Large Spikes in SGD: A Large-Deviations View of Catapults

Training loss, non-convexity, and implicit bias

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Based on joint work with D. Heydecker

Roadmap

1. Recap: Supervised learning, overparameterization and implicit bias
2. Recap: Full-batch gradient descent (GD) - deterministic catapults at large learning rates, neural tangent kernen (NTK).
   (Lewkowycz, A., Bahri, Y., Dyer, E., Sohl-Dickstein, J., & Gur-Ari, G. (2020). The large learning rate phase of deep learning: the catapult mechanism. arXiv:2003.02218)
3. Recap: Empirics for catapults in stochastic gradient descent (SGD)
   (Zhu, L., Liu, C., Radhakrishnan, A., & Belkin, M. (ICML 2024). Catapults in SGD: spikes in the training loss and their impact on generalization through feature learning)
4. Main findings:
   1. internal structure of SGD catapult region.
   2. Catapults and curvature decrease
5. Intuition: multiplicative random walk + Cramér exponent.

Supervised learning: data, model, empirical risk

Data. We observe labelled examples

$$\mathcal{S}_m = \{(s_i, y_i)\}_{i=1}^{m}, \qquad s_i \in \mathbb{R}^d, \quad y_i \in \mathbb{R}.$$

The sample is a finite proxy for the unknown population distribution $\mathcal{D}$.

Model. A neural network is a parametrized function

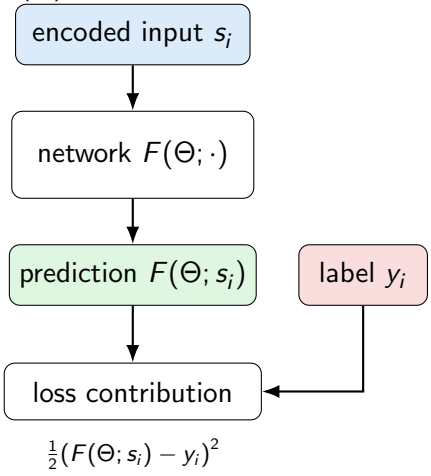
$$F : \mathbb{R}^{2n} \times \mathbb{R}^d \to \mathbb{R}, \qquad (\Theta, s) \mapsto F(\Theta; s),$$

where $\Theta \in \mathbb{R}^{2n}$ denotes the trainable weights.

Training loss. For squared loss, the empirical risk is

$$L(\Theta) = \frac{1}{m} \sum_{i=1}^{m} \big(F(\Theta; s_i) - y_i\big)^2.$$

Learning means moving Θ so that $L(\Theta)$ decreases.



Training is optimization: gradient descent and SGD

Ideal objective. The population loss is

$$\mathcal{L}(\Theta) = \frac{1}{2}\mathbb{E}_{(s,y)\sim\mathcal{D}}\big(F(\Theta; s) - y\big)^2,$$

but $\mathcal{D}$ is unknown, hence $\mathcal{L}$ is not computable.

Empirical loss. For $\mathcal{S}_m = \{(s_i, y_i)\}_{i=1}^m$,

$$L(\Theta) = \frac{1}{m}\sum_{i=1}^{m}\big(F(\Theta; s_i) - y_i\big)^2.$$

How to find Θ? Full-batch gradient descent computes the complete empirical gradient:

$$\Theta_{t+1} = \Theta_t - \eta\nabla L(\Theta_t), \qquad \eta > 0.$$

Practically impossible when m is enormous.

$\eta =$ "learning rate"

Stochastic gradient descent. Choose one index uniformly at random,

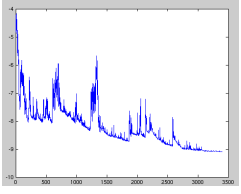
$$i(t+1) \in \{1, \dots, m\}.$$

For the single-sample loss

$$\ell_i(\Theta) = \frac{1}{2}\big(F(\Theta; s_i) - y_i\big)^2, \qquad L(\Theta) = \frac{1}{m}\sum_{i=1}^{m}\ell_i(\Theta).$$

The SGD update is

$$\Theta_{t+1} = \Theta_t - \eta\nabla_\Theta \ell_{i(t+1)}(\Theta_t).$$

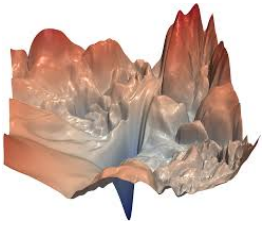


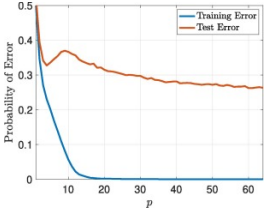
It is an unbiased random estimate of full-batch GD:

$$\mathbb{E}\big[g_t \mid \Theta_t\big] = \nabla L(\Theta_t).$$

Non-convexity and overparameterization

Non-convexity. The empirical loss $L(\Theta)$ is typically non-convex, so optimization can encounter complicated loss landscapes.





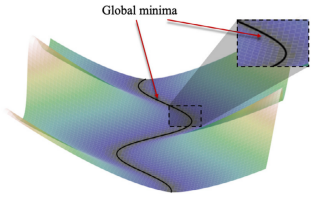
How can this work? Overparameterization and degenerate minima. In the regime $2n \gg m$, there are often many interpolating parameters with

$$F(\Theta; s_i) = y_i, \qquad i = 1, \ldots, m.$$

Hence

$$\mathcal{M} := \{\Theta \in \mathbb{R}^{2n} : L(\Theta) = 0\}$$

form a whole valley (or manifold) of minima rather than a single isolated minimizer.



(b) Loss landscape of over-parameterized models

Empirical risk only a proxy for population loss

$$\mathcal{L}(\Theta) = \frac{1}{2}\mathbb{E}_{(s,y)\sim\mathcal{D}}\big(F(\Theta; s) - y\big)^2,$$

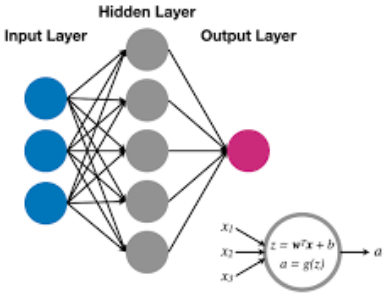
Implicit bias: which point in this degenerate set is selected by GD/SGD?

Recap: Neural tangent kernel (NTK)

Model case, consider one-hidden-layer linear network

$$F(\Theta; s) = \frac{1}{\sqrt{n}} \sum_{r=1}^{n} a_r \, \phi(w_r s), \qquad \Theta = ((w_r, a_r))_{r=1}^{n}.$$

Here n is the width (number of neurons in the hidden layer), $a \in \mathbb{R}^n$ and $w \in \mathbb{R}^n$ are the model parameters (collectively denoted Θ), and $s \in \mathbb{R}$ is the data. At initialization, the weights are drawn from $\mathcal{N}(0, 1)$.



One-sample, one-hidden-layer linear network ($s = 1, y = 0$) with linear activation $\phi(w) = w$: Set new variables

$$\text{prediction } \mu = \frac{1}{\sqrt{n}} a^\top w, \quad L = \tfrac{1}{2}\mu^2, \quad \text{sharpness } \lambda = \frac{1}{n}(\|a\|_2^2 + \|w\|_2^2).$$

Recap: Neural tangent kernel (NTK)

Full-batch GD yields in new variables:

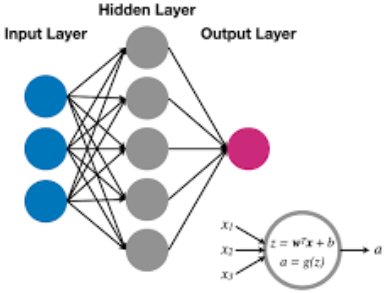
$$\mu(t+1) = \left(1 - \eta\lambda(t) + \eta\frac{\mu^2(t)}{n}\right)\mu(t),$$

$$\lambda(t+1) = \lambda(t) + \eta\frac{\mu^2(t)}{n}(\eta\lambda(t) - 4).$$

Observe: NKT limit (infinite width $n \to \infty$)

$$\mu(t+1) = (1 - \eta\lambda(t))\,\mu(t),$$
$$\lambda(t+1) = \lambda(t).$$

Threshold: $\eta_{\text{crit}} = 2/\lambda_0$.
But also note threshold: $\eta_{\text{max}} = 4/\lambda_0$.

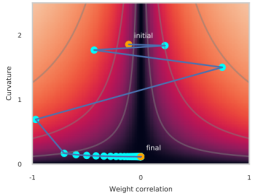


Recap: "catapult mechanism"

Recall

$$\mu(t+1) = \left(1 - \eta\lambda(t) + \eta\frac{\mu^2(t)}{n}\right)\mu(t),$$

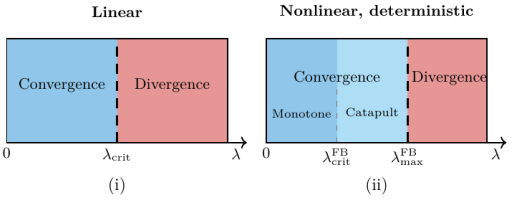
$$\lambda(t+1) = \lambda(t) + \eta\frac{\mu^2(t)}{n}(\eta\lambda(t) - 4).$$



(Source: Lewkowycz et. al. 2020)

Training wide networks with MSE exhibits learning-rate phases determined by the initial curvature scale (top NTK eigenvalue) λ_0:

- **Lazy / NTK phase:** $\eta < 2/\lambda_0$ (linearized dynamics stable).
- **Catapult phase:** $2/\lambda_0 < \eta < 4/\lambda_0$ (loss can rise then converge; curvature collapses).
- **Divergent phase:** $\eta > 4/\lambda_0$.

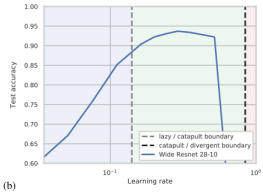


Recap: Catapult mechanism and sharpness

Recall

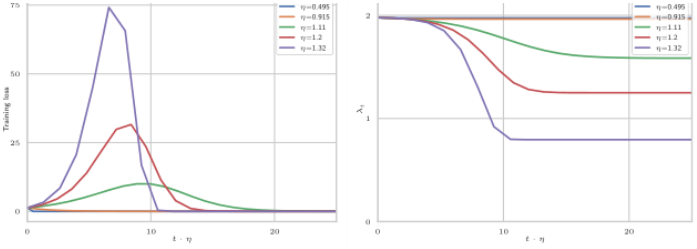
$$\mu(t+1) = \left(1 - \eta\lambda(t) + \eta\frac{\mu^2(t)}{n}\right)\mu(t),$$

$$\lambda(t+1) = \lambda(t) + \eta\frac{\mu^2(t)}{n}(\eta\lambda(t) - 4).$$

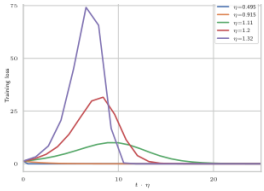


(Source: Lewkowycz et. al. 2020)

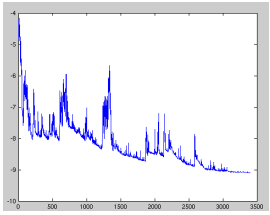
Observe: During spikes sharpness decreases. Large LR can yield a transient loss increase and then better solutions inside a narrow stable window.



Empirical Observation: Spikes in SGD



(Source: Lewkowycz et. al. 2020)



(Source:wikipedia)

Question: Why does SGD exhibit repeated sharp spikes in training loss, while GD shows only a single catapult? Smaller batch $\rightarrow$ higher variance of NTK eigenvalues $\rightarrow$ more frequent violations of

$$\eta < \eta_{\text{crit}}(s_{\text{batch}})$$

Hence:

$$\text{Small batch} \Rightarrow \text{More catapults}$$

Empirically confirmed across FCNs, CNNs, WideResNets, ViTs. (Zhu, Liu, Radhakrishnan, Belkin, 2024)

Model and two scalar state variables (linear activation case)

Shallow NTK-scaled model:

$$F(\Theta; s) = \frac{1}{\sqrt{n}} \sum_{r=1}^{n} a_r \, \phi(w_r s), \qquad \Theta = ((w_r, a_r))_{r=1}^{n}.$$

Dataset $\{(s_i, 0)\}_{i=1}^{m}$ sampled i.i.d. with probabilities $\{p_i\}$ (minibatch size $b = 1$).

For **linear activation** $\phi(w) = w$, define

$$\mu(t) = \frac{1}{\sqrt{n}} \sum_{r=1}^{n} a_r(t) w_r(t), \qquad \lambda(t) = \frac{1}{n} \sum_{r=1}^{n} (a_r(t)^2 + w_r(t)^2).$$

Think: loss $\ell(t) \propto \mu(t)^2$, curvature/NTK scale $\sim \lambda(t)$. Get

$$\mu(t+1) = \left(1 - \eta \lambda(t) s_{i(t+1)}^2 + \frac{\eta^2 s_{i(t+1)}^4 \mu(t)^2}{n}\right) \mu(t);$$

$$\lambda(t+1) = \lambda(t) + \frac{\mu(t)^2 \eta}{n} (\eta \lambda(t) s_{i(t+1)}^4 - 4 s_{i(t+1)}^2).$$

If $\frac{\eta^2 s_{i(t+1)}^4 \mu(t)^2}{n}$, $\frac{\mu(t)^2 \eta}{n} << 1$ then enter linear regime.

Stochastic GD: If

$$\frac{\eta^2 s_{i(t+1)}^4 \mu(t)^2}{n}, \frac{\mu(t)^2 \eta}{n} << 1$$

then

$$\mu(t+1) = \left(1 - \eta\lambda(t) s_{i(t+1)}^2\right) \mu(t);$$
$$\lambda(t+1) = \lambda(t).$$

and $\mu(t)$ approximately evolves by a **multiplicative random walk**:

$$\mu(t+1) \approx \left(1 - \eta\lambda(0) s_{i(t+1)}^2\right) \mu(t)$$
$$= \mu_0 \prod_{u=1}^{t} \left(1 - \eta\lambda_0 s_{i(u)}^2\right)$$
$$\log|\mu(t)| \approx \log|\mu_0| + \sum_{u=1}^{t} \log|1 - \eta\lambda_0 s_{i(u)}^2|$$
$$\approx_{LLN} \log|\mu_0| + t \underbrace{\mathbb{E}_s \log|1 - \eta\lambda_0 s^2|}_{=:G(\lambda_0)}$$

Full batch GD: If

$$\frac{\eta^2 (\mathbb{E}_s s^2)^2 \mu(t)^2}{n}, \frac{\mu(t)^2 \eta}{n} << 1$$

then

$$\mu(t+1) = \left(1 - \eta\lambda(t) \mathbb{E}_s s^2\right) \mu(t);$$
$$\lambda(t+1) = \lambda(t).$$

and

$$\mu(t) \approx \mu_0 \prod_{u=1}^{t} \left(1 - \eta\lambda_0 \mathbb{E}_s s^2\right)$$
$$= \mu_0 \left(1 - \eta\lambda_0 \mathbb{E}_s s^2\right)^t$$
$$\log|\mu(t)| \approx \log|\mu_0| + t \underbrace{\log|1 - \eta\lambda_0 \mathbb{E}_s s^2|}_{=:G_{FB}(\lambda_0)}$$

Related dynamical system perspective: [Chemnitz, Engel, JMLR; 2025]

Stochastic GD:

$$\log|\mu(t)| \approx \log|\mu_0| + t\underbrace{\mathbb{E}_s \log|1-\eta\lambda_0 s^2|}_{=:G(\lambda_0)}$$

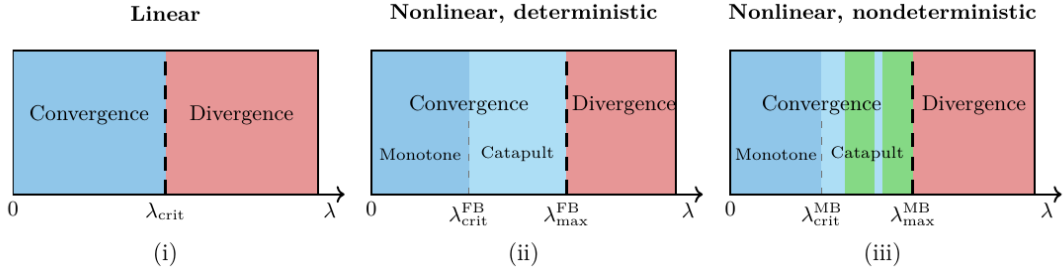
Full batch GD:

$$\log|\mu(t)| \approx \log|\mu_0| + t\underbrace{\log|1-\eta\lambda_0 \mathbb{E}_s s^2|}_{=:G_{FB}(\lambda_0)}$$

Spikes correspond to $|\mu(t)|$ getting large.

- **Inflationary:** $G(\lambda_0) > 0 \Rightarrow$ spikes are typical/guaranteed.
- **Deflationary:** $G(\lambda_0) < 0 \Rightarrow$ spikes are large-deviation events.

Since $\log|\cdot|$ is neither convex nor concave, G and G_{FB} are not comparable.



Example: $G(\lambda)$ can be non-monotone (sign changes)

Consider datapoints

$$\text{i)} \quad \{(s_i, p_i)\} = \{(1, 0.5), (1.3, 0.5)\}$$
$$\text{ii)} \quad \{(s_i, p_i)\} = \{(1, 0.83), (\sqrt{2}, 0.17)\}$$

and recall

$$G(\lambda) := \sum_{i=1}^{m} p_i \log \left|1 - \eta\lambda s_i^2\right|.$$

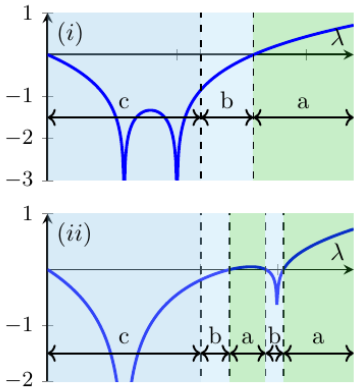


FIGURE 2. Plots of $G(\lambda)$ for the examples (1.17 - 1.18)

Even for two datapoints, $G(\lambda)$ can change sign multiple times: increasing curvature can make spikes *more* or *less* likely (non-monotonicity).

Deflationary regime $G(\lambda_0) < 0$: Large deviations and polynomial spike probability.

Define the **Cramér/LDP exponent**

$$\vartheta(\lambda) := \text{the unique positive root of } \sum_i p_i |1 - \eta\lambda s_i^2|^\theta = 1.$$

Recall: **Deflationary:** $G(\lambda_0) < 0 \Rightarrow$ spikes are rare events, but only *polynomially* rare:

Theorem

In particular, at the medium **spike scale** $M \sim \sqrt{n/\eta}$*: (up to polylogs)*

$$\mathbb{P}(\textit{medium large spike}) \approx (n/\eta)^{-\vartheta(\lambda_0)/2}.$$

Linear regime: $\frac{\eta^2 s_{i(t+1)}^4 \mu(t)^2}{n}$, $\frac{\mu(t)^2 \eta}{n} << 1$

Plot: $\vartheta(\lambda)$ and the resulting probability scale

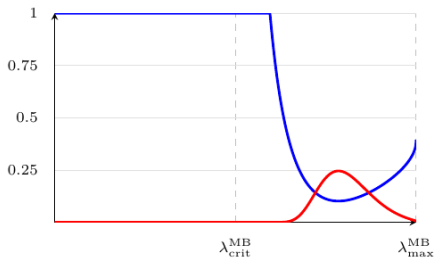


FIGURE 3. $\vartheta(\lambda)$ (blue) and $n^{-\vartheta(\lambda)/2}$ with $n = 10^{12}$ (red) for the dataset (1.26).

Large Spikes and curvature decrease

Assume:

- $\lambda_{MB}^{\text{crit}} < \lambda_0 < \lambda_{MB}^{\max}$
- Moderate spike has reached scale: $M \lesssim \frac{1}{\log^{1/\beta}(n/\eta)} \sqrt{\frac{n}{\eta}}$
- Let $\vartheta(\lambda_0) = \sup\left\{\theta \geq 0 : \sum_{i=1}^{m} p_i \left|1 - \lambda_0 s_i^2\right|^\theta \leq 1\right\} > 0.$

Theorem 5 (Large Spikes)

Conditional on reaching a moderate spike, the probability of a *large spike* that reduces curvature from λ_0 to λ decays at most polynomially:

$$\mathbb{P}(\text{large spike reducing } \lambda_0 \to \lambda) \gtrsim \left(\frac{\sqrt{n/\eta}}{|\mu_0|}\right)^{-\vartheta(\lambda_0)} (\lambda_0 - \lambda)^\alpha$$

Why spikes trigger curvature reduction (the catapult mechanism, stochastic edition)

At spike heights $|\mu(t)| \sim \sqrt{n/\eta}$, curvature updates become $O(1)$:

$$\lambda(t+1) - \lambda(t) = \frac{\eta}{n}\mu(t)^2\big(\eta\lambda(t)s_{i(t+1)}^4 - 4s_{i(t+1)}^2\big).$$

In the minibatch catapult window $\lambda(t) < 4/(\eta s_\star^2)$, for all i,

$$\eta\lambda(t)s_i^4 - 4s_i^2 \le s_i^2(\eta\lambda(t)s_\star^2 - 4) < 0,$$

so a large spike forces $\lambda(t)$ down.

Message: the same geometric story (instability $\Rightarrow$ spike $\Rightarrow$ curvature collapse) persists, but the spike itself may be typical or LDP-rare.

However: In principle, sharpness could also gradually decrease

Summary: catapults in SGD

1. Inside the catapult-capable region, the drift

$$G(\lambda_0) = \sum_i p_i \log|1 - \eta\lambda_0 s_i^2|$$

   splits behavior into inflationary (spikes typical) vs deflationary (spikes LDP-rare).
2. Deflationary spikes remain *polynomially likely*: (large spike) $\approx (n/\eta)^{-\vartheta(\lambda_0)/2}$.
3. Significant curvature reduction without spikes is exponentially unlikely: spikes are the dominant escape mechanism.

Extension: ReLu activation.

References

S. Gess, M. Heydecker, *Large spikes in SGD: a large-deviations view of catapults*, arXiv, 2026.