Welcome to the Zoo: Fast Rates in Statistical and Online Learning

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Statistical Learning

$$\begin{pmatrix} Y_1 \\ \boldsymbol{X}_1 \end{pmatrix}, \dots, \begin{pmatrix} Y_N \\ \boldsymbol{X}_N \end{pmatrix} \qquad \text{independently distributed} \sim P$$

$$\downarrow$$

$$\hat{f} = f_{\hat{\theta}} \in \mathcal{F} = \{f_\theta \mid \theta \in \Theta\} \qquad \text{(estimator inside model)}$$

$$\downarrow$$

Small risk $\quad R(\hat{\theta}) = \mathop{\mathbb{E}}_{(\boldsymbol{X}, Y) \sim P}[\ell(\boldsymbol{X}, Y, \hat{\theta})]$

Compared to minimizer $\theta^* = \arg\min_{\theta \in \Theta} R(\theta)$ of risk

Minimax Rate:

Rate for most difficult possible P

$$\min_{\hat{\theta}} \max_{P} \; \mathbb{E}[R(\hat{\theta})] - R(\theta^*)$$

Classification

Given $\boldsymbol{X} \in \mathbb{R}^d$, predict binary label $Y \in \{0, 1\}$

$$\ell(\boldsymbol{X}, Y, \theta) = \begin{cases} 0 & \text{if } f_\theta(\boldsymbol{X}) = Y, \\ 1 & \text{if } f_\theta(\boldsymbol{X}) \neq Y \end{cases}$$

$$R(\theta) = P(f_\theta(\boldsymbol{X}) \neq Y)$$

Minimax Rate:

For worst-case P, learning is slow:

$$\mathbb{E}[R(\hat{\theta})] - R(\theta^*) \asymp \sqrt{\frac{\text{complexity}_N(\Theta)}{N}}$$

But Faster Rates Are Common

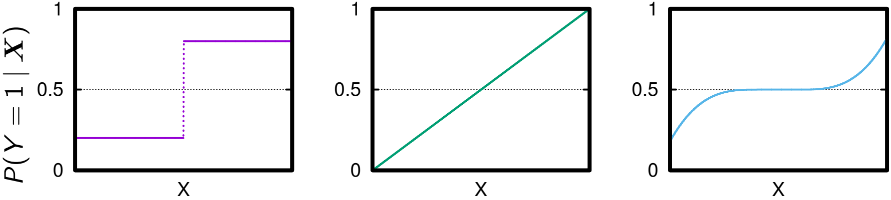
- Worst-case distribution: $P(Y = 1 \mid \boldsymbol{X})$ very close to $\frac{1}{2}$
- But then learning is (almost) useless!

The Margin Condition: [Tsybakov, 2004]

- Common case: $P(Y = 1 \mid \boldsymbol{X})$ not too close to $\frac{1}{2}$
- Assume $f_{\theta^*}(\boldsymbol{X}) = f_{\mathsf{B}}(\boldsymbol{X}) = \arg\max_y P(Y = y \mid \boldsymbol{X})$
- Learning can be much faster depending on $\alpha \in [0, \infty]$:

$$\mathbb{E}[R(\hat{\theta})] - R(\theta^*) = O\left(\frac{\text{complexity}_N(\Theta)}{N}\right)^{\frac{1+\alpha}{2+\alpha}}$$

The Margin Condition



easy $\alpha = \infty$

moderate $\alpha = 1$

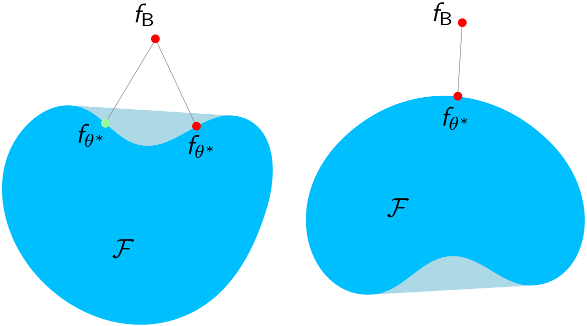
hard $\alpha = 0$

$$P_{\boldsymbol{X}}\left(|P(Y \mid \boldsymbol{X}) - \tfrac{1}{2}| \leq t\right) \leq ct^{\alpha}$$

Fast Rates in Misspecified Regression

Bounded regression: given $\boldsymbol{X} \in \mathbb{R}^d$, predict $Y, f_\theta(\boldsymbol{X}) \in [-B, +B]$

$$\ell(\boldsymbol{X}, Y, \theta) = (Y - f_\theta(\boldsymbol{X}))^2, \qquad f_{\mathrm{B}}(\boldsymbol{X}) = \mathbb{E}[Y \mid \boldsymbol{X}]$$



Non-convex
Projection not unique
Slow rate: $O(\frac{1}{\sqrt{N}})$

Convex
Projection unique
Fast rate: $\tilde{O}(\frac{1}{N})$

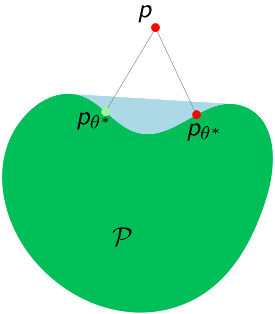
Conclusion: **convex** $\mathcal{F}$ always safe to get fast rates [Lee et al., 1998].

Fast Rates for Misspecified Density Estimation I

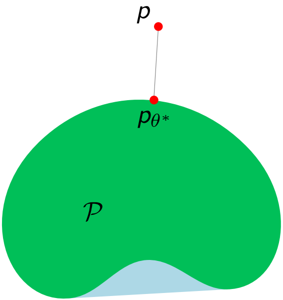
Estimate the best density from $\mathcal{P} = \{p_\theta \mid \theta \in \Theta\}$

$$\ell(Y, \theta) = -\log p_\theta(Y)$$

Assume all densities uniformly bounded: $1/c \leq p_\theta(Y) \leq c$



Non-convex
ERM gets slow rate
depending on P



Convex
ERM gets fast rate:
$\tilde{O}(\frac{\text{complexity}_N(\mathcal{P})}{N})$

Fast Rates for Misspecified Density Estimation II

Fast rates follow from the following supermartingale-like property:

$$\mathop{\mathbb{E}}_{P}\left[\frac{p_\theta}{p_{\theta^*}}\right] \leq 1 \qquad \text{for all } p_\theta \in \mathcal{P}. \tag{1}$$

NB. If $p \in \mathcal{P}$, then $p_{\theta^*} = p$, so $\mathbb{E}_P\left[\frac{p_\theta}{p_{\theta^*}}\right] = 1$.

Lemma ([Li, 1999])

Convexity of $\mathcal{P}$ implies (1).

Proof.

- For arbitrary p_θ, let $p_\lambda = (1-\lambda)p_{\theta^*} + \lambda p_\theta$ and $h(\lambda) = \mathbb{E}[-\log p_\lambda(Y)]$.
- Convexity: h is minimized at $\lambda = 0$, so $0 \leq h'(0) = 1 - \mathbb{E}\left[\frac{p_\theta}{p_{\theta^*}}\right]$.

□

Online Learning

For $t = 1, \dots, T$:

1. Predict parameter vector $\hat{\theta}_t \in \Theta \subset \mathbb{R}^d$
2. Observe outcome $(\boldsymbol{X}_t, Y_t)$ and update $\hat{\theta}_t \to \hat{\theta}_{t+1}$

Goal: achieve small **regret**

$$\text{Regret}_T^{\theta^*} = \sum_{t=1}^{T} \ell(\boldsymbol{X}_t, Y_t, \hat{\theta}_t) - \sum_{t=1}^{T} \ell(\boldsymbol{X}_t, Y_t, \theta^*)$$

with respect to the 'best' parameters $\theta^* \in \Theta$.
Assume losses bounded and convex in θ, and Θ convex with bounded diameter.

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Minimax Rate:

Rate for most difficult possible data:

$$\min_{\hat{\theta}_1} \max_{\boldsymbol{X}_1, Y_1} \min_{\hat{\theta}_2} \max_{\boldsymbol{X}_2, Y_2} \cdots \min_{\hat{\theta}_T} \max_{\boldsymbol{X}_T, Y_T} \max_{\theta^* \in \Theta} \text{Regret}_T^{\theta^*} = O(\sqrt{T})$$

Fast Rates for Exp-concave and Mixable Losses

We can get a much faster $O(\frac{d}{\eta} \log T)$ rate in the following cases:

Exp-concavity:

$$\theta \mapsto e^{-\eta \ell(\boldsymbol{X}_t, Y_t, \theta)} \qquad \text{should be concave.}$$

E.g. logistic loss: $\log(1 + e^{-Y_t \theta^\intercal \boldsymbol{X}_t})$

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Mixability:

Without knowing $\boldsymbol{X}_t, Y_t$, we can map any probability distribution π on Θ to a prediction $\theta_\pi \in \Theta$ such that

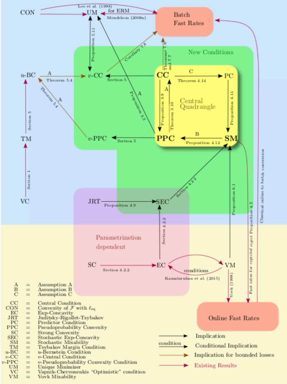
$$e^{-\eta \ell(\boldsymbol{X}_t, Y_t, \theta_\pi)} \geq \int e^{-\eta \ell(\boldsymbol{X}_t, Y_t, \theta)} \mathrm{d}\pi(\theta)$$

- Intuition: allows being unsure
- Exp-concavity is a special case: $\theta_\pi = \mathbb{E}_\pi[\theta]$.

Welcome to the Zoo

How can we understand all these different cases?

- We made a map...
- ...but the zoo is huge and the routes are long.

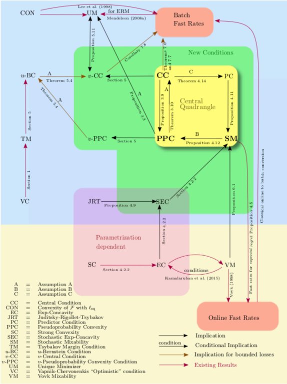


A full map of the zoo [Van Erven, Grünwald, Mehta, Reid, and Williamson, 2015]

Welcome to the Zoo

How can we understand all these different cases?

- We made a map...
- ...but the zoo is huge and the routes are long.
- The summary: for bounded losses, they are all special cases of (more or less) one **central condition**.
- Let me give you a tour.



A full map of the zoo [Van Erven, Grünwald, Mehta, Reid, and Williamson, 2015]

The Central Condition

Central Condition

For some $\eta > 0$,

$$\mathop{\mathbb{E}}_{P}\left[e^{-\eta\left(\ell(\boldsymbol{X},Y,\theta)-\ell(\boldsymbol{X},Y,\theta^*)\right)}\right] \leq 1 \qquad \text{for all } \theta \in \Theta.$$

- Controls the left tail of $\ell(\boldsymbol{X}, Y, \theta) - \ell(\boldsymbol{X}, Y, \theta^*)$.

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Specialize to Density Estimation

- $\ell(Y, \theta) = -\log p_\theta(Y) \leftrightarrow p_\theta(Y) = e^{-\ell(Y,\theta)}$
- For $\eta = 1$, CC specializes to $\mathbb{E}_P\left[\frac{p_\theta(Y)}{p_{\theta^*}(Y)}\right] \leq 1$.
- Convex $\mathcal{P}$: $\min_{\pi(\theta)} \mathbb{E}[-\log \int p_\theta(Y)\,\mathrm{d}\pi(\theta)] = \min_\theta \mathbb{E}[-\log p_\theta(Y)]$.

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Theorem

For general losses, CC is equivalent to **pseudo-probability convexity***:*

$$\min_{\pi(\theta)} \mathbb{E}[-\log \int e^{-\eta\ell(\boldsymbol{X},Y,\theta)}\,\mathrm{d}\pi(\theta)] = \min_\theta \mathbb{E}[-\log e^{-\eta\ell(\boldsymbol{X},Y,\theta)}]$$

Understanding Online Learning Conditions

Mixability

Without knowing $\boldsymbol{X}_t$, Y_t, we can map any probability distribution π on Θ to a prediction $\theta_\pi \in \Theta$ such that

$$e^{-\eta\ell(\boldsymbol{X}_t, Y_t, \theta_\pi)} \geq \int e^{-\eta\ell(\boldsymbol{X}_t, Y_t, \theta)} \mathrm{d}\pi(\theta)$$

$$\ell(\boldsymbol{X}_t, Y_t, \theta_\pi) \leq -\frac{1}{\eta} \log \int e^{-\eta\ell(\boldsymbol{X}_t, Y_t, \theta)} \mathrm{d}\pi(\theta)$$

Stochastic Mixability

Without knowing P, we can map any probability distribution π on Θ to a prediction $\theta_\pi \in \Theta$ such that

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Theorem

Stochastic mixability implies the central condition, and under technical conditions the reverse also holds.

The Technical Conditions...

$$S_\pi(P,\theta) = \mathop{\mathbb{E}}_{(\boldsymbol{X},Y)\sim P,\theta'\sim\pi}\left[e^{\eta(\ell(X,Y,\theta)-\ell(X,Y,\theta'))}\right]$$

Theorem (Detailed)

Stochastic mixability w.r.t. all $P \in \mathcal{P}$ implies the central condition for all $P \in \mathcal{P}$ if, for all π,

$$\sup_{P\in\mathcal{P}} \inf_{\theta\in\Theta} S_\pi(P,\theta) \leq 1 \qquad \Longrightarrow \qquad \inf_{\theta\in\Theta} \sup_{P\in\mathcal{P}} S_\pi(P,\theta) \leq 1. \qquad (*)$$

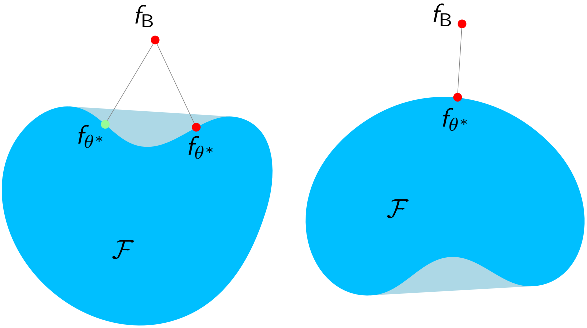
Sufficient Conditions for (*):

1. $\ell(X,Y,\theta)$ continuous in (X,Y) in Polish space
2. $\ell(X,Y,\theta)$ or $e^{\eta\ell(X,Y,\theta)}$ convex in θ
3. $\mathcal{P}$ closed, convex and tight in weak topology
4. $\xi_\theta(X,Y) = \mathbb{E}_{\theta'\sim\pi}\left[e^{\eta(\ell(X,Y,\theta)-\ell(X,Y,\theta'))}\right]$ uniformly integrable over $\theta \in \Theta, P \in \mathcal{P}$.

Understanding Regression

Bounded regression: given $\boldsymbol{X} \in \mathbb{R}^d$, predict $Y, f_\theta(\boldsymbol{X}) \in [-B, +B]$

$$\ell(\boldsymbol{X}, Y, \theta) = (Y - f_\theta(\boldsymbol{X}))^2$$



Proposition

For convex $\mathcal{F}$ parametrized by $\theta = f_\theta$, the squared loss is exp-concave with $\eta \propto 1/B^2$.

exp-concavity $\rightarrow$ mixability $\rightarrow$ stochastic mixability $\rightarrow$ central condition

Another Way to See the Central Condition

Abbreviate $\Delta_\theta = \ell(\boldsymbol{X}, Y, \theta) - \ell(\boldsymbol{X}, Y, \theta^*)$. Then

$$\mathbb{E}[\Delta_\theta] = R(\theta) - R(\theta^*)$$

Central Condition

$$\mathbb{E}[e^{-\eta \Delta_\theta}] \leq 1$$

$(B, 1)$-Bernstein Condition

The closer $R(\theta)$ to $R(\theta^*)$, the smaller the variance:

$$\mathbb{E}[\Delta_\theta^2] \leq B \, \mathbb{E}[\Delta_\theta]$$

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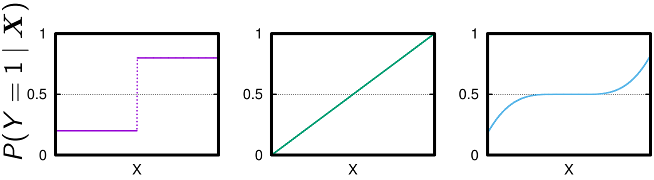
Proposition

For bounded losses, CC and $(B, 1)$-Bernstein are equivalent for $B \propto 1/\eta$.

Proof.

By $e^{-z} \approx 1 - z + \frac{1}{2} z^2$ applied to $z = \eta \Delta_\theta$. □

Understanding Classification



easy — $\alpha = \infty$ | moderate — $\alpha = 1$ | hard — $\alpha = 0$

$$P_{\boldsymbol{X}}\left(|P(Y \mid \boldsymbol{X}) - \tfrac{1}{2}| \leq t\right) \leq ct^{\alpha} \qquad (\alpha\text{-margin})$$

Lemma (Tsybakov)

If $f_B \in \mathcal{F}$. Then, for 0/1-loss, α-margin is equivalent to the **(B, β)-Bernstein condition**:

$$\mathbb{E}[\Delta_\theta^2] \leq B\, \mathbb{E}[\Delta_\theta]^{\beta}$$

with $\beta = \frac{\alpha}{1+\alpha} \in [0, 1]$ and some $B \geq 0$.

Intermediate Rates

Abbreviate $\Delta_\theta = \ell(\boldsymbol{X}, Y, \theta) - \ell(\boldsymbol{X}, Y, \theta^*)$

Generalized Central Condition

For all $\epsilon \geq 0$

$$\mathbb{E}[e^{-\eta_\epsilon \Delta_\theta}] \leq e^{\eta_\epsilon \epsilon}$$

(B, β)-Bernstein Condition

For some $B \geq 0, \beta \in [0, 1]$:

$$\mathbb{E}[\Delta_\theta^2] \leq B\, \mathbb{E}[\Delta_\theta]^\beta$$

Theorem

For bounded losses, generalized CC and (B, β)-Bernstein are equivalent for $\eta_\epsilon \propto \epsilon^{1-\beta}/B$.

Online Learning: Prediction with Expert Advice

Prediction with Expert Advice

- Interpret the components of $\boldsymbol{X}_t \in [0,1]^d$ as predictions of d **experts**, who are predicting $Y_t \in \{0,1\}$.
- Our choice P_θ is a probability distribution on these d experts
- $\ell(\boldsymbol{X}_t, Y_t, \theta) = |Y_t - \mathbb{E}_{P_\theta(i)}[X_{t,i}]| = \mathbb{E}_{P_\theta(i)}[|Y_t - X_{t,i}|]$

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Suppose i.i.d. expert losses...

- Suppose $|Y_t - X_{t,i}|$ are i.i.d. with mean $\mu_i = \mathbb{E}_{\boldsymbol{X}_t, Y_t}[|Y_t - X_{t,i}|]$.
- Let $i^* = \arg\min_i \mu_i$.

Proposition ([Koolen, Grünwald, and van Erven, 2016])

Then the $(B,1)$-Bernstein condition is satisfied with

$$B = \min_{i \neq i^*} \frac{\mathbb{E}_{Y_t, X_{t,i}}[(|Y_t - X_{t,i}| - |Y_t - X_{t,i^*}|)^2]}{\mu_i - \mu_{i^*}}$$

Achieving Fast Rates in Prediction with Expert Advice

Theorem ([Koolen, Grünwald, and van Erven, 2016])

If the (B, β)-Bernstein condition is satisfied for **prediction with expert advice**, *then the* **Squint** *algorithm [Koolen and van Erven, 2015] achieves (pseudo)-regret*

$$\mathbb{E}[\mathrm{Regret}_T^{i^*}] = O\big((B \log d)^{\frac{1}{2-\beta}}\, T^{\frac{1-\beta}{2-\beta}}\big)$$

$$\mathrm{Regret}_T^{i^*} = O\big((B \log d - \log \delta)^{\frac{1}{2-\beta}}\, T^{\frac{1-\beta}{2-\beta}}\big) \qquad w.p. \geq 1 - \delta$$

w.r.t. $i^* = \arg\min_i \mu_i$.

Bernstein Condition for General Online Learning

Linearizing Losses

In online learning it is common to perform linear approximations of the loss:

$$\tilde{\ell}(\boldsymbol{X}_t, Y_t, \theta) = \ell(\boldsymbol{X}_t, Y_t, \theta_t) + (\theta - \theta_t)^\intercal \nabla_\theta \ell(\boldsymbol{X}_t, Y_t, \theta_t),$$

which overestimates the regret.

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which overestimates the regret.

Hinge Loss

- Suppose (X_t, Y_t) are i.i.d., and let $\theta, \boldsymbol{X}_t$ in the d-dimensional unit ball
- Hinge loss: $\ell(\boldsymbol{X}_t, Y_t, \theta) = \max\{Y_t - \theta^\intercal \boldsymbol{X}_t, 0\}$

Theorem ([Koolen, Grünwald, and van Erven, 2016])

Then the $(B, 1)$-Bernstein condition is satisfied for $\tilde{\ell}$ with

$$B = \frac{2\lambda_{max}(\mathbb{E}[\boldsymbol{X}\boldsymbol{X}^\intercal])}{\|\mathbb{E}[Y\boldsymbol{X}]\|}$$

Achieving Fast Rates in General Online Learning

Theorem ([Koolen, Grünwald, and van Erven, 2016])

If the (B, β)-Bernstein condition is satisfied for $\tilde{\ell}$ in general **online learning***, then the* **MetaGrad** *algorithm [Van Erven and Koolen, 2016] achieves (pseudo)-regret*

$$\mathbb{E}[\mathrm{Regret}_T^{\theta^*}] = O\big((Bd \log T)^{\frac{1}{2-\beta}} \, T^{\frac{1-\beta}{2-\beta}}\big)$$

$$\mathbb{E}[\mathrm{Regret}_T^{\theta^*}] = O\big((Bd \log T - \log \delta)^{\frac{1}{2-\beta}} \, T^{\frac{1-\beta}{2-\beta}}\big) \qquad \textit{w.p. } \geq 1 - \delta$$

w.r.t. $\theta^* = \arg\min_{\theta \in \Theta} \mathbb{E}[\ell(\boldsymbol{X}, Y, \theta)]$.

Achieving Fast Rates in Statistical Learning

- Simplest example: **prior π** on **countable model** $\Theta = \{\theta_1, \theta_2, \ldots\}$.
- **Penalized ERM** $\hat{\theta}$ minimizes

$$\sum_{i=1}^{N} \ell(\boldsymbol{X}_i, Y_i, \theta) + \lambda \log \frac{1}{\pi(\theta)}$$

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Proposition (Bernstein Condition Rate)

Under (B, β)-Bernstein condition, bounded loss, $\lambda = \left(\frac{N}{B \log \frac{1}{\pi(\theta^*)}}\right)^{\frac{1-\beta}{2-\beta}}$ *achieves*

$$R(\hat{\theta}) - R(\theta^*) = O\left(\frac{B \log \frac{1}{\delta \pi(\theta^*)}}{N}\right)^{\frac{1}{2-\beta}} \qquad \text{w.p.} \geq 1 - \delta.$$

Achieving Fast Rates in Statistical Learning

- Simplest example: **prior** π on **countable model** $\Theta = \{\theta_1, \theta_2, \ldots\}$.
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- **Simple approach**: estimate λ using cross-validation
- Or **sophisticated approaches**:
  - Slope heuristic (Birgé, Massart)
  - Lepski's method
  - Safe Bayes (Grünwald)

Summary

Conditions for fast rates **all the same or closely related:**

- **Central Condition**: density estimation
- Pseudo-probability convexity: convex set of pseudo-probabilities
- Stochastic mixability (stronger): bounded squared loss (convex model)
- Bernstein Condition: classification
- Bernstein for Online Learning: gap in prediction with expert advice, hinge loss

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Achieving these **fast rates**:

- In statistical learning: use **cross-validation** to select regularization parameter
- In online learning: **Squint** (experts), **MetaGrad** (general online learning)

Papers

- Van Erven, Grünwald, Mehta, Reid, Williamson. **Fast Rates in Statistical and Online Learning.** Journal of Machine Learning Research, 2015. (Special issue dedicated to the memory of Alexey Chervonenkis.)
- Koolen, Grünwald, Van Erven. **Combining adversarial guarantees and stochastic fast rates in online learning.** In Advances in Neural Information Processing Systems 29 (NIPS), pages 4457–4465, 2016.

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