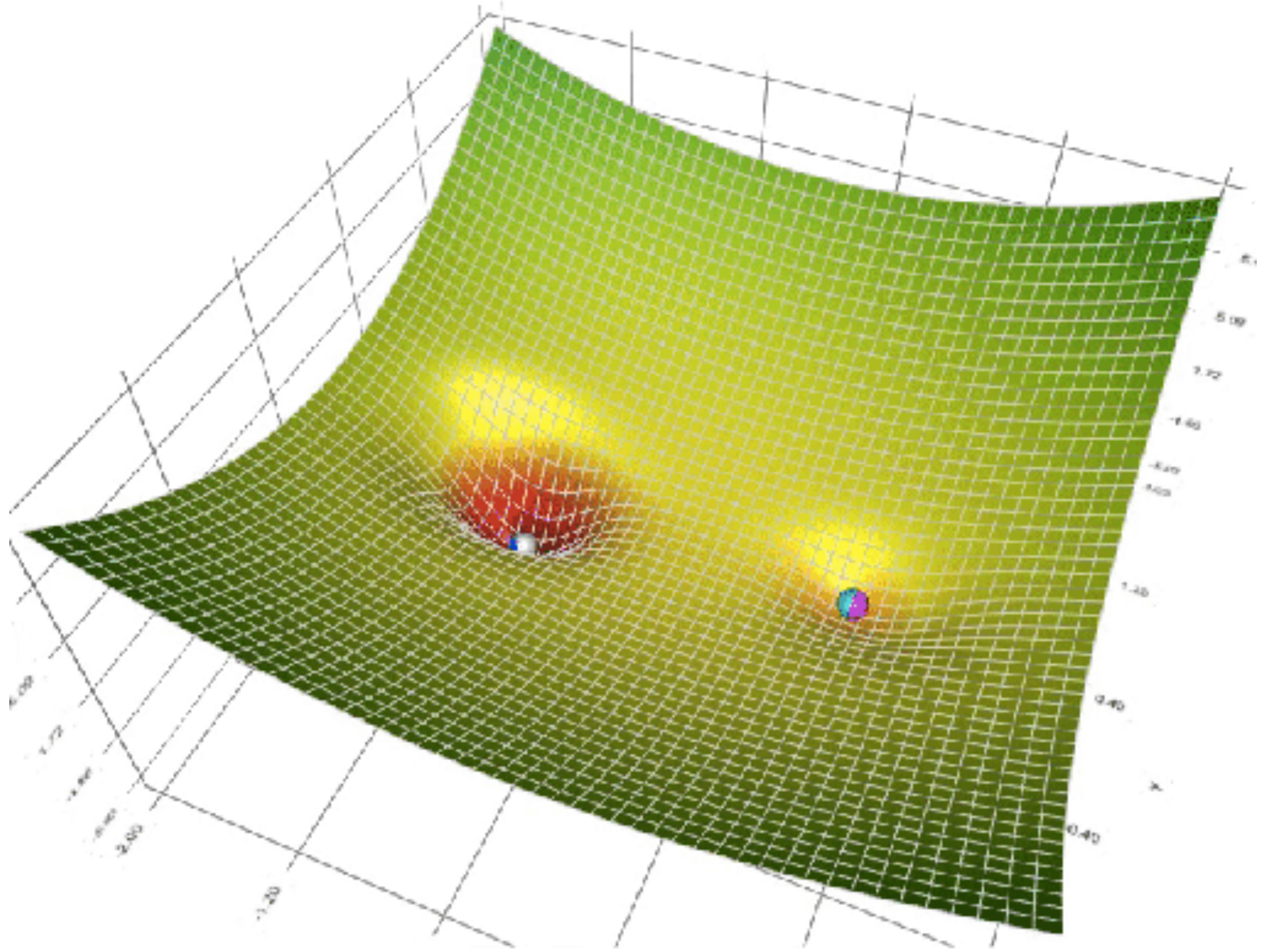
Why is the gradient term negative?

Batch vs stochastic vs minibatch



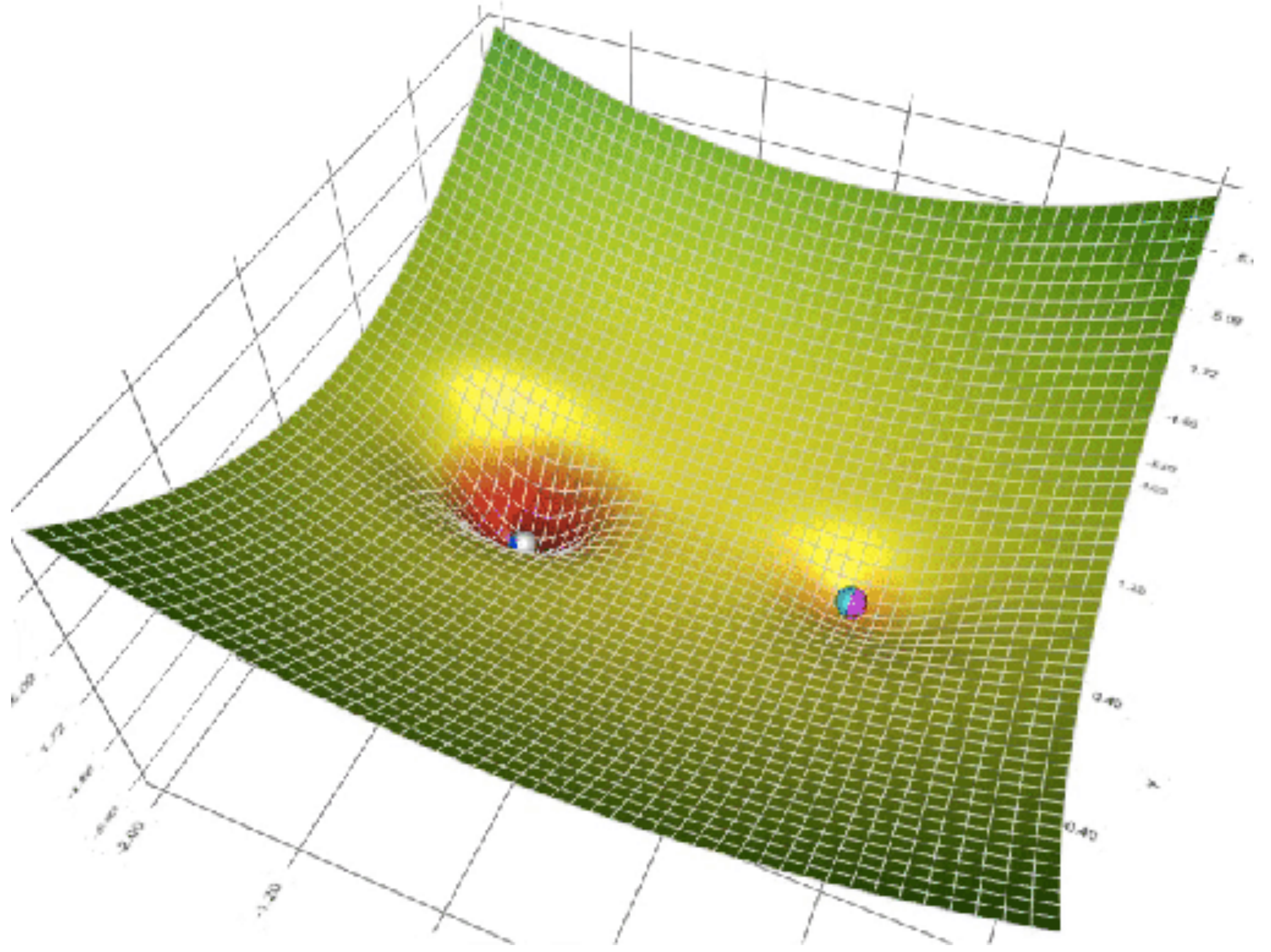
- Batch gradient descent
  - Takes all the training data, calculate gradient, take a step
  - Lots of memory required!
  - $\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \nabla_{\mathbf{w}} \mathscr{L}\left(\mathbf{w}; \mathbf{X}; \mathbf{y}\right)$

Batch vs stochastic vs minibatch



- Stochastic gradient descent
  - Pick a random data point in training, calculate gradient, take a step
  - Little memory required!
  - Not as accurate, Not repeatable
  - $\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \nabla_{\mathbf{w}} \mathscr{L}\left(\mathbf{w}; \mathbf{x}^{(i)}; y^{(i)}\right)$

Batch vs stochastic vs minibatch

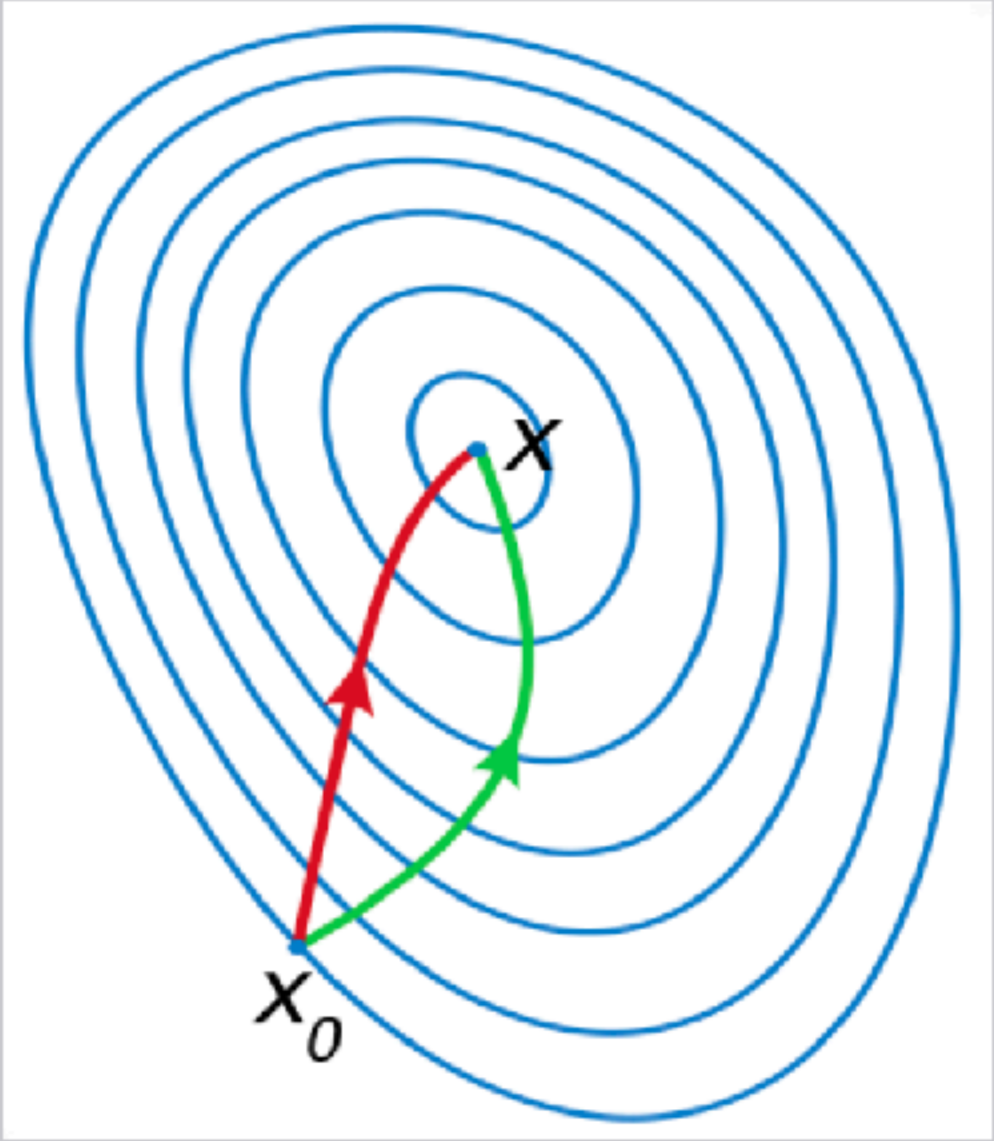


- Miniatch gradient descent (ONLINE)
  - Takes a chunk of training data, calculate gradient, take a step
  - Goldilocks zone for memory, time, accuracy, repeatability
  - $\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \nabla_{\mathbf{w}} \mathscr{L} \left(\mathbf{w}; \mathbf{X}^{(i:i+n)}; \mathbf{y}^{(i:i+n)} \right)$

Higher order terms

Newton's method in optimization

In calculus, Newton's method is an iterative method for finding the roots of a differentiable function F, which are solutions to the equation $F(x) = 0$. As such, Newton's method can be applied to the derivative f' of a twice-differentiable function f to find the roots of the derivative (solutions to $f'(x) = 0$), also known as the critical points of f. These solutions may be minima, maxima, or saddle points; see section "Several variables" in Critical point (mathematics) and also section "Geometric interpretation" in this article. This is relevant in optimization, which aims to find (global) minima of the function f.



A comparison of gradient descent (green) and Newton's method (red) for minimizing a function (with small step sizes). Newton's method uses curvature information (i.e. the second derivative) to take a more direct route.

Newton's method [edit]

The central problem of optimization is minimization of functions. Let us first consider the case of univariate functions, i.e., functions of a single real variable. We will later consider the more general and more practically useful multivariate case.

Given a twice differentiable function $f : \mathbb{R} \to \mathbb{R}$, we seek to solve the optimization problem

$$\min_{x \in \mathbb{R}} f(x).$$

Newton's method attempts to solve this problem by constructing a sequence $\{x_k\}$ from an initial guess (starting point) $x_0 \in \mathbb{R}$ that converges towards a minimizer x_* of f by using a sequence of second-order Taylor approximations of f around the iterates. The second-order Taylor expansion of f around x_k is

$$f(x_k + t) \approx f(x_k) + f'(x_k)t + \frac{1}{2} f''(x_k)t^2.$$

The next iterate x_{k+1} is defined so as to minimize this quadratic approximation in t, and setting $x_{k+1} = x_k + t$. If the second derivative is positive, the quadratic approximation is a convex function of t, and its minimum can be found by setting the derivative to zero. Since

Newton's method in optimization

From Wikipedia, the free encyclopedia

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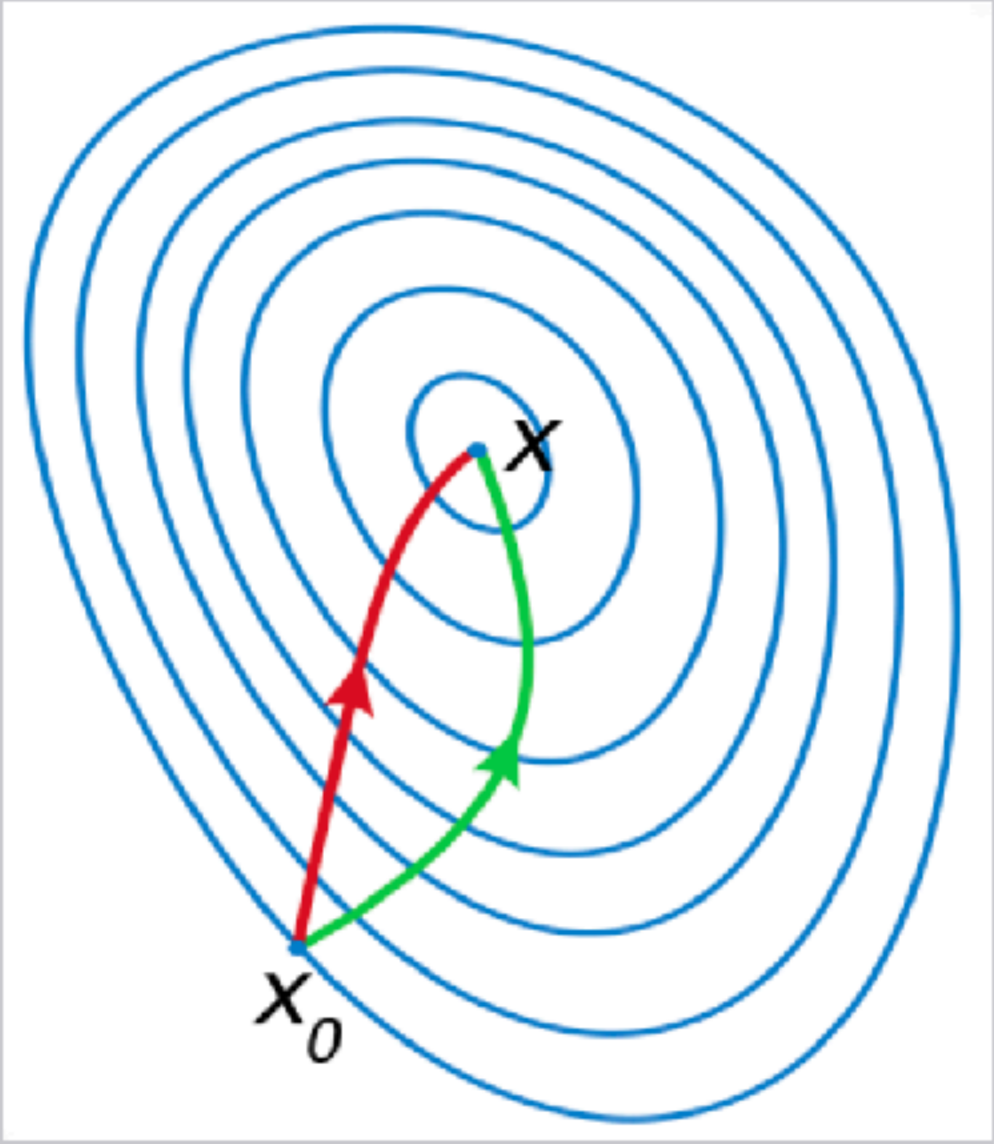

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Quasi-Newton method

Quasi-Newton methods are methods used to either find zeroes or local maxima and minima of functions, as an alternative to Newton's method. They can be used if the Jacobian or Hessian is unavailable or is too expensive to compute at every iteration. The "full" Newton's method requires the Jacobian in order to search for zeros, or the Hessian for finding extrema.

As in Newton's method, one uses a second-order approximation to find the minimum of a function $f(x)$. The Taylor series of $f(x)$ around an iterate is

$$f(x_k + \Delta x) \approx f(x_k) + \nabla f(x_k)^{\mathrm{T}}\, \Delta x + \frac{1}{2} \Delta x^{\mathrm{T}} B\, \Delta x,$$

where (∇f) is the gradient, and B an approximation to the Hessian matrix.[4] The gradient of this approximation (with respect to Δx) is

$$\nabla f(x_k + \Delta x) \approx \nabla f(x_k) + B\, \Delta x,$$

and setting this gradient to zero (which is the goal of optimization) provides the Newton step:

$$\Delta x = -B^{-1} \nabla f(x_k).$$

The Hessian approximation B is chosen to satisfy

$$\nabla f(x_k + \Delta x) = \nabla f(x_k) + B\, \Delta x,$$

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Limited-memory BFGS (**L-BFGS** or **LM-BFGS**) is an optimization algorithm in the family of quasi-Newton methods that approximates the Broyden–Fletcher–Goldfarb–Shanno algorithm (BFGS) using a limited amount of computer memory.[1] It is a popular algorithm for parameter estimation in machine learning.[2][3] The algorithm's target problem is to minimize $f(\mathbf{x})$ over unconstrained values of the real-vector $\mathbf{x}$ where f is a differentiable scalar function.

Like the original BFGS, L-BFGS uses an estimate of the inverse Hessian matrix to steer its search through variable space, but where BFGS stores a dense $n \times n$ approximation to the inverse Hessian (n being the number of variables in the problem), L-BFGS stores only a few vectors that represent the approximation implicitly. Due to its resulting linear memory requirement, the L-BFGS method is particularly well suited for optimization problems with many variables. Instead of the inverse Hessian $\mathbf{H}_k$, L-BFGS maintains a history of the past m updates of the position $\mathbf{x}$ and gradient $\nabla f(\mathbf{x})$, where generally the history size m can be small (often $m < 10$). These updates are used to implicitly do operations requiring the $\mathbf{H}_k$-vector product.

Momentum

See https://distill.pub/2017/momentum/

Adaptive step sizes

See https://www.ruder.io/optimizing-gradient-descent/

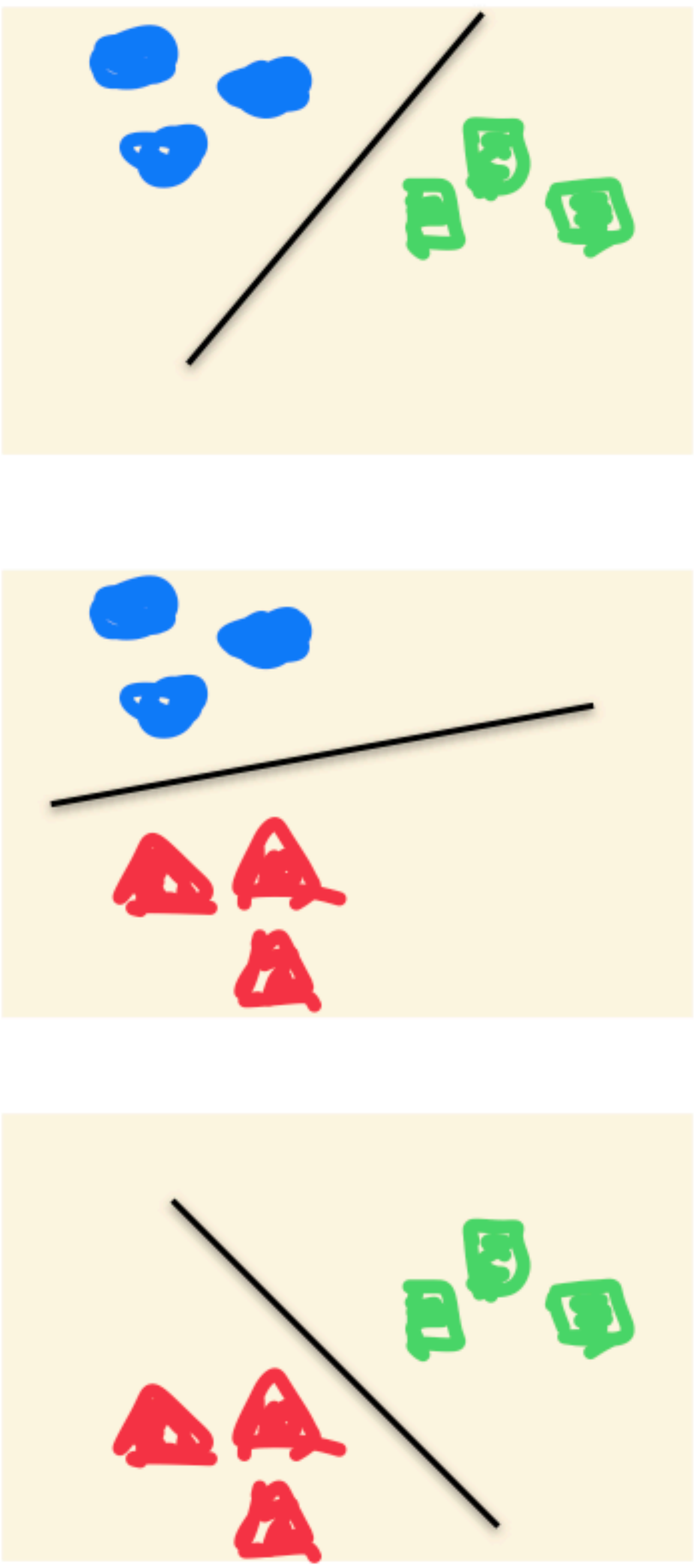
Extending binary classification to multi-class situations

$K=3$ classes

One v One uses class with highest confidence score

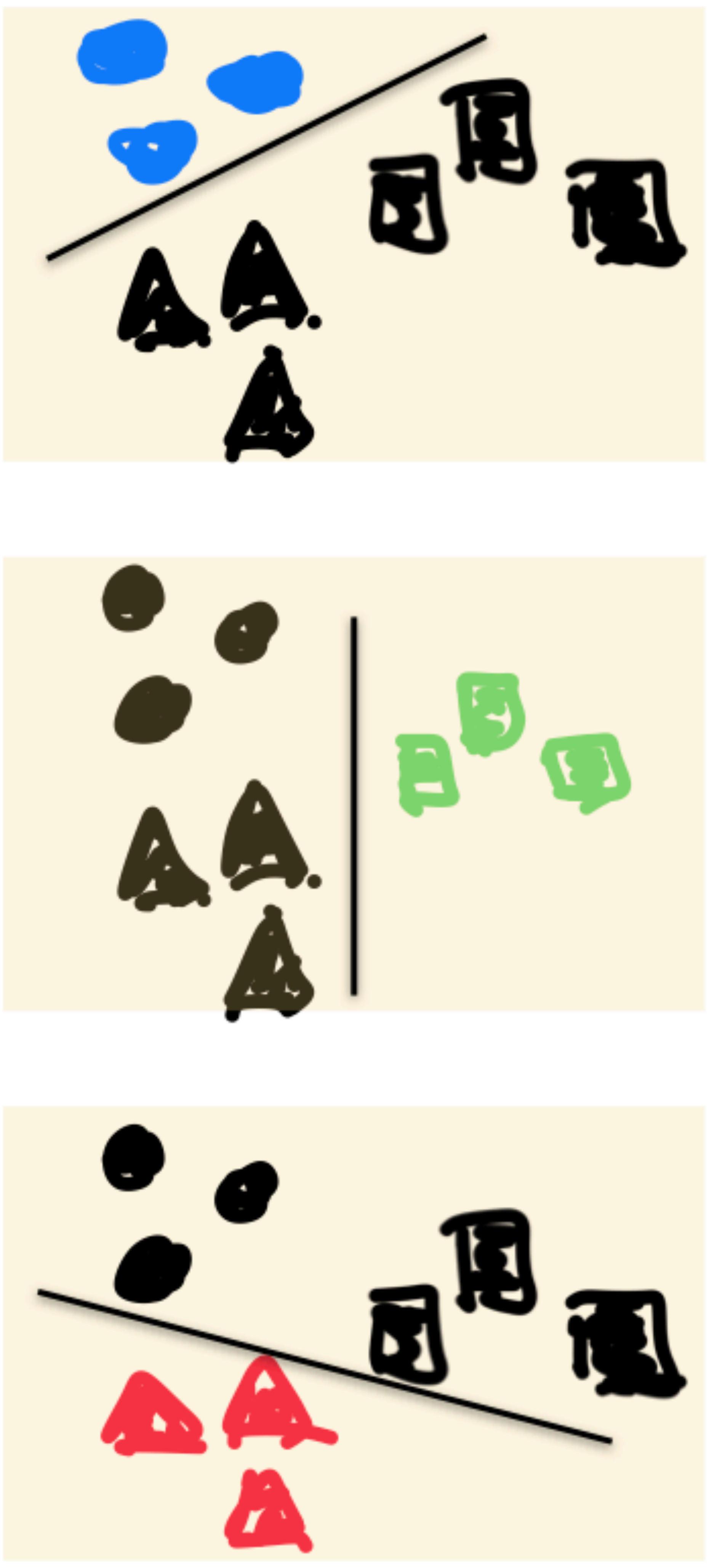
One v Rest uses plurality (mode) vote, tie breaker with confidence score

One v. One



$\frac{K(K-1)}{2}$ classifiers

One v. Rest



K classifiers

Multi-ball!

https://scikit-learn.org/stable/modules/multiclass.html