Our First Hyperparameters: Mini-batching, Regularization, and Momentum

CS6787 Lecture 3 — Fall 2019

Where we left off

- We talked about how we can compute gradients easily and efficiently using ML frameworks.

- We talked about **overfitting**, which can negatively impact generalization from the training set to the test set.

- We saw in the paper we read that **early stopping** is one way that overfitting can be prevented.
  - It's an important technique, but I won't cover it in today's lecture since we already covered it in the paper.

How to address overfitting

- **Many, many techniques** to deal with overfitting
  - Have varying computational costs

- But this is a systems course…so what can we do **with little or no extra computational cost?**

- Notice from the demo that **some loss functions do better than others**
  - E.g. the linear loss function did better than the polynomial loss function
  - Can we **modify our loss function** to prevent overfitting?

Regularization

- Add an extra **regularization term** to the objective function

- Most popular type: **L2 regularization**

$$h(w) = \frac{1}{N}\sum_{i=1}^{N} f(w; x_i) + \sigma^2 \|w\|_2^2 = \frac{1}{N}\sum_{i=1}^{N} f(w; x_i) + \sigma^2 \sum_{k=1}^{d} x_k^2$$

- Also popular: **L1 regularization**

$$h(w) = \frac{1}{N}\sum_{i=1}^{N} f(w; x_i) + \gamma \|w\|_1 = \frac{1}{N}\sum_{i=1}^{N} f(w; x_i) + \gamma \sum_{k=1}^{d} \|x_k\|$$

Benefits of Regularization

- **Cheap to compute**
  - For SGD and L2 regularization, there's just an extra scaling

$$w_{t+1} = (1 - 2\alpha_t \sigma^2) w_t - \alpha_t \nabla f(w_t; x_{i_t})$$

- **L2 regularization makes the objective strongly convex**
  - This makes it easier to get and prove bounds on convergence

- **Helps with overfitting**

Demo

How to choose the regularization parameter?

- One way is to use an independent **validation set** to estimate the test error, and set the regularization parameter manually so that it is high enough to avoid overfitting
  - This is what we saw in the demo

- But doing this naively can be **computationally expensive**
  - Need to re-run learning algorithm many times

- Yet another use case for **hyperparameter optimization**

More general forms of regularization

- **Regularization** is used more generally to describe anything that helps prevent overfitting
  - By biasing learning by making some models more desirable *a priori*

- Many techniques that give throughput improvements also have a regularizing effect
  - Sometimes: a **win-win** of better statistical and hardware performance

Mini-Batching

Gradient Descent vs. SGD

- Gradient descent: **all examples at once**

$$w_{t+1} = w_t - \alpha_t \frac{1}{N} \sum_{i=1}^{N} \nabla f(w_t; x_i)$$

- Stochastic gradient descent: **one example at a time**

$$w_{t+1} = w_t - \alpha_t \nabla f(w_t; x_{i_t})$$

- Is it really **all or nothing**? Can we do something intermediate?

Mini-Batch Stochastic Gradient Descent

- An intermediate approach

$$w_{t+1} = w_t - \alpha_t \frac{1}{|B_t|} \sum_{i \in B_t} \nabla f(w_t; x_i)$$

where B_t is sampled uniformly from the set of all subsets of {1, … , N} of size b.

  - The b parameter is the **batch size**
  - Typically choose b << N.

- Also called **mini-batch gradient descent**

How does runtime cost of Mini-Batch compare to SGD and Gradient Descent?

- Takes **less time to compute each update** than gradient descent
  - Only needs to sum up b gradients, rather than N

$$w_{t+1} = w_t - \alpha_t \frac{1}{|B_t|} \sum_{i \in B_t} \nabla f(w_t; x_i)$$

- But takes **more time for each update** than SGD
  - So what's the benefit?

- It's more like gradient descent, so **maybe it converges faster** than SGD?

Mini-Batch SGD Converges

- Start by breaking up the update rule into expected update and noise

$$w_{t+1} - w^* = w_t - w^* - \alpha_t \left(\nabla h(w_t) - \nabla h(w^*) \right)$$
$$- \alpha_t \frac{1}{|B_t|} \sum_{i \in B_t} \left(\nabla f(w_t; x_i) - \nabla h(w_t) \right)$$

- Second moment bound

$$\mathbf{E}\left[\|w_{t+1} - w^*\|^2 \right] = \mathbf{E}\left[\|w_t - w^* - \alpha_t \left(\nabla h(w_t) - \nabla h(w^*) \right) \|^2 \right]$$
$$+ \alpha_t^2 \mathbf{E}\left[\left\| \frac{1}{|B_t|} \sum_{i \in B_t} \left(\nabla f(w_t; x_i) - \nabla h(w_t) \right) \right\|^2 \right]$$

Mini-Batch SGD Converges (continued)

Let $\Delta_i = \nabla f(w_t; x_i) - \nabla h(w_t)$

$$\mathbf{E}\left[\left\|\frac{1}{|B_t|}\sum_{i \in B_t}\left(\nabla f(w_t; x_i) - \nabla h(w_t)\right)\right\|^2\right]$$

$$= \mathbf{E}\left[\left\|\frac{1}{|B_t|}\sum_{i \in B_t}\Delta_i\right\|^2\right]$$

Mini-Batch SGD Converges (continued)

- Because we sampled B uniformly at random, for **i ≠ j**

$$\mathbf{E}\left[\beta_i \beta_j\right] = \mathbf{P}\left(i \in B \wedge j \in B\right) = \mathbf{P}\left(i \in B\right) \mathbf{P}\left(j \in B | i \in B\right) = \frac{b}{N} \cdot \frac{b-1}{N-1}$$

$$\mathbf{E}\left[\beta_i^2\right] = \mathbf{P}\left(i \in B\right) = \frac{b}{N}$$

- So we can bound our square error term as

$$\mathbf{E}\left[\left\| \frac{1}{|B_t|} \sum_{i \in B_t} \left(\nabla f(w_t; x_i) - \nabla h(w_t)\right) \right\|^2\right] = \frac{1}{|B_t|^2} \mathbf{E}\left[\sum_{i=1}^{N} \sum_{j=1}^{N} \beta_i \beta_j \Delta_i^T \Delta_j\right]$$

$$= \frac{1}{b^2} \mathbf{E}\left[\sum_{i \neq j} \frac{b(b-1)}{N(N-1)} \Delta_i^T \Delta_j + \sum_{i=1}^{N} \frac{b}{N} \|\Delta_i\|^2\right]$$

Mini-Batch SGD Converges (continued)

$$\mathbf{E}\left[\left\|\frac{1}{|B_t|}\sum_{i\in B_t}\left(\nabla f(w_t;x_i)-\nabla h(w_t)\right)\right\|^2\right]=\frac{1}{bN}\mathbf{E}\left[\frac{b-1}{N-1}\sum_{i\neq j}\Delta_i^T\Delta_j+\sum_{i=1}^{N}\|\Delta_i\|^2\right]$$

Mini-Batch SGD Converges (continued)

$$\mathbf{E}\left[\left\|\frac{1}{|B_t|}\sum_{i\in B_t}(\nabla f(w_t;x_i)-\nabla h(w_t))\right\|^2\right]=\frac{N-b}{b(N-1)}\mathbf{E}\left[\frac{1}{N}\sum_{i=1}^{N}\|\Delta_i\|^2\right]$$

- Compared with SGD, **squared error term decreased by a factor of b**

Mini-Batch SGD Converges (continued)

- Recall that SGD converged to a noise ball of size

$$\lim_{T \to \infty} \mathbf{E}\left[\|w_T - w^*\|^2\right] \le \frac{\alpha M}{2\mu - \alpha\mu^2}$$

- Since mini-batching decreases error term by a factor of **b**, it will have

$$\lim_{T \to \infty} \mathbf{E}\left[\|w_T - w^*\|^2\right] \le \frac{\alpha M}{(2\mu - \alpha\mu^2)b}$$

  - **Noise ball smaller** by the same factor!

Advantages of Mini-Batch (reprise)

- Takes **less time to compute each update** than gradient descent
  - Only needs to sum up b gradients, rather than N

$$w_{t+1} = w_t - \alpha_t \frac{1}{|B_t|} \sum_{i \in B_t} \nabla f(w_t; x_i)$$

- Converges to a **smaller noise ball** than stochastic gradient descent

$$\lim_{T \to \infty} \mathbf{E}\left[\|w_T - w^*\|^2\right] \le \frac{\alpha M}{(2\mu - \alpha\mu^2) b}$$

How to choose the batch size?

- **Mini-batching is not a free win**
  - Naively, compared with SGD, it takes **b** times as much effort to get a **b**-times-as-accurate answer
  - But we could have gotten a **b**-times-as-accurate answer by just running SGD for **b** times as many steps with a step size of $\alpha/\mathbf{b}$.

- But it still makes sense to run it for **systems** and **statistical** reasons
  - Mini-batching exposes more parallelism
  - Mini-batching lets us estimate statistics about the full gradient more accurately

- Another use case for **hyperparameter optimization**

Mini-Batch SGD is very widely used

- Including in basically all neural network training

- **b = 32** is a typical default value for batch size
  - From “Practical Recommendations for Gradient-Based Training of Deep Architectures,” Bengio 2012.

Another class of technique: Acceleration and Momentum

How does the step size affect convergence?

- Let's go back to gradient descent

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

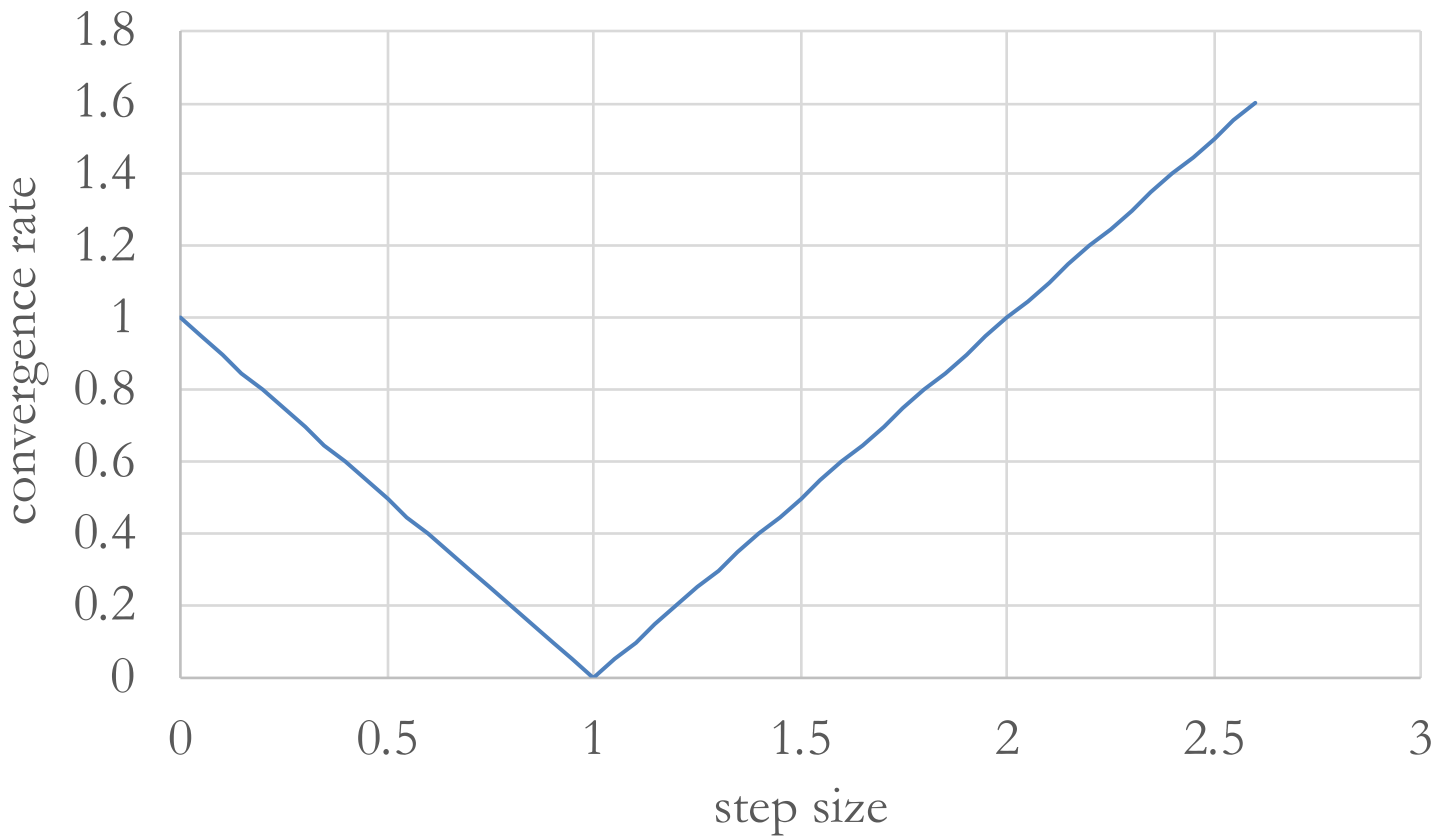
- Simplest possible case: a quadratic function

$$f(x) = \frac{1}{2} x^2$$

$$x_{t+1} = x_t - \alpha x_t = (1 - \alpha) x_t$$

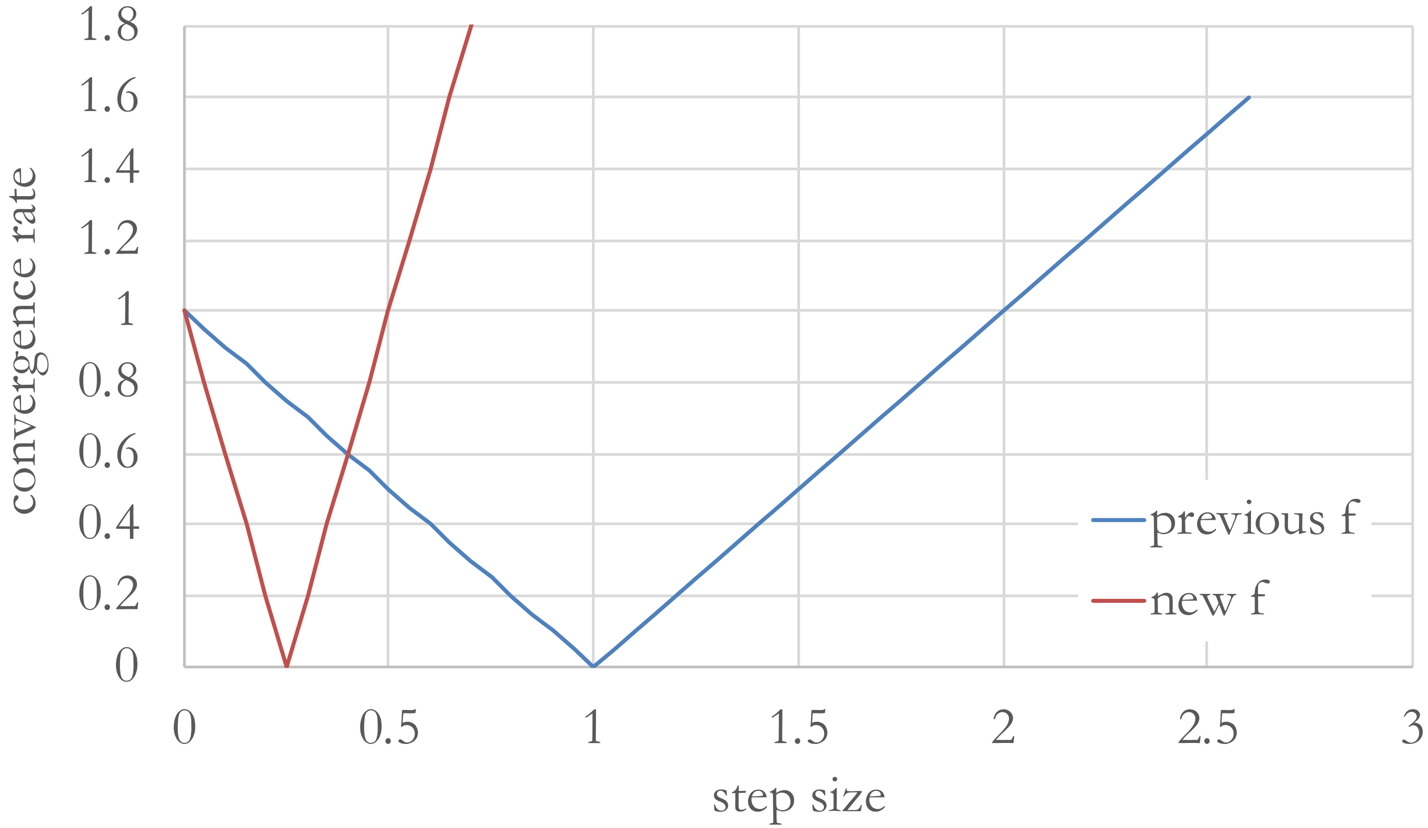
Step size vs. convergence: graphically

$$|x_{t+1} - 0| = |1 - \alpha| \, |x_t - 0|$$



What if the curvature is different?

$$f(x) = 2x^2 \qquad x_{t+1} = x_t - 4\alpha x_t = (1 - 4\alpha)x_t$$



Step size vs. curvature

- For these one-dimensional quadratics, how we should set **the step size depends on the curvature**
  - More curvature → smaller ideal step size

- What about higher-dimensional problems?
  - Let's look at a really simple quadratic that's just a sum of our examples.

$$f(x, y) = \frac{1}{2}x^2 + 2y^2$$

Simple two dimensional problem

$$f(x,y) = \frac{1}{2}x^2 + 2y^2$$

- Gradient descent:

$$\begin{aligned} \begin{bmatrix} x_{t+1} \\ y_{t+1} \end{bmatrix} &= \begin{bmatrix} x_t \\ y_t \end{bmatrix} - \alpha \begin{bmatrix} x_t \\ 4y_t \end{bmatrix} \\ &= \begin{bmatrix} 1-\alpha & 0 \\ 0 & 1-4\alpha \end{bmatrix} \begin{bmatrix} x_t \\ y_t \end{bmatrix} \end{aligned}$$

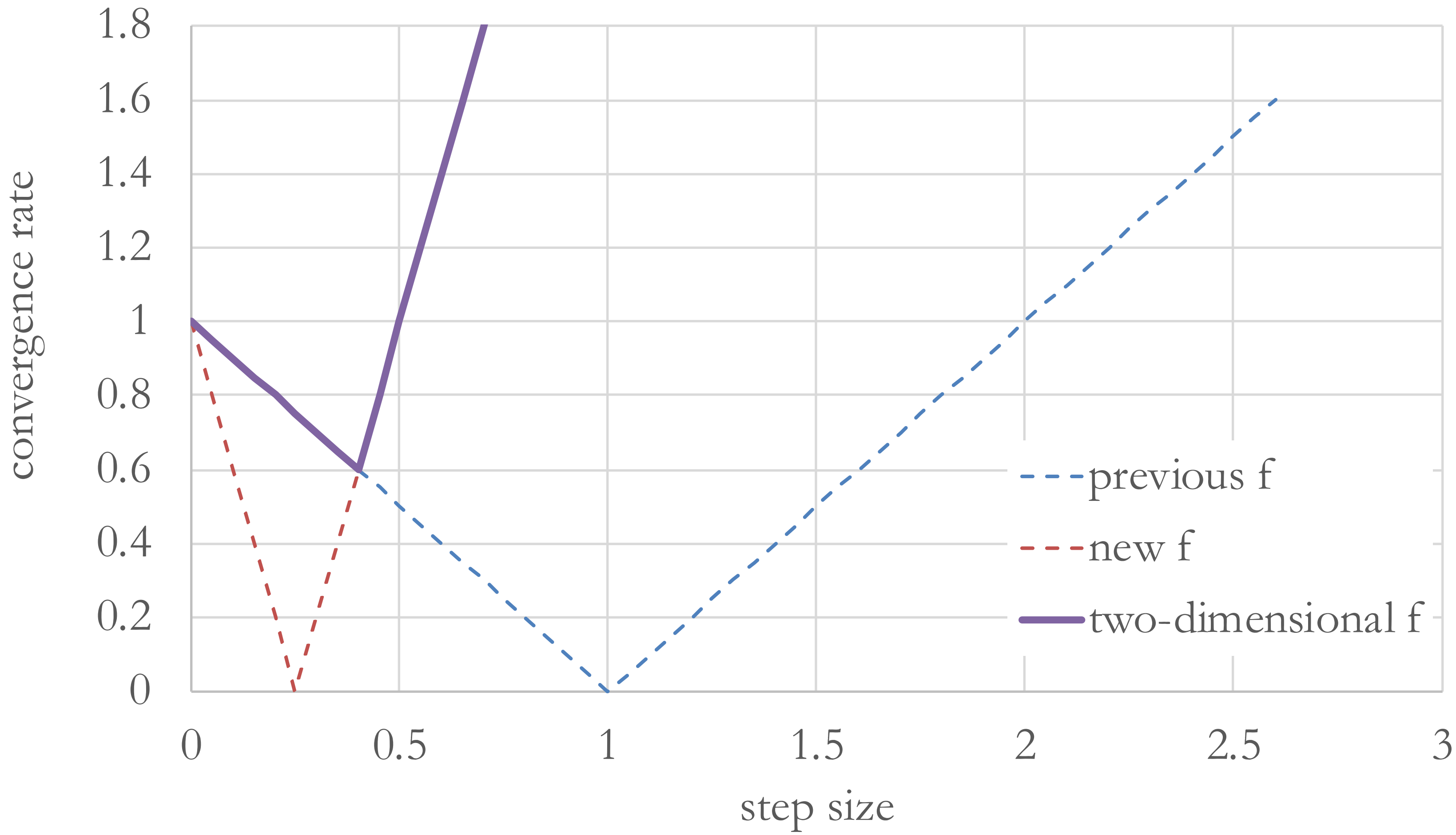
What's the convergence rate?

- Look at the worst-case contraction factor of the update

$$\max_{x,y} \frac{\left\| \begin{bmatrix} 1-\alpha & 0 \\ 0 & 1-4\alpha \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \right\|}{\left\| \begin{bmatrix} x \\ y \end{bmatrix} \right\|} = \max(|1-\alpha|, |1-4\alpha|)$$

- Contraction is maximum of previous two values.

Convergence of two-dimensional quadratic



What does this example show?

- We'd like to set the step size larger for dimension with less curvature, and smaller for the dimension with more curvature.

- But we can't, because there is **only a single step-size parameter**.

- There's a **trade-off**
  - Optimal convergence rate is **substantially worse than** what we'd get in each scenario individually — individually we converge in one iteration.

For general quadratics

- For PSD symmetric A,

$$f(x) = \frac{1}{2}x^T Ax$$

- Gradient descent has update step

$$x_{t+1} = x_t - \alpha A x_t = (I - \alpha A)x_t$$

- What does the convergence rate look like in general?

Convergence rate for general quadratics

$$
\begin{aligned}
\max_x \frac{\|(I - \alpha A)x\|}{\|x\|} &= \max_x \frac{1}{\|x\|} \left\| \left(I - \alpha \sum_{i=1}^{n} \lambda_i u_i u_i^T \right) x \right\| \\
&= \max_x \frac{\|\sum_{i=1}^{n} (1 - \alpha \lambda_i) u_i u_i^T x\|}{\|\sum_{i=1}^{n} u_i u_i^T x\|} \\
&= \max_i |1 - \alpha \lambda_i| \\
&= \max(1 - \alpha \lambda_{\min}, \alpha \lambda_{\max} - 1)
\end{aligned}
$$

Optimal convergence rate

- Minimize:

$$\max(1 - \alpha\lambda_{\min}, \alpha\lambda_{\max} - 1)$$

- Optimal value occurs when

$$1 - \alpha\lambda_{\min} = \alpha\lambda_{\max} - 1 \Rightarrow \alpha = \frac{2}{\lambda_{\max} + \lambda_{\min}}$$

- Optimal rate is

$$\max(1 - \alpha\lambda_{\min}, \alpha\lambda_{\max} - 1) = \frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}}$$

What affects this optimal rate?

$$\text{rate} = \frac{\lambda_{\text{max}} - \lambda_{\text{min}}}{\lambda_{\text{max}} + \lambda_{\text{min}}} = \frac{\lambda_{\text{max}}/\lambda_{\text{min}} - 1}{\lambda_{\text{max}}/\lambda_{\text{min}} + 1} = \frac{\kappa - 1}{\kappa + 1}.$$

- Here, κ is called the **condition number** of the matrix **A**.

$$\kappa = \frac{\lambda_{\text{max}}}{\lambda_{\text{min}}}$$

- Problems with larger condition numbers converge slower.
  - Called **poorly conditioned**.

Poorly conditioned problems

- Intuitively, these are problems that are **highly curved in some directions but flat in others**

- Happens pretty often in machine learning
  - Measure something unrelated → low curvature in that direction
  - Also affects stochastic gradient descent

- **How do we deal with this?**

Momentum

Motivation

- Can we tell the difference between the curved and flat directions using information that is already available to the algorithm?
- Idea: in the one-dimensional case, if the gradients are **reversing sign**, then the step size is too large
  - Because we're **over-shooting the optimum**
  - And if the gradients stay in the same direction, then step size is too small
- Can we leverage this to make steps smaller when gradients reverse sign and larger when gradients are consistently in the same direction?

Polyak Momentum

- Add extra **momentum term** to gradient descent

$$x_{t+1} = x_t - \alpha \nabla f(x_t) + \beta(x_t - x_{t-1})$$

- Intuition: if current gradient step is in same direction as previous step, then move a little further in that direction.
  - And if it's in the opposite direction, move less far.

- Also known as the **heavy ball method**.

Momentum for 1D Quadratics

$$f(x) = \frac{\lambda}{2} x^2$$

- Momentum gradient descent gives

$$\begin{aligned} x_{t+1} &= x_t - \alpha\lambda x_t + \beta(x_t - x_{t-1}) \\ &= (1 + \beta - \alpha\lambda) x_t - \beta x_{t-1} \end{aligned}$$

Characterizing momentum for 1D quadratics

- Start with $x_{t+1} = (1 + \beta - \alpha\lambda)x_t - \beta x_{t-1}$

- Trick: let $x_t = \beta^{t/2} z_t$

$$\beta^{(t+1)/2} z_{t+1} = (1 + \beta - \alpha\lambda)\beta^{t/2} z_t - \beta \cdot \beta^{(t-1)/2} z_{t-1}$$

$$z_{t+1} = \frac{1 + \beta - \alpha\lambda}{\sqrt{\beta}} z_t - z_{t-1}$$

Characterizing momentum (continued)

- Let

$$u = \frac{1 + \beta - \alpha\lambda}{2\sqrt{\beta}}$$

- Then we get the simplified characterization

$$z_{t+1} = 2uz_t - z_{t-1}$$

- This is a degree-***t*** polynomial in **u**

Chebyshev Polynomials

- If we initialize such that $z_0 = 1,\ z_1 = u$ then these are a special family of polynomials called the **Chebyshev polynomials**

$$z_{t+1} = 2uz_t - z_{t-1}$$

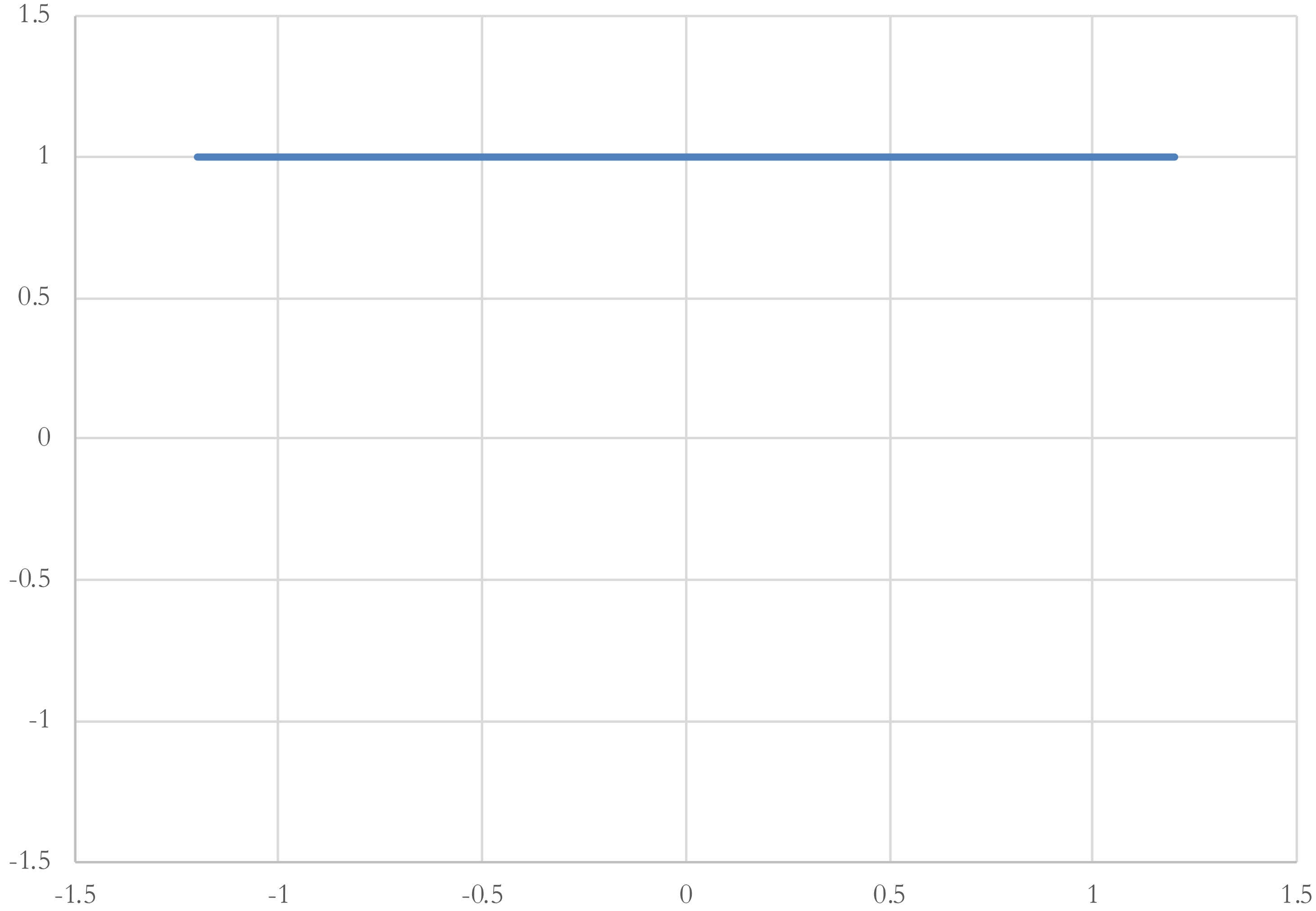
- Standard notation:

$$T_{t+1}(u) = 2uT_t(u) - T_{t-1}(u)$$

- These polynomials have an important property: for all **t**

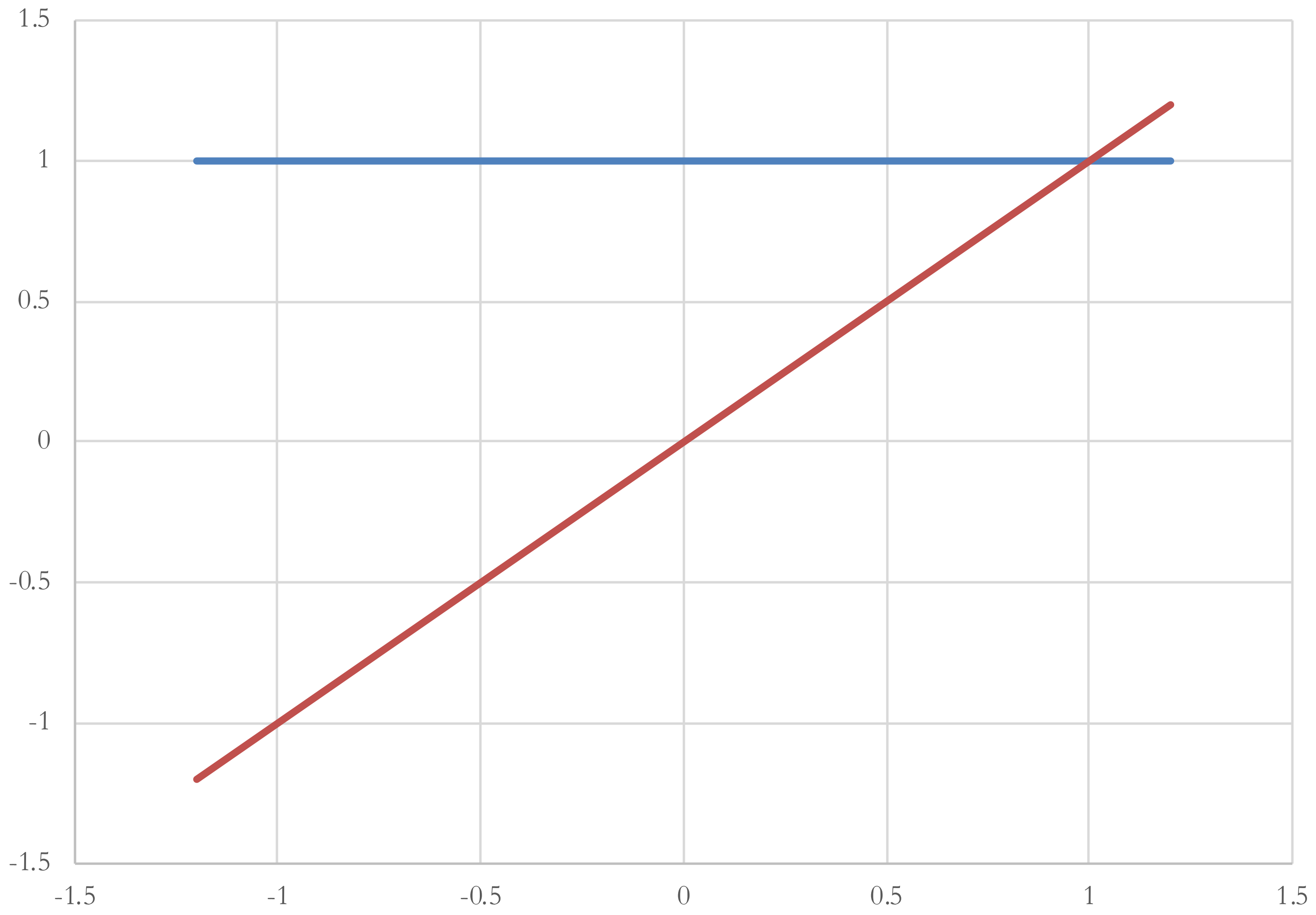
$$-1 \leq u \leq 1 \Rightarrow -1 \leq z_t \leq 1$$

Chebyshev Polynomials



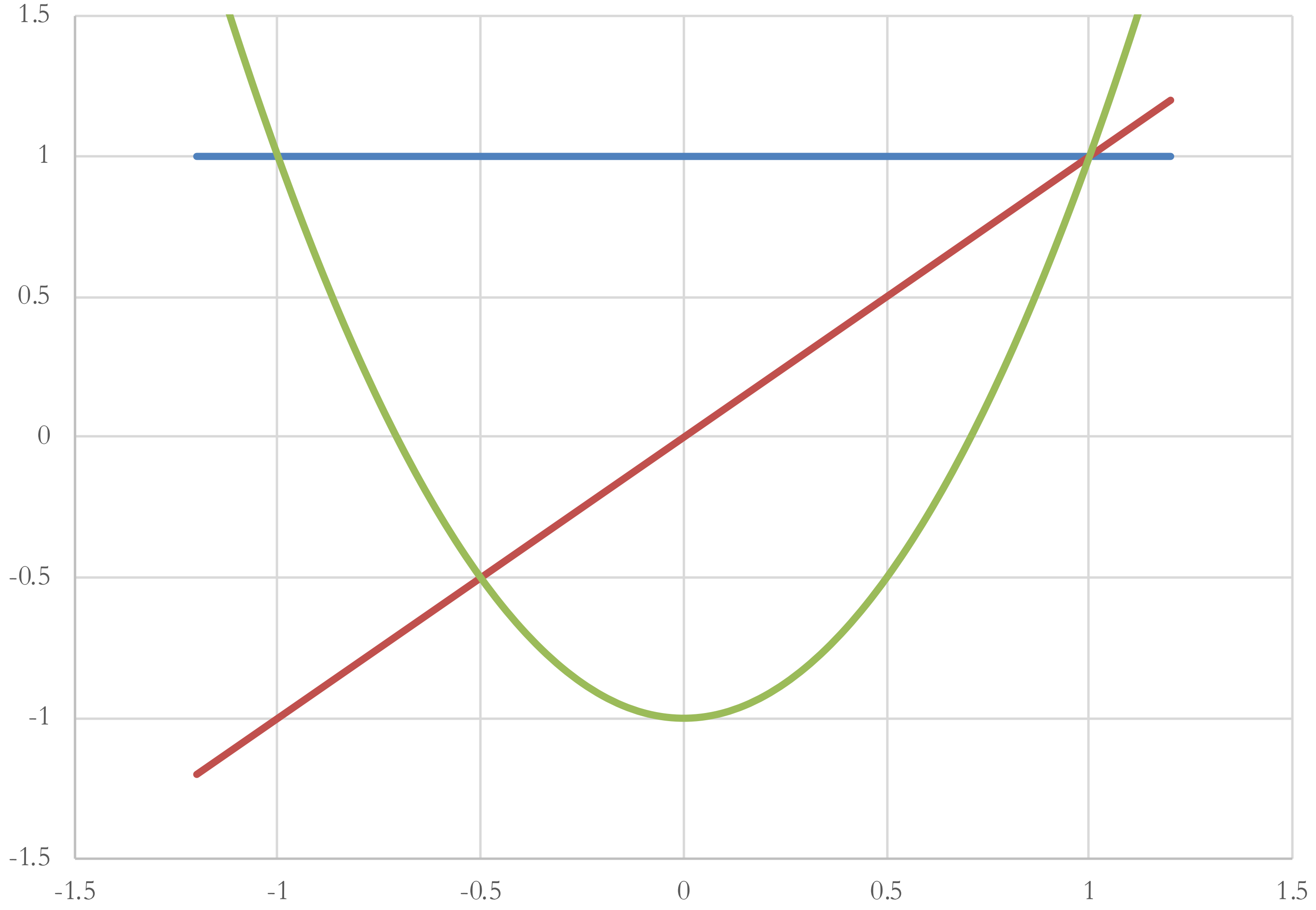
$$T_0(u) = 1$$

Chebyshev Polynomials



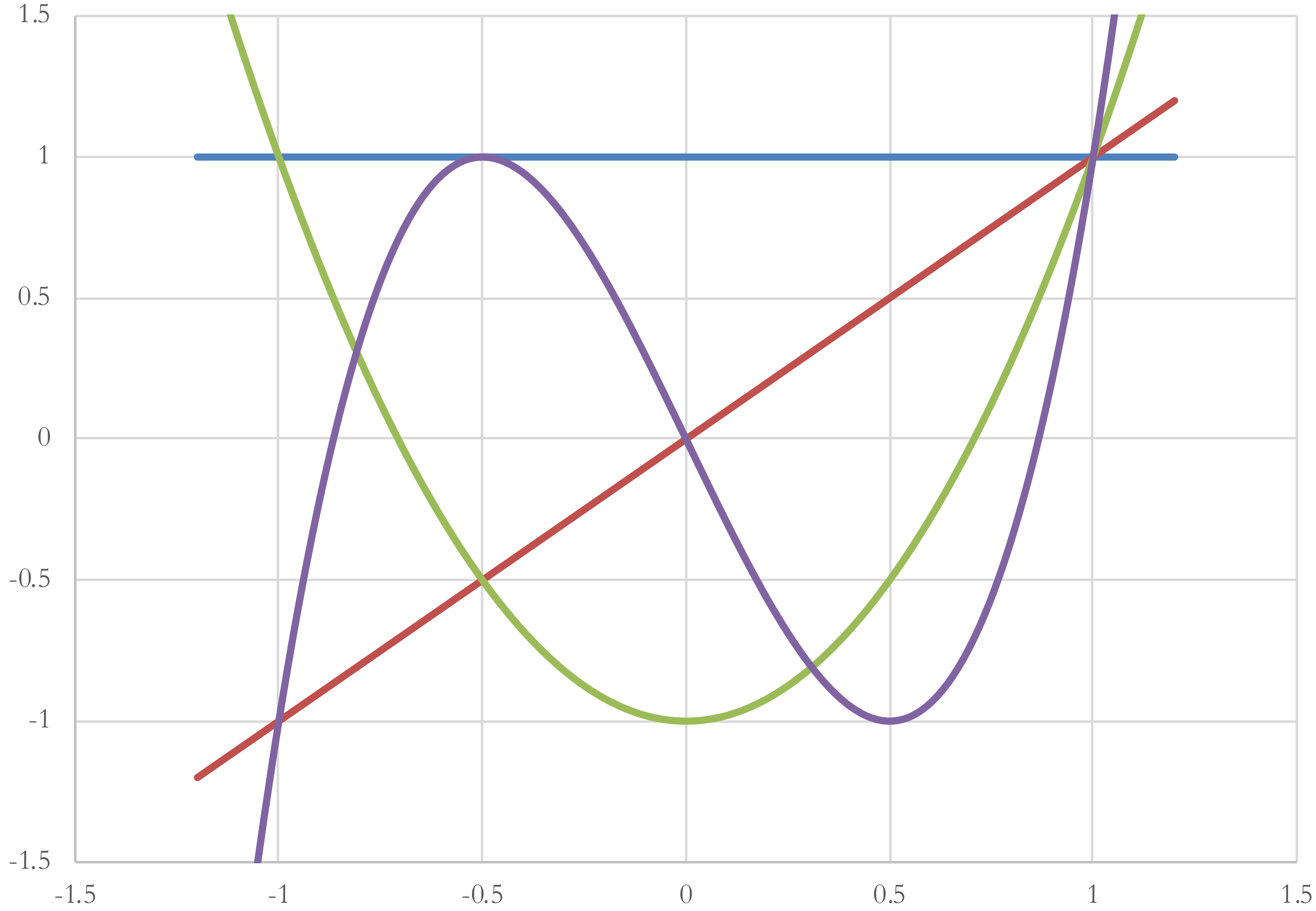
$$T_1(u) = u$$

Chebyshev Polynomials

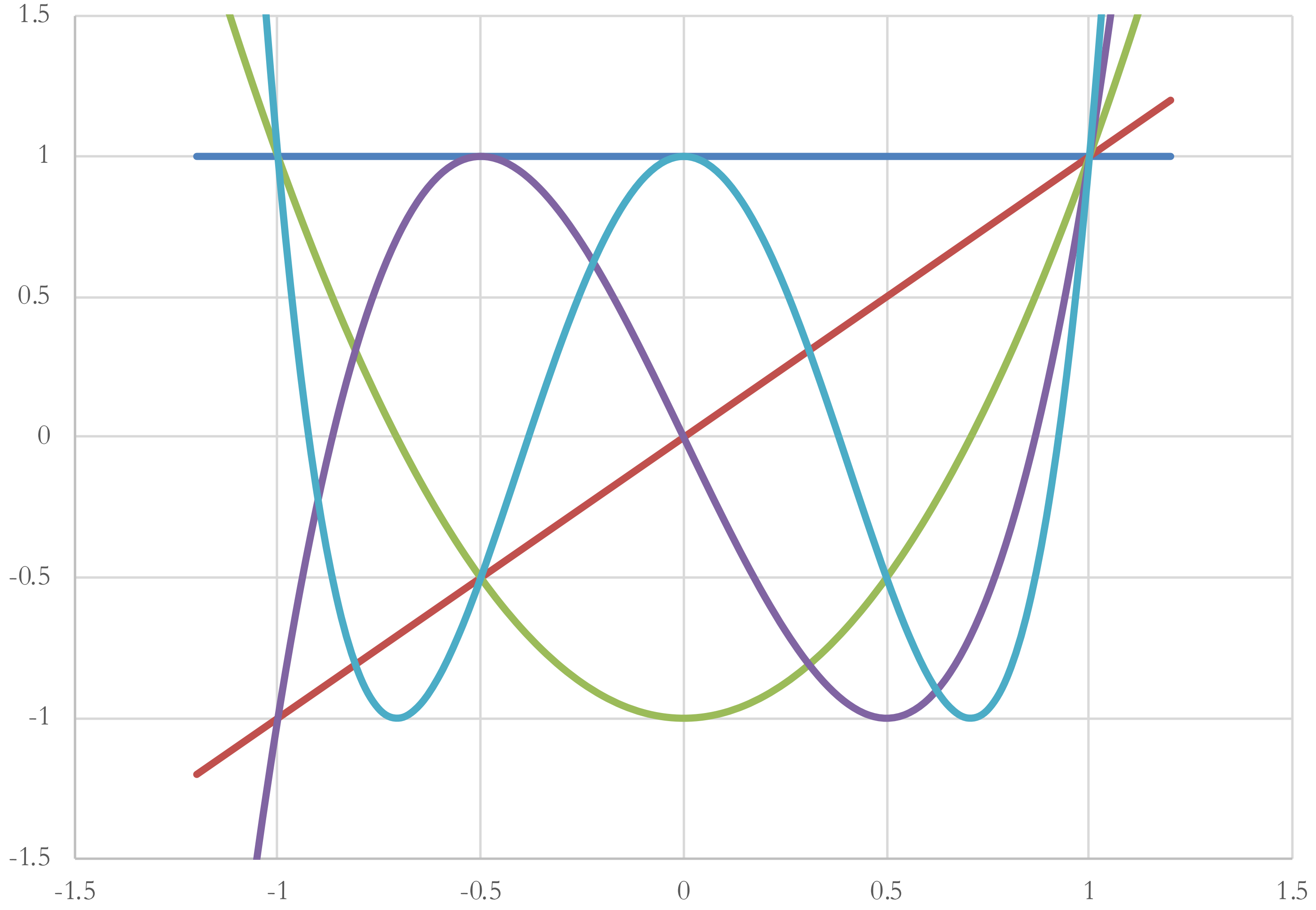


$$T_2(u) = 2u^2 - 1$$

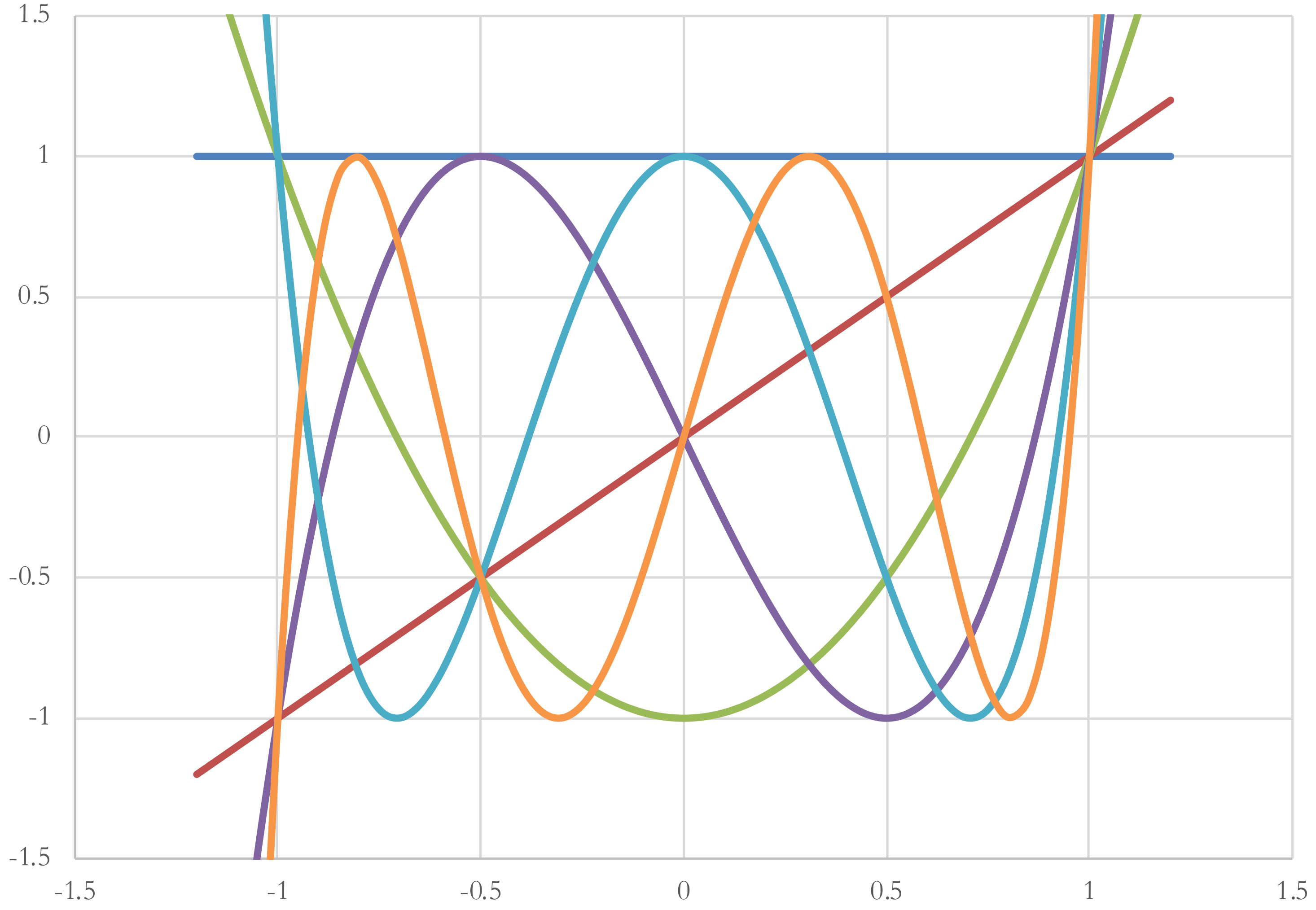
Chebyshev Polynomials



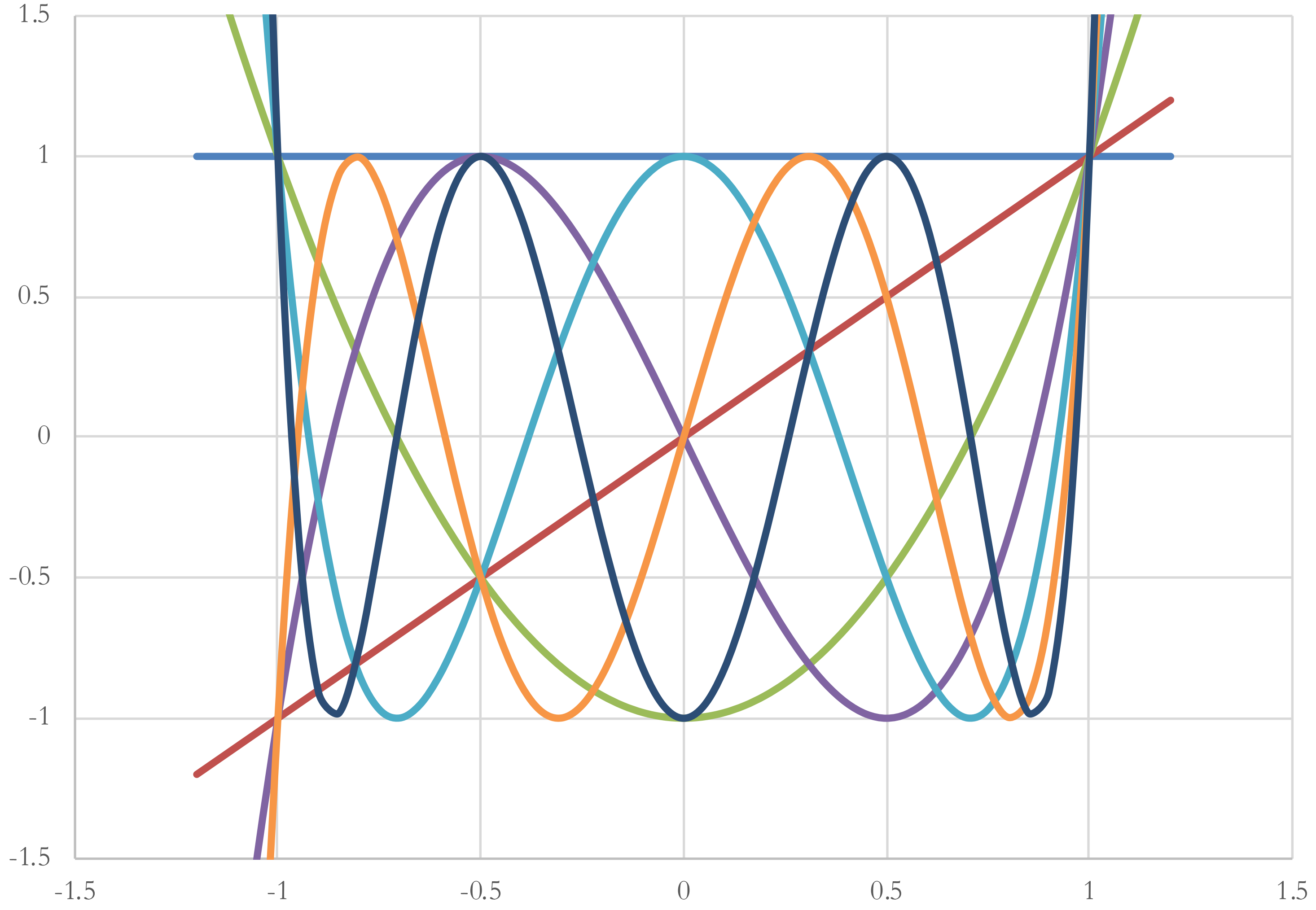
Chebyshev Polynomials



Chebyshev Polynomials



Chebyshev Polynomials



Characterizing momentum (continued)

- What does this mean for our 1D quadratics?
  - Recall that we let $x_t = \beta^{t/2} z_t$

$$x_t = \beta^{t/2} \cdot x_0 \cdot T_t(u)$$
$$= \beta^{t/2} \cdot x_0 \cdot T_t\left(\frac{1+\beta-\alpha\lambda}{2\sqrt{\beta}}\right)$$

- So

$$-1 \leq \frac{1+\beta-\alpha\lambda}{2\sqrt{\beta}} \leq 1 \Rightarrow |x_t| \leq \beta^{t/2} |x_0|$$

Consequences of momentum analysis

- Convergence rate depends **only on momentum parameter β**
  - Not on step size or curvature.

- We **don't need to be that precise in setting the step size**
  - It just needs to be within a window
  - Pointed out in "*YellowFin and the Art of Momentum Tuning*" by Zhang et. al.

- If we have a multidimensional quadratic problem, the **convergence rate will be the same in all directions**
  - This is different from the gradient descent case where we had a trade-off

Choosing the parameters

- How should we **set the step size and momentum parameter** if we only have bounds on λ ?

- Need: $$-1 \leq \frac{1+\beta-\alpha\lambda}{2\sqrt{\beta}} \leq 1$$

- Suffices to have:

$$-1 = \frac{1+\beta-\alpha\lambda_{\max}}{2\sqrt{\beta}} \text{ and } \frac{1+\beta-\alpha\lambda_{\min}}{2\sqrt{\beta}} = 1$$

Choosing the parameters (continued)

- Adding both equations:

$$0 = \frac{2 + 2\beta - \alpha\lambda_{\max} - \alpha\lambda_{\min}}{2\sqrt{\beta}}$$

$$0 = 2 + 2\beta - \alpha\lambda_{\max} - \alpha\lambda_{\min}$$

$$\alpha = \frac{2 + 2\beta}{\lambda_{\max} + \lambda_{\min}}$$

Choosing the parameters (continued)

- Subtracting both equations:

$$\frac{1+\beta-\alpha\lambda_{\min}-1-\beta+\alpha\lambda_{\max}}{2\sqrt{\beta}}=2$$

$$\frac{\alpha(\lambda_{\max}-\lambda_{\min})}{2\sqrt{\beta}}=2$$

Choosing the parameters (continued)

- Combining these results:

$$\alpha = \frac{2 + 2\beta}{\lambda_{\text{max}} + \lambda_{\text{min}}} \qquad \frac{\alpha(\lambda_{\text{max}} - \lambda_{\text{min}})}{2\sqrt{\beta}} = 2$$

$$\frac{2 + 2\beta}{\lambda_{\text{max}} + \lambda_{\text{min}}} \cdot \frac{(\lambda_{\text{max}} - \lambda_{\text{min}})}{2\sqrt{\beta}} = 2$$

$$0 = 1 - 2\sqrt{\beta}\frac{\lambda_{\text{max}} + \lambda_{\text{min}}}{\lambda_{\text{max}} - \lambda_{\text{min}}} + \beta$$

Choosing the parameters (continued)

- Quadratic formula: $$0 = 1 - 2\sqrt{\beta}\frac{\lambda_{\max} + \lambda_{\min}}{\lambda_{\max} - \lambda_{\min}} + \beta$$

$$\begin{aligned}\sqrt{\beta} &= \frac{\kappa+1}{\kappa-1} - \sqrt{\left(\frac{\kappa+1}{\kappa-1}\right)^2 - 1} \\ &= \frac{\kappa+1}{\kappa-1} - \sqrt{\frac{4\kappa}{\kappa^2 - 2\kappa + 1}} \\ &= \frac{\kappa+1}{\kappa-1} - \frac{2\sqrt{\kappa}}{\kappa-1} = \frac{(\sqrt{\kappa}-1)^2}{\kappa-1} = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\end{aligned}$$

Gradient Descent versus Momentum

- Recall: gradient descent had a convergence rate of

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

- But with momentum, the optimal rate is

$$\sqrt{\beta} = \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}$$

- This is called **convergence at an accelerated rate**

Demo

Setting the parameters

- How do we set the momentum in practice for machine learning?

- One method: **hyperparameter optimization**

- Another method: just set $\beta = 0.9$
  - Works across a range of problems
  - Actually quite popular in deep learning

Nesterov momentum

What about more general functions?

- Previous analysis was for quadratics

- Does this work for general convex functions?

- Answer: **not in general**
  - We need to do something slightly different

Nesterov Momentum

- Slightly different rule

$$x_{t+1} = y_t - \alpha \nabla f(y_t)$$
$$y_{t+1} = x_{t+1} + \beta(x_{t+1} - x_t)$$

- Main difference: separate the momentum state from the point that we are calculating the gradient at.

Nesterov Momentum Analysis

- Converges at an accelerated rate **for ANY convex problem**

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

- Optimal assignment of the parameters:

$$\alpha = \frac{1}{\lambda_{\max}}, \ \beta = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}$$

Nesterov Momentum is Also Very Popular

- People use it in practice for deep learning all the time

- Significant speedups in practice

Demo

What about SGD?

- All our above analysis was for **gradient descent**
- But momentum still produces empirical improvements when used with stochastic gradient descent
- And we'll see how in one of the papers we're reading on **Wednesday**

Questions?

- Upcoming things
  - Paper 1 review **due Today**
  - Next paper presentations **on Wednesday**