

Today

1. Complexity

- Individual Sequence Prediction with Log-Loss: the NML distribution and Complexity
- Extending the Right-Hand Side of Zhang's Bound

2. Safe Probability, Safe Statistics

Three Complexity Notions

- Shtarkov or NML Complexity
 - central notion in **nonstochastic log-loss** individual sequence prediction.
- PAC-Bayesian Complexity
 - right-hand side in a strong **excess risk bound** in (**stochastic**) statistical learning for **arbitrary loss** fns
 - especially suited for (pseudo-) Bayesian methods but **not for very large classes**
- Rademacher Complexity
 - right-hand side in stochastic excess risk bound that deals well with large classes but **not with log-loss and priors**

The Shtarkov/MDL Complexity

- **Minimax Cumulative Regret for Individual Sequence Prediction with Log Loss** (Shtarkov '88, Rissanen '96), also known as **Shtarkov complexity** or **MDL/stochastic complexity**:

$$\mathcal{M} = \{P_\theta : \theta \in \Theta\}$$

$$\text{comp}_n(\mathcal{M}) = \log \sum_{y^n \in \mathcal{Y}^n} p_{\hat{\theta}(y^n)}(y^n)$$

On-Line “Probabilistic” Prediction

- Consider sequence y_1, y_2, \dots , all $y_i \in \mathcal{Y}$
- **Goal:** sequentially predict y_i given past $y^{i-1} = y_1, \dots, y_{i-1}$ using a ‘probabilistic prediction’ P_i (distribution on \mathcal{Y})
- prediction strategy S is function mapping, for all i , ‘histories’ y_1, \dots, y_{i-1} to distributions for i -th outcome

$$S : \cup_{n=1}^{\infty} \mathcal{Y}^n \rightarrow \text{set of distributions on } \mathcal{Y}$$

prediction strategy = distribution

- If we think that $Y_1, \dots, Y_n \sim P$ (not necessarily i.i.d !)
then should predict Y_i using conditional distribution

$$P(\cdot | y^{i-1}) := P(Y_i = \cdot | Y_1 = y_1, \dots, Y_{i-1} = y_{i-1})$$

- note that then joint probability mass/density is equal to the product of the predictions:

$$P(y^n) = \prod_{i=1}^n P(y_i | y^{i-1})$$

prediction strategy = distribution

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- note that then joint probability mass/density is equal to the product of the predictions: $P(y^n) = \prod_{i=1}^n P(y_i | y^{i-1})$

Conversely, **every** prediction strategy S may be thought of as a distribution on (Y_1, \dots, Y_n) , by defining:

$$P(\cdot | y^{i-1}) := S(y^{i-1})$$

$$P(y_1, \dots, y_n) := \prod_{i=1}^n P(y_i | y^{i-1})$$

Logarithmic Loss

- To compare **performance** of different prediction strategies, we need a measure of prediction quality
- One popular measure of quality is the **log loss**:

$$\text{loss}(y, P) := -\log_2 P(y)$$

$$\text{loss}(y_1 \dots, y_n, S) := \sum_{i=1}^n \text{loss}(y_i, S(y_1, \dots, y_{i-1}))$$

- corresponds to two important practical settings:
 - **data compression**: $\text{loss}(y_1 \dots, y_n, S)$ is number of bits needed to encode y_1, \dots, y_n using **code** S
 - **'Kelly' gambling**: $\text{loss} = \log$ capital growth factor

Log loss & likelihood

- For every “prediction strategy” P , all n ,

$$\sum_{i=1}^n \text{loss}(y_i, P(\cdot | y^{i-1})) = \sum_{i=1}^n -\log P(y_i | y^{i-1}) = -\log P(y_1, \dots, y_n)$$



$$\sum_{i=1}^n -\log P(y_i | y^{i-1}) = -\log \prod_{i=1}^n P(y_i | y^{i-1}) = -\log \prod \frac{P(y_i)}{P(y^{i-1})} = -\log P(y_1, \dots, y_n)$$

Log loss & likelihood

- For every “prediction strategy” P , all n ,

$$\sum_{i=1}^n \text{loss}(y_i, P(\cdot | y^{i-1})) = \sum_{i=1}^n -\log P(y_i | y^{i-1}) = -\log P(y_1, \dots, y_n)$$

- **Accumulated log loss = minus log likelihood**

Dawid '84, Rissanen '84

Universal Prediction

- Let $\mathcal{M} = \{P_\theta : \theta \in \Theta\}$ be a set of predictors (identified with probability distributions on \mathcal{Y}^∞)
 - Simplest example: \mathcal{M} is the Bernoulli model
 - Nonparametric example: \mathcal{Y} is unit interval, \mathcal{M} is set of all monotonically decreasing probability densities
- GOAL: given \mathcal{M} , construct a new predictor predicting data 'almost as well' as any of the $P_\theta \in \mathcal{M}$ *no matter what data arrive* (a nonstochastic setting!)

Universal Prediction

- More concretely: find, for fixed n , the predictor P achieving the **minimax cumulative log-loss regret**

$$\min_P \left\{ \sup_{y^n \in \mathcal{Y}^n} \left(\text{loss}(y^n, P) - \left[\inf_{\theta \in \Theta} \text{loss}(y^n, P_\theta) \right] \right) \right\}$$

where $\text{loss}(y^n, Q) = \sum_{i=1}^n -\log Q(y_i | y^{i-1})$

- Solution was given by Shtarkov in 1988 (!)

Universal Prediction

- More concretely: find, for fixed n , the predictor P achieving the **minimax cumulative log-loss regret**

$$\begin{aligned} & \min_P \left\{ \sup_{y^n \in \mathcal{Y}^n} \left(\text{loss}(y^n, P) - \left[\inf_{\theta \in \Theta} \text{loss}(y^n, P_\theta) \right] \right) \right\} \\ &= \min_P \left\{ \sup_{y^n \in \mathcal{Y}^n} \left(-\log P(y^n) - \left[\inf_{\theta \in \Theta} -\log P_\theta(y^n) \right] \right) \right\} \\ &= \min_P \left\{ \sup_{y^n \in \mathcal{Y}^n} \left(-\log P(y^n) + \log P_{\hat{\theta}(y^n)}(y^n) \right) \right\} \end{aligned}$$

Universal Prediction

$$\min_P \left\{ \sup_{y^n \in \mathcal{Y}^n} \left(-\log P(y^n) + \log P_{\hat{\theta}(y^n)}(y^n) \right) \right\}$$

- uniquely achieved* by **Shtarkov** or **NML** (Normalized Maximum Likelihood) Distribution, given by

$$P_{\text{nml}}(y^n) = \frac{P_{\hat{\theta}(y^n)}(y^n)}{\sum_{y^n \in \mathcal{Y}^n} P_{\hat{\theta}(y^n)}(y^n)}$$

- ...and its regret satisfies, for all $y^n \in \mathcal{Y}^n$,

$$-\log P_{\text{nml}}(y^n) - [-\log P_{\hat{\theta}(y^n)}(y^n)] = \text{comp}_n(\mathcal{M}) = \log \sum_{y^n \in \mathcal{Y}^n} p_{\hat{\theta}y^n}(y^n)$$

Complexity for Parametric Models

- So $\text{comp}_n(\mathcal{M}) = \log \sum_{y^n \in \mathcal{Y}^n} p_{\hat{\theta}(y^n)}(y^n)$

is cumulative minimax regret relative to model \mathcal{M}

For d -dimensional exponential families with bounded density ratios (Rissanen '96, G. '07),

$$\text{comp}_n(\mathcal{M}) = \frac{d}{2} \log \frac{n}{2\pi} + \log \int \sqrt{\det I(\theta)} + o(1) = O(\log n)$$

Complexity for Parametric Models

$$\text{comp}_n(\mathcal{M}) = \frac{d}{2} \log \frac{n}{2\pi} + \log \int \sqrt{\det I(\theta)} + o(1) = O(\log n)$$

...whereas the Bayesian marginal likelihood

$$P_{\text{Bayes}}(y^n) = \int P_{\theta}(y^n) w(\theta) d\theta$$

is known to satisfy*

$$-\log P_{\text{Bayes}}(y^n) - [-\log P_{\hat{\theta}(y^n)}(y^n)] =$$

$$\frac{d}{2} \log \frac{n}{2\pi} - \log w(\theta) + \log \sqrt{\det I(\theta)} + o(1) = O(\log n)$$

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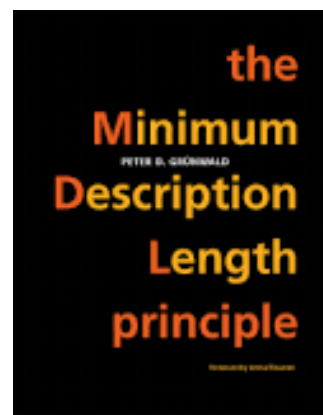
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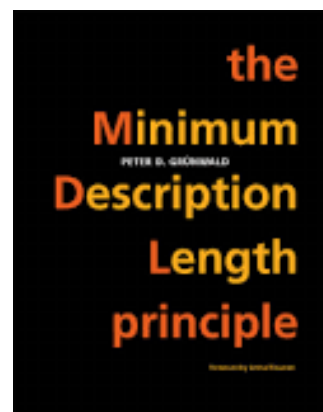
$$\frac{d}{2} \log \frac{n}{2\pi} - \log w(\theta) + \log \sqrt{\det I(\theta)} + o(1) = O(\log n)$$

for **Jeffreys' prior**, $w(\theta) \propto \sqrt{\det I(\theta)}$ asymptotically same!

Aside

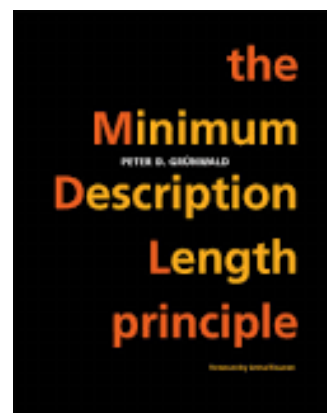


- In its simplest form, the MDL Principle (Rissanen, '89) states that to compare 2 statistical models $\mathcal{M}_0, \mathcal{M}_1$ for the same data, one should associate them both with a lossless universal code (i.e. a code that gives small codelengths whenever 'the model fits the data well' ...)
- ... and then pick the model which allows for the shortest codelength of the data
- A lossless code is just a sequential log-loss prediction strategy... It is a good universal code if it has small regret



Aside

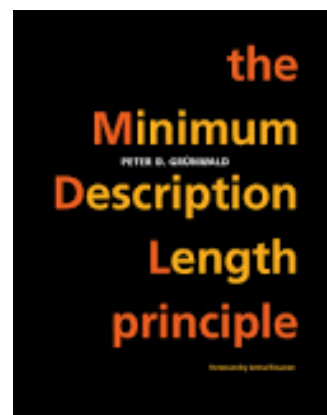
- pick the model \mathcal{M}_j which allows for shortest codelength of data if encoded with good universal code
- A lossless code is just a sequential log-loss prediction strategy... it is a good universal code if it has small regret
- i.e. MDL tells you to pick \mathcal{M}_1 with 'confidence' $K > 0$ iff
$$-\log P_{\text{nml}}(y^n | \mathcal{M}_1) - (-\log P_{\text{nml}}(y^n | \mathcal{M}_0)) \leq -K$$



Aside

- pick the model \mathcal{M}_j which allows for shortest codelength of data if encoded with good universal code
- A lossless code is just a sequential log-loss prediction strategy... it is a good universal code if it has small regret
- i.e. MDL tells you to pick \mathcal{M}_1 with 'confidence' $K > 0$ iff
$$-\log P_{\text{nml}}(y^n | \mathcal{M}_1) - (-\log P_{\text{nml}}(y^n | \mathcal{M}_0)) \leq -K$$

$$\text{i.e. } \frac{P_{\text{nml}}(y^n | \mathcal{M}_1)}{P_{\text{nml}}(y^n | \mathcal{M}_0)} \geq 2^K$$



Aside

- pick \mathcal{M}_1 with 'confidence' $K > 0$ iff

$$S = \frac{P_{\text{nml}}(y^n | \mathcal{M}_1)}{P_{\text{nml}}(y^n | \mathcal{M}_0)} \geq 2^K$$

- If null model is simple, then S is an S-value ($\mathbf{E}[S] \leq 1$)
- ... More generally, one also allows ratios of other P 's that correspond to codes with small regret, such as Bayesian, 'prequential', 'switch'
- Ryabko & Monarev:

$$S = \frac{P_{\text{gzip}}(y^n)}{P_0(y^n)}$$

Complexity for Parametric Models

$$\text{comp}_n(\mathcal{M}) = \frac{d}{2} \log \frac{n}{2\pi} + \log \int \sqrt{\det I(\theta)} + o(1) = O(\log n)$$

...whereas the Bayesian marginal likelihood

$$P_{\text{Bayes}}(y^n) = \int P_{\theta}(y^n) w(\theta) d\theta$$

is known to satisfy*

$$-\log P_{\text{Bayes}}(y^n) - [-\log P_{\hat{\theta}(y^n)}(y^n)] =$$

$$\frac{d}{2} \log \frac{n}{2\pi} - \log w(\theta) + \log \sqrt{\det I(\theta)} + o(1) = O(\log n)$$

for **Jeffreys' prior**, $w(\theta) \propto \sqrt{\det I(\theta)}$ asymptotically same!

Nonparametric Models

- Opper & Haussler ('96), Cesa-Bianchi & Lugosi ('01) and more recently Rakhlin and Sridharan ('15) gave bounds using chaining based on L_∞ -covering nrs:

$$\text{comp}_n(\mathcal{M}) \leq \inf_{\epsilon > 0} \log N_\infty(\mathcal{M}, \epsilon) + 24 \int_0^\epsilon \sqrt{\log N_\infty(\mathcal{M}, \delta)} d\delta$$

- If the model is i.i.d., then $N_\infty(\mathcal{M}, \epsilon)$ is ϵ -covering nr under metric $d(P, Q) = \sup_{y \in \mathcal{Y}} | -\log P(Y) + \log Q(Y) |$

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- With this bound they obtained for variety of nonparametric models $\text{comp}_n(\mathcal{M}) = O(n^\gamma)$

Two Observations

$$\text{comp}_n(\mathcal{M}) \leq \inf_{\epsilon > 0} \log N_\infty(\mathcal{M}, \epsilon) + 24 \int_0^\epsilon \sqrt{\log N_\infty(\mathcal{M}, \delta)} d\delta$$

- Bound is often **better** than best regret bound that can be given for prediction by Bayes marginal likelihood (n^γ vs. n^β for $\beta > \gamma$)
 - ...and for some models it is indeed known that Bayesian prediction has larger worst-case regret
- ...yet bound is **void** if $N_\infty(\mathcal{M}, \epsilon) = \infty$

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$$\text{comp}_n(\mathcal{M}) \leq \inf_{\epsilon > 0} \log N_\infty(\mathcal{M}, \epsilon) + 24 \int_0^\epsilon \sqrt{\log N_\infty(\mathcal{M}, \delta)} d\delta$$

1. Bound is often **better** than best regret bound that can be given for prediction by Bayes marginal likelihood (n^γ vs. n^β for $\beta > \gamma$)
 - ...and for some \mathcal{M} it is indeed known that Bayesian prediction has larger worst-case regret
2. ...yet bound is **void** if $N_\infty(\mathcal{M}, \epsilon) = \infty$
 - Take e.g. \mathcal{M} to be all i.i.d. extensions of monotonically decreasing densities (bounded away from 0 and ∞) on unit interval

Two Complexity Notions, Two Results

- Shtarkov or NML Complexity
 - central notion in log-loss individual sequence prediction. Existing bounds are in terms of L_∞ -entropy nrs; we have bound in terms of $L_{1/2}(P)$ nrs.
- PAC-**Bayesian** Complexity
 - right-hand side in a strong excess risk bound in (**stochastic**) statistical learning for arbitrary loss fns; **not suited for very large classes**. We will unify with Shtarkov Complexity and thus make bound suitable for large classes.

Zhang's Excess Risk Bound

For every learning algorithm $\hat{\Pi}_n := \hat{\Pi}|Z^n$ that outputs a **distribution** on model \mathcal{F} , every 'prior' Π_0 every $\eta > 0$:

$$\mathbf{E}_{f \sim \hat{\Pi}_n} \mathbf{E}_{Z \sim P}^{\text{ann}, \eta} [r_f(Z)] \leq_{\eta n} \mathbf{E}_{f \sim \hat{\Pi}_n} \left[\frac{1}{n} \sum_{i=1}^n r_f(Z_i) \right] + \frac{\text{KL}(\hat{\Pi}_n \| \Pi_0)}{\eta \cdot n}$$

- G. & Mehta 2016 mostly about extending the left-hand side
- **TODAY: G. & Mehta 2017a; mostly about the right-hand side**

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$r_f(Z) := \ell_f(Z) - \ell_{f^*}(Z)$ is excess loss on Z

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$r_f(Z) := \ell_f(Z) - \ell_{f^*}(Z)$ is excess loss on Z

ℓ can be any loss function

e.g. $Z = (X, Y)$, $\ell_f((X, Y)) = |Y - f(X)|$ (0/1-loss)

$Z = (X, Y)$, $\ell_f((X, Y)) = (Y - f(X))^2$ (sq. Err. loss)

$\ell_f(Z) = -\log p_f(Z)$ (log loss)

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$r_f(Z) := \ell_f(Z) - \ell_{f^*}(Z)$ is excess loss on Z

ℓ can be any loss function (0/1, square, log-loss, ...)

f^* is risk minimizer in \mathcal{F} :

$$f^* := \arg \min_{f \in \mathcal{F}} \mathbf{E}_{Z \sim P} [\ell_f(Z)]$$

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where $p'_{f, \eta}(z) = p(z) \cdot e^{-\eta r_f(z)} = p(z) \cdot e^{-\eta(\ell_f(z) - \ell_f^*(z))}$
 are the 'entropified' probabilities we discussed earlier

Zhang's Excess Risk Bound

For every 'prior' Π_0 , every $0 < \eta$, for the **generalized η -Bayesian posterior**, every 'prior' Π_0 every $\eta > 0$:

$$\mathbf{E}_{f \sim \hat{\Pi}_n} \mathbf{E}_{Z \sim P}^{\text{ann}, \eta} [r_f(Z)] \leq_{\eta n} C_\eta \cdot \left(\mathbf{E}_{f \sim \hat{\Pi}_n} \left[\frac{1}{n} \sum_{i=1}^n r_f(Z_i) \right] + \frac{\text{KL}(\hat{\Pi}_n \| \Pi_0)}{\eta \cdot n} \right) - \frac{1}{\eta \cdot n} \cdot \log \frac{\int_{\mathcal{F}} p'_{f, \eta}(Z^n) d\Pi_0(f)}{p'_{f^*, \eta}(Z^n)}$$

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Insight: excess risk bound in terms of the cumulative log-loss of a Bayesian prediction strategy

Two Observations

$$\text{comp}_n(\mathcal{M}) \leq \inf_{\epsilon > 0} \log N_\infty(\mathcal{M}, \epsilon) + 24 \int_0^\epsilon \sqrt{\log N_\infty(\mathcal{M}, \delta)} d\delta$$

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Recall: Two Complexity Notions

- Shtarkov or NML Complexity
 - central notion in log-loss individual sequence prediction
- PAC-**Bayesian** Complexity
 - right-hand side in a strong excess risk bound in (**stochastic**) statistical learning for arbitrary loss fns; **not suited for very large classes. We will unify with Shtarkov Complexity and thus make bound suitable for large classes.**

G & M Excess Risk Bound (Thm)

For every $\hat{\Pi}_n = \hat{\Pi} \mid Z^n$, every prior Π_0 , every $\eta > 0$:

$$\mathbf{E}_{f \sim \hat{\Pi}_n} \mathbf{E}_{Z \sim P}^{\text{ann}, \eta} [r_f(Z)] \triangleleft_{\eta n}$$

$$\mathbf{E}_{f \sim \hat{\Pi}_n} \left[\frac{1}{n} \sum_{i=1}^n r_f(Z_i) \right] + \frac{\text{KL}(\hat{\Pi}_n \parallel \Pi_0)}{\eta \cdot n}$$

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For every $\hat{\Pi}_n = \hat{\Pi} \mid Z^n$, every prior Π_0 , every $\eta > 0$:

$$\mathbf{E}_{f \sim \hat{\Pi}_n} \mathbf{E}_{Z \sim P}^{\text{ann}, \eta} [r_f(Z)] \triangleq_{\eta n}$$

$$\mathbf{E}_{f \sim \hat{\Pi}_n} \left[\frac{1}{n} \sum_{i=1}^n r_f(Z_i) \right] + \frac{\text{KL}(\hat{\Pi}_n \parallel \Pi_0)}{\eta \cdot n}$$

G & M Excess Risk Bound

For every $\hat{\Pi}_n = \hat{\Pi} \mid Z^n$, every **luckiness function** w , every $\eta > 0$:

$$\mathbf{E}_{f \sim \hat{\Pi}_n} \mathbf{E}_{Z \sim P}^{\text{ann}, \eta} [r_f(Z)] \triangleleft_{\eta n}$$

$$\mathbf{E}_{f \sim \hat{\Pi}_n} \left[\frac{1}{n} \sum r_f(Z_i) \right] + \text{COMP}_\eta(\mathcal{F}, \hat{\Pi}, w, Z^n)$$

$$\text{COMP}_\eta(\mathcal{F}, \hat{\Pi}_n, w, Z^n) = \frac{1}{\eta} \cdot \left(\mathbf{E}_{f \sim \hat{\Pi}_n} [-\log w(z^n, f)] + \log S(\mathcal{F}, \hat{\Pi}, w) \right)$$

data-dependent part

data-independent part

Bounding the novel complexity

- By different choices of w , $\text{COMP}_\eta(\mathcal{F}, \hat{\Pi}, w, Z^n)$ can be further bounded so as to become a
 - **KL divergence between prior and posterior** (recovering and improving Zhang's bound)
 - **Normalized Maximum Likelihood (NML) or Shtarkov Integral**
*which can be further bounded in terms of **Rademacher complexity**, VC dim, entropy nrs (right rates for polynomial entropy classes)*
 - **Luckiness NML** (useful for penalized estimators e.g. Lasso)

Bounding COMP for ERM/ML \hat{f}

- Let us take $\hat{\Pi} \equiv \hat{f}$ to be ERM (note that for the log loss, this is just maximum likelihood)
- and let us take $w(z^n, f) \equiv 1$ *constant*
Assume bounded losses here!

G & M Excess Risk Bound

For every $\hat{\Pi}_n = \hat{\Pi} \mid Z^n$, every luckiness fn w , every $\eta > 0$:

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$$\mathbf{E}_{f \sim \hat{\Pi}_n} \left[\frac{1}{n} \sum r_f(Z_i) \right] + \text{COMP}_{\eta}(\mathcal{F}, \hat{\Pi}, w, Z^n)$$

$$\text{COMP}_{\eta}(\mathcal{F}, \hat{\Pi}_n, w, Z^n) = \frac{1}{\eta} \cdot \left(\mathbf{E}_{f \sim \hat{\Pi}_n} [-\log w(z^n, f)] + \log S(\mathcal{F}, \hat{\Pi}, w) \right)$$

G & M Excess Risk Bound

For every **deterministic** \hat{f} , every luckiness fn w , $\eta > 0$:

~~$$\mathbf{E}_{f \sim \hat{\Pi}_n} \mathbf{E}_{Z \sim P}^{\text{ann}, \eta} \left[r_{\hat{f}|Z^n} (Z) \right] \leq_{\eta n}$$~~

~~$$\mathbf{E}_{f \sim \hat{\Pi}_n} \left[\frac{1}{n} \sum r_{\hat{f}|Z^n} (Z_i) \right] + \text{COMP}_{\eta}(\mathcal{F}, \hat{\Pi}, w, Z^n)$$~~

$$\text{COMP}_{\eta}(\mathcal{F}, \hat{\Pi}_n, w, Z^n) = \frac{1}{\eta} \cdot \left(\mathbf{E}_{f \sim \hat{\Pi}_n} [-\log w(z^n, f)] + \log S(\mathcal{F}, \hat{\Pi}, w) \right)$$

G & M Excess Risk Bound

For every **deterministic \hat{f}** , constant $w \equiv 1$, $\eta > 0$:

~~$$\mathbf{E}_{f \sim \hat{\Pi}_n} \mathbf{E}_{Z \sim P}^{\text{ann}, \eta} \left[r_{\hat{f}|Z^n} (Z) \right] \leq_{\eta n}$$~~

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data-dependent part disappears

G & M Excess Risk Bound

For **ERM** \hat{f} , constant $w \equiv 1$, $\eta > 0$:

~~$$\mathbf{E}_{f \sim \hat{\Pi}_n} \mathbf{E}_{Z \sim P}^{\text{ann}, \eta} \left[r_{\hat{f}|Z^n}(Z) \right] \leq_{\eta n}$$~~

~~$$\mathbf{E}_{f \sim \hat{\Pi}_n} \left[\frac{1}{n} \sum r_{\hat{f}|Z^n}(Z_i) \right] + \text{COMP}_{\eta}(\mathcal{F}, \hat{\Pi}, w, Z^n)$$~~

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data-dependent part disappears

Excess Risk Bound for ERM

$$\mathbf{E}_{Z \sim P}^{\text{ann}, \eta} \left[r_{\hat{f}|Z^n}(Z) \right] \leq_{\eta n} \eta^{-1} \cdot \log S(\mathcal{F}, \hat{f}, w_{\text{uniform}})$$

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...to define S , define probability density fns q_f as

$$q_f(z) := p(z) \cdot \frac{e^{-\eta r_f(z)}}{\int p(z) e^{-\eta r_f(z)} d\nu(z)}$$

[note that with log-loss and $\eta = 1$ and a correctly specified model, $q_f(z) = p_f(z)$!]

Then

$$S(\mathcal{F}; \hat{f}, w_{\text{uniform}}) := \int q_{\hat{f}|z^n}(z^n) d\nu(z^n) \leq \int q_{\hat{f}_{\text{ML}}|z^n}(z^n) d\nu(z^n)$$

Excess Risk Bound for ERM

$$\mathbf{E}_{Z \sim P}^{\text{ann}, \eta} \left[r_{\hat{f}|Z^n} (Z) \right] \leq_{\eta n} \eta^{-1} \cdot \log S(\mathcal{F}, \hat{f}, w_{\text{uniform}})$$

...where

$$S(\mathcal{F}; \hat{f}, w_{\text{uniform}}) \leq S(\mathcal{F}; \hat{f}_{\text{ML}}, w_{\text{uniform}}) = \int q_{\hat{f}_{\text{ML}}|z^n}(z^n) d\nu(z^n)$$

$\log S$ is **cumulative minimax individual sequence regret** for log-loss prediction relative to the set of densities $\{q_f : f \in \mathcal{F}\}$

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$\log S$ is cumulative minimax individual sequence regret for log-loss prediction relative to the set of densities $\{q_f : f \in \mathcal{F}\}$

...a.k.a. as **Shtarkov** or **NML (normalized ML) complexity**

G & M Excess Risk Bound

For every $\hat{\Pi}_n = \hat{\Pi} \mid Z^n$, every luckiness fn w , every $\eta > 0$:

$$\mathbf{E}_{f \sim \hat{\Pi}_n} \mathbf{E}_{Z \sim P}^{\text{ann}, \eta} [r_f(Z)] \triangleleft_{\eta n}$$

$$\mathbf{E}_{f \sim \hat{\Pi}_n} \left[\frac{1}{n} \sum r_f(Z_i) \right] + \text{COMP}_{\eta}(\mathcal{F}, \hat{\Pi}, w, Z^n)$$

$$\text{COMP}_{\eta}(\mathcal{F}, \hat{\Pi}_n, w, Z^n) = \frac{1}{\eta} \cdot \left(\mathbf{E}_{f \sim \hat{\Pi}_n} [-\log w(z^n, f)] + \log S(\mathcal{F}, \hat{\Pi}, w) \right)$$

G & M Excess Risk Bound

For every **deterministic** \hat{f} , every luckiness fn w , $\eta > 0$:

~~$$\mathbf{E}_{f \in \hat{\Pi}_n} \mathbf{E}_{Z \sim P}^{\text{ann}, \eta} \left[r_{\hat{f}|Z^n}(Z) \right] \leq_{\eta n}$$~~

~~$$\mathbf{E}_{f \in \hat{\Pi}_n} \left[\frac{1}{n} \sum r_{\hat{f}|Z^n}(Z_i) \right] + \text{COMP}_{\eta}(\mathcal{F}, \hat{f}, w, Z^n)$$~~

$$\text{COMP}_{\eta}(\mathcal{F}, \hat{f}, w, z^n) = \frac{1}{\eta} \cdot \left(-\log w(z^n, \hat{f}|z^n) + \log S(\mathcal{F}, \hat{f}, w) \right)$$

G & M Excess Risk Bound

For every **deterministic \hat{f}** , every **simple luckiness fn w** :

~~$$\mathbf{E}_{f \in \hat{\Pi}_n} \mathbf{E}_{Z \sim P}^{\text{ann}, \eta} \left[r_{\hat{f}|Z^n} (Z) \right] \leq_{\eta n}$$~~

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G & M Excess Risk Bound

~~$$\mathbf{E}_{f \in \hat{\Pi}_n} \mathbf{E}_{Z \sim P}^{\text{ann}, \eta} \left[r_{\hat{f}|Z^n}(Z) \right] \leq \eta n$$~~

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...and now

$$S(\mathcal{F}, \hat{f}, w) := \int q_{\hat{f}|z^n}(z^n) w(z^n) d\nu(z^n)$$

Bounds for Penalized ERM

For every **deterministic** \hat{f} , every simple luckiness fn w :

$$\mathbf{E}_{Z \sim P}^{\text{ann}, \eta} \left[r_{\hat{f}|Z^n}(Z) \right] \leq_{\eta n} \frac{1}{n} \sum r_{\hat{f}|Z^n}(Z_i) + \text{COMP}_{\eta}(\mathcal{F}, \hat{f}, w, Z^n)$$

$$\text{COMP}_{\eta}(\mathcal{F}, \hat{f}, w, z^n) = \frac{1}{\eta} \cdot \left(-\log w(z^n) + \log S(\mathcal{F}, \hat{f}, w) \right)$$

Taking $w(z^n) = \exp(-\text{PEN}(\hat{f}|_{z^n}))$ for a penalization function PEN the bound is optimized if we take

$$\hat{f}|_{z^n} := \arg \min_{f \in \mathcal{F}} \sum_{i=1}^n \ell_f(z_i) + \eta^{-1} \text{PEN}(f)$$

Bounds for Penalized ERM

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....we get (sharp!) bounds for Lasso and friends. We see that **multiplier in Lasso is 'just like' learning rate in Bayes**

Bounds for ‘Posteriors’ including generalized Bayes

For every $\hat{\Pi}_n = \hat{\Pi} \mid Z^n$, every luckiness fn w , every $\eta > 0$:

$$\mathbf{E}_{f \sim \hat{\Pi}_n} \mathbf{E}_{Z \sim P}^{\text{ann}, \eta} [r_f(Z)] \triangleleft_{\eta n}$$

$$\mathbf{E}_{f \sim \hat{\Pi}_n} \left[\frac{1}{n} \sum r_f(Z_i) \right] + \text{COMP}_{\eta}(\mathcal{F}, \hat{\Pi}, w, Z^n)$$

$$\text{COMP}_{\eta}(\mathcal{F}, \hat{\Pi}_n, w, Z^n) = \frac{1}{\eta} \cdot \left(\mathbf{E}_{f \sim \hat{\Pi}_n} [-\log w(z^n, f)] + \log S(\mathcal{F}, \hat{\Pi}, w) \right)$$

$$S(\mathcal{F}, \hat{\Pi}, w) := \mathbf{E}_{Z^n \sim P} \left[\exp \left(-\mathbf{E}_{f \sim \hat{\Pi} \mid Z^n} [\eta r_f(Z^n) + \log C(f) - \log w(Z^n, f)] \right) \right]$$

Proposition

- Take arbitrary estimator $\hat{\Pi}$ that outputs distribution over \mathcal{F} and arbitrary prior Π_0 . If we take

$$w(z^n, f) := \frac{\pi_0(f)}{\pi(f|z^n)} \text{ then we have}$$

$$S(\mathcal{F}, \hat{\Pi}, w) \leq 1$$

(Proof is just Jensen)

Now we reduce to Zhang...

For every $\hat{\Pi}_n = \hat{\Pi} \mid Z^n$, luckiness fn $w(z^n, f) := \frac{\pi_0(f)}{\pi(f|z^n)}$

$$\mathbf{E}_{f \sim \hat{\Pi}_n} \mathbf{E}_{Z \sim P}^{\text{ann}, \eta} [r_f(Z)] \triangleleft_{\eta n}$$

$$\mathbf{E}_{f \sim \hat{\Pi}_n} \left[\frac{1}{n} \sum r_f(Z_i) \right] + \text{COMP}_\eta(\mathcal{F}, \hat{\Pi}, w, Z^n)$$

$$\text{COMP}_\eta(\mathcal{F}, \hat{\Pi}_n, w, Z^n) = \frac{1}{\eta} \cdot \left(\mathbf{E}_{f \sim \hat{\Pi}_n} [-\log w(z^n, f)] + \log S(\mathcal{F}, \hat{\Pi}, w) \right)$$

$$\mathbf{E}_{f \sim \hat{\Pi}_n} \left[-\log \frac{\pi_0(f)}{\hat{\pi}(f|z^n)} \right] = \text{KL}(\hat{\Pi}_n \parallel \Pi_0)$$

Excess Risk \leq Codelength Diff.

- If we estimate by generalized Bayesian posterior, RHS has a log-Bayesian marginal likelihood interpretation = codelength under Bayesian code
- If we take deterministic \hat{f} and constant w then RHS has a NML codelength interpretation
- If we take deterministic \hat{f} and nonconstant w then RHS has a ‘luckiness NML’ (Bartlett et al. 2013) codelength interpretation

... Bayes and NML are two most important ‘universal coding strategies’ for data compression (G. 07)

General insight: **right-hand side of bound always has a codelength interpretation**, different w 's corresponding to different codes

More Remarks on Bound

Bound is sharp! Why?

- It says $\text{LHS} \triangleleft_{\eta n} \text{RHS}$

$$\text{i.e. } \mathbf{E} \left[e^{\eta \cdot (\text{LHS} - \text{RHS})} \right] \leq 1$$

...but the proof (which is straightforward rewriting!) actually gives that

$$\mathbf{E} \left[e^{\eta \cdot (\text{LHS} - \text{RHS})} \right] = 1$$

$$\text{LHS} = \mathbf{E}_{f \sim \hat{\Pi}_n} \mathbf{E}_{Z \sim P}^{\text{ann}, \eta} [r_f(Z)]$$

$$\text{RHS} = \mathbf{E}_{f \sim \hat{\Pi}_n} \left[\frac{1}{n} \sum r_f(Z_i) \right] + \text{COMP}_{\eta}(\mathcal{F}, \hat{\Pi}, w, Z^n)$$

Two Observations

$$\text{comp}_n(\mathcal{M}) \leq \inf_{\epsilon > 0} \log N_\infty(\mathcal{M}, \epsilon) + 24 \int_0^\epsilon \sqrt{\log N_\infty(\mathcal{M}, \delta)} d\delta$$

1. Bound is often **better** than best regret bound that can be given for prediction by Bayes marginal likelihood (n^γ vs. n^β for $\beta > \gamma$)
 - ...and for some \mathcal{M} it is indeed known that Bayesian prediction has larger worst-case regret
2. ...yet bound is **void** if $N_\infty(\mathcal{M}, \epsilon) = \infty$
 - Take e.g. \mathcal{M} to be all i.i.d. extensions of monotonically decreasing densities (bounded away from 0 and ∞) on unit interval

Two Complexity Notions, Two Results

- Shtarkov or NML Complexity
 - central notion in log-loss individual sequence prediction. Existing bounds are in terms of L_∞ -entropy nrs; we have comparable bound in terms of $L_{1/2}(P)$ nrs. (but haven't shown you)
- PAC-**Bayesian** Complexity
 - right-hand side in a strong excess risk bound in (**stochastic**) statistical learning for arbitrary loss fns with Bayesian codelength interpretation; **not suited for very large classes**. We have unified with Shtarkov Complexity (smaller codelengths) and thus made bound suitable for large classes.

Three Complexity Notions

- Shtarkov or NML Complexity
 - central notion in **nonstochastic log-loss** individual sequence prediction.
- PAC-Bayesian Complexity
 - right-hand side in a strong **excess risk bound** in (**stochastic**) statistical learning for **arbitrary loss** fns
 - especially suited for (pseudo-) Bayesian methods but **not for very large classes**
- Rademacher Complexity
 - right-hand side in stochastic excess risk bound that deals well with large classes but **not with log-loss and priors**

Thm 2: Shtarkov bounded by Rademacher Complexity

- Fix arbitrary $f^\circ \in \mathcal{F}$ and define $\mathcal{G} = \{\ell_f - \ell_{f^\circ} : f \in \mathcal{F}\}$
- Define centered empirical process

$$T_n := \sup_{f \in \mathcal{F}} \left\{ \sum_{j=1}^n (\ell_{f^\circ}(Z_j) - \ell_f(Z_j)) - \mathbf{E}_{Z^n \sim Q_{f^\circ}} \left[\sum_{j=1}^n (\ell_{f^\circ}(Z_j) - \ell_f(Z_j)) \right] \right\}.$$

- For arbitrary deterministic estimators \hat{f} ,

$$\begin{aligned} \text{COMP}_\eta(\mathcal{F}, \hat{f}, w_{\text{UNIFORM}}) &\leq 3 \cdot \mathbf{E}_{Z^n \sim Q_{f^\circ}} [T_n] + n \cdot \eta \cdot C \cdot \epsilon^2 \\ &\leq 6n \cdot \mathbf{E}_{Z^n \sim Q_{f^\circ}} [\text{RAD}_n(\mathcal{G} \mid Z^n)] + n \cdot \eta \cdot C \cdot \epsilon^2 \end{aligned}$$

where ϵ is diameter of \mathcal{F} in $L_2(P)$ -pseudometric

$$\text{RAD}_n(\mathcal{G} \mid Z^n) := \mathbf{E}_{\epsilon_1, \dots, \epsilon_n} \left[\sup_{g \in \mathcal{G}} \left| \frac{1}{n} \sum_{i=1}^n \epsilon_i g(Z_i) \right| \right]$$

Bounding excess risk, minimax regret in terms of L_2 entropy nrs

- Recall Lugosi/Cesa-Bianchi log-loss result:

$$\text{COMP}_1(\mathcal{F}, \hat{f}, w_{\text{UNIFORM}}) \leq$$

$$\inf_{\epsilon > 0} \log N_{\infty}(\mathcal{F}, \epsilon) + 24 \int_0^{\epsilon} \sqrt{\log N_{\infty}(\mathcal{F}, \delta)} d\delta$$

- Via existing bounds on Rademacher using chaining we get

$$\text{COMP}_{\eta}(\mathcal{F}, \hat{f}, w_{\text{UNIFORM}}) \leq$$

$$\inf_{\epsilon > 0} \log N_{L_2(P)}(\mathcal{F}, \epsilon) + 24 \int_0^{\epsilon} \sqrt{\log N_{L_2(P)}(\mathcal{F}, \delta)} d\delta + Cn\eta\epsilon^2$$

For class of monotone decreasing densities, now get $O(n^{1/3})$ which is tight; previous bound was void

Today

1. Complexity

- Individual Sequence Prediction with Log-Loss: the NML distribution and Complexity
- Extending the Right-Hand Side of Zhang's Bound

2. Safe Inference

Safe Bayes, Safe Probability

- In previous work, I used phrase ‘safe Bayes’ in two senses:
 1. Specific algorithm for **learning** η from the data
(‘G. ‘12, **The Safe Bayesian**; G. and vOmmen ‘17)
 2. General idea that in practice probabilities should not be taken fully seriously; their application should be restricted to **safe** uses
(G., **Safe Probability**, JSPI ‘18)

Two Extreme Views on Learning – yet using almost same methods

- **Vapnik's ML Theory**
(**'statistical learning theory', 50000 citations**)
*Can only do one single thing with the function
learned from data*



- **Bayesian Inference (at least De Finetti brand)**
*Every single inference task that can be
formulated in terms of measurable fns on my
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Example: Ridge/Lasso Regression

$$\hat{\beta}_n := \arg \min_{\beta \in \mathbb{R}^k} \sum_{i=1}^n (y_i - \beta^T x_i)^2 + \lambda \|\beta\|_2^2$$

- **V**: assume X_i, Y_i i.i.d. $\sim P$. For large enough n , ‘right’ λ , we have

$$\mathbf{E}_{(X,Y) \sim P} (Y - \hat{\beta}_n^T X)^2 \approx \min_{\beta \in \mathbb{R}^k} \mathbf{E}_{(X,Y) \sim P} (Y - \beta^T X)^2$$

- “Hence I can get small squared error when predicting a new Y based on a new X **from the same distribution**”



$$\hat{\beta}_n := \arg \min_{\beta \in \mathbb{R}^k} \sum_{i=1}^n (y_i - \beta^T x_i)^2 + \lambda \|\beta\|_2^2$$

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- “Hence I can get small squared error when predicting a new Y based on a new X from the same distribution”
- Q: What if new X drawn from different distribution?
- V: You can’t say anything!



$$\hat{\beta}_n := \arg \min_{\beta \in \mathbb{R}^k} \sum_{i=1}^n (y_i - \beta^T x_i)^2 + \lambda \|\beta\|_2^2$$

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- “Hence I can get small squared error when predicting a new Y based on a new X from the same distribution”
- Q: What if new X drawn from different distribution?
- V: You can't say anything!
- Q: Does $\hat{\beta}_n^T X$ give a good estimate of $\mathbf{E}[Y|X]$?
- V: Can't say!

$$\hat{\beta}_n := \arg \min_{\beta \in \mathbb{R}^k} \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta^T x_i)^2 + \frac{\lambda}{\sigma^2} \|\beta\|_2^2$$

- B: $\hat{\beta}_n$ is also posterior mean (even with prior on σ^2)
- So I agree that I can get small squared error when predicting a new Y based on a new X from same distr.
- Q: What if new X drawn from different distribution?
- B: You'll still be o.k.!
- Q: Does $\hat{\beta}_n^T X$ give a good estimate of $\mathbf{E}[Y|X]$?
- B: Of course!



$$\hat{\beta}_n := \arg \min_{\beta \in \mathbb{R}^k} \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta^T x_i)^2 + \frac{\lambda}{\sigma^2} \|\beta\|_2^2$$

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- Q: Does $\hat{\beta}_n^T X$ give a good estimate of $\mathbf{E}[Y|X]$?
- B: Of course!
- Q: Does $\hat{\beta}_n^T X$ give good estimate of median of Y given X ?
- B: Of course!
- Q: Is $P(Y|X)$ unimodal? B: Of course! etc etc



V&B use almost same method but draw very weak vs very strong conclusions!

$$\hat{\beta}_n := \arg \min_{\beta \in \mathbb{R}^k} \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta^T x_i)^2 + \frac{\lambda}{\sigma^2} \|\beta\|_2^2$$

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- B: Of course!
- Q: Is $P(Y|X)$ unimodal? B: Of course! Etc etc



Safe Statistics: Go Inbetween

- If I do η –Bayesian linear regression with normal prior on β , standard prior on variance σ^2 and $\eta < \bar{\eta}$, then if data i.i.d. I can guarantee convergence to KL optimal $f^*(x) = \beta^{*T}x$ and σ^* s.t.:

- **Optimality** of squared error predictions of p_{f^*}

$$\mathbf{E}_{(X,Y) \sim P} [(Y - f^*(X))^2] = \min_{f \in \mathcal{F}} \mathbf{E}_{(X,Y) \sim P} [(Y - f(X))^2]$$

- **Safety** of your error assessment thereof

$$\mathbf{E}_{Y \sim p_{f^*}} [(Y - f^*(X))^2 \mid X] = \sigma_2^* = \mathbf{E}_{(X,Y) \sim P} [(Y - f^*(X))^2]$$

Safe Statistics: Go Inbetween

- If I assume data i.i.d. I can guarantee
- **Optimality** of squared error predictions of p_{f^*}
- **Safety** of error assessment thereof
- If(f) I am further willing to assume that \mathcal{F} contains Bayes-optimal decision rule...
$$\arg \min_{f: \mathcal{X} \rightarrow \mathbb{R}} \mathbf{E}_{(X,Y) \sim P} (Y - f(X))^2$$
-then I can guarantee that $f^*(X) = \mathbf{E}[Y | X]$
- If on top I want to assume that $P(Y|X)$ is symmetric then I can guarantee that $f^*(X)$ is **median** of $P(Y | X)$

I have a Dream

- Imagine a world in which statisticians/data analysts would, as a matter of principle, be asked to **express what their probability model can be used for and what not.**
- **Then indeed we would have a safer statistics**
- ...in the paper 'Safe Probability' I make a first attempt to develop a **formal language for specifying this**

Hypothesis Testing

- Suppose you test between two models using a Bayes factor
- If you choose $\bar{p}_0(y^n) = \int p_\theta(y^n)w_0(\theta)d\theta$ because your prior w_0 really expresses prior knowledge, and $\bar{p}_0(y^n) \gg \bar{p}_1(y^n)$, then you might be willing to use the Bayes posterior $w_0(\theta|y^n)$ for making actual predictions: you might **claim it is safe for all bounded loss fns.**
- But if you choose \bar{p}_0 because it is the RIPr of \bar{p}_1 , then you definitely cannot trust the poster and you do not want to make such claims!

New Mathematical Questions/Concepts

- **Optimality:** If I assume $\langle X \rangle$, for what inference/prediction tasks am I (sufficiently) optimal?
- Some scattered nontrivial results exist in machine learning theory literature.

New Mathematical Questions/Concepts

- **Optimality:** If I assume $\langle X \rangle$, for what inference/prediction tasks am I (sufficiently) optimal?
- Some scattered nontrivial results exist in machine learning theory literature. For example:
if you do **logistic regression** and you are really interested in classification, then your KL optimal parameters (to which you'll converge) also give you the smallest expected 0/1-loss when used for classification **if your model contains the Bayes optimal classifier** (Bartlett, Jordan, McAullife '06)

New Mathematical Questions/Concepts

- **Optimality:** If I assume $\langle X \rangle$, for what inference/prediction tasks am I (sufficiently) optimal?
- **Safety:** central concept of G. 2018.

A distribution \tilde{P} is **safe** for predicting against loss function L with 'true' distribution P if it holds that

$$\mathbf{E}_{Z \sim P} [L(Z, \delta_{\tilde{P}})] = \mathbf{E}_{Z \sim \tilde{P}} [L(Z, \delta_{\tilde{P}})]$$

where $\delta_{\tilde{P}}$ is the Bayes act according to \tilde{P}

Safe Probability

- **Safety:** Simplest form:

A distribution \tilde{P} is **safe** for predicting against loss function L with ‘true’ distribution P if it holds that

$$\mathbf{E}_{Z \sim P} [L(Z, \delta_{\tilde{P}})] = \mathbf{E}_{Z \sim \tilde{P}} [L(Z, \delta_{\tilde{P}})]$$

where $\delta_{\tilde{P}}$ is the Bayes act according to \tilde{P}

If you act as your model prescribes, the world behaves as your model predicts, even though your model may be wrong and there may be better predictions!

Example

- If I do η –Bayesian linear regression with normal prior on β , standard prior on variance σ^2 and $\eta < \bar{\eta}$, then if data i.i.d. I can guarantee convergence to KL optimal $f^*(x) = \beta^{*T}x$ and σ^* s.t.:

- **Optimality** of squared error predictions of p_{f^*}

$$\mathbf{E}_{(X,Y) \sim P} [(Y - f^*(X))^2] = \min_{f \in \mathcal{F}} \mathbf{E}_{(X,Y) \sim P} [(Y - f(X))^2]$$

- **Safety** of your error assessment thereof

$$\mathbf{E}_{Y \sim p_{f^*}} [(Y - f^*(X))^2 \mid X] = \sigma_2^* = \mathbf{E}_{(X,Y) \sim P} [(Y - f^*(X))^2]$$

Example 2

- The Weather Forecaster!

Monty Hall (3-door) Problem

Monty Hall 1970



Monty Hall



- There are three doors in the TV studio. Behind one door is a car, behind both other doors a goat. You choose one of the doors. Monty Hall opens one of the other two doors, and shows that there is a goat behind it. You are now allowed to switch to the other door that is still closed. Is it smart to switch?

Monty Hall: The Wikipedia Wars

- I am interested in understanding the **Wikipedia Wars** (Gill 11, Mlodinow 08) on Monty Hall
 - Both sides agree that switching is smart and increases your chances of winning from $1/3$ to $2/3$!
 - The “war” is about how to *prove* this:
 - “strictly Bayesian”: via conditioning (in the right space, with additional assumption that Monty chooses by tossing a fair coin) (“MaxEnt-style assumption”)
 - Without additional assumptions, via decision-theoretic argument

Safe Probability applied to Monty Hall

- Under a **symmetric** loss function as in the original formulation of the problem, assuming that Monty flips a fair coin if he has a choice and then conditioning is **safe** and **minimax optimal**
 - ‘asymmetric’ means e.g. that if the car is behind door B, it is a **Ferrari**; if it is behind door C, it is a **Fiat Panda**
- Still holds if same candidate plays each week and can reinvest his prize, hedging over several doors (**horse race losses**), even if prizes asymmetric
- But *not* if loss functions are asymmetric and reinvestment impossible

Thank you!

Further Reading:

- G. and T. van Ommen, Inconsistency of Bayesian Inference for Misspecified Linear Models, and a Proposal for Repairing It. *Bayesian Analysis*, Dec. 2017
- G. and N. Mehta, Fast Rates for Unbounded Losses, arXiv (2016)
- G. and N. Mehta. A Tight Excess Risk bound in terms of a Unified PAC-Bayesian-Rademacher-MDL Complexity, arXiv (2017)
- G. Safe Probability, *Journal of Stat. Planning and Inference*, 2018
- T. van Ommen, W. Koolen and G. *Robust Probability Updating*, *Intern. Journ. of Approx. Reasoning*, 2016