Constrained Relative Entropy Minimization with Applications to Multitask Learning

Dissertation Defense

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Probabilistic Inference

Quantify uncertainty about x as $P(x)$.

Principle of maximum entropy

Choose $P(x)$ that captures known information and is as difficult as possible to discriminate from uniform[a] (Jaynes, 1957).

[a] Uniform distribution represents complete ignorance.

Principle of minimum discrimination information

Given $P(x)$, choose $Q(x)$ that captures new information and is as difficult to discriminate from $P(x)$ as possible (Kullback, 1959).

Comparison with Bayesian Inference

Why do we need (yet) another inference rule?

Bayesian Inference:

- Solid conceptual framework derived from axioms of probability.
- Provides rules for updating $P(x)$ given data samples $\mathcal{D}$.
- Can impose support constraints by defining appropriate $P(x)$.
- Support constraints are preserved by $P(x) \mapsto P(x|\mathcal{D})$.

But:

- Other kinds of structure (e.g. moment constraints) generally do not propagate.
- Bayesian inference does not provide a formal approach for updating P with new *constraint* information.

Prior Work

Relative entropy inference

- MAXENT for natural language processing (Berger et al., 1996).
- l_1 and l_2 norm ball constraints (Dudík et al., 2007).
- Banach norm constraints (Altun and Smola, 2006).
- Margin constraints ("probabilistic support vector machines"):
  - Maximum entropy discrimination (Jaakkola et al., 1999).
  - MED-LDA (Zhu et al., 2009).
  - Link prediction (Zhu, 2012).

Multitask Learning

An overview

Given multiple (related) learning tasks:

$$f_1 : x \mapsto y_1, \quad f_2 : x \mapsto y_2, \quad f_3 : x \mapsto y_3, \quad \ldots$$

Single task learning:

- Learn $f_1, f_2, f_3, \ldots$ separately.

Multiple task learning:

- Learn $F : x \mapsto Y$ jointly.
- Exploits inter-task relationships to improve performance
- When F is a bilinear function, MTL can be posed as a *matrix* estimation task.

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Main Contributions

Constrained Inference

A framework for probabilistic inference subject to expectation constraints:

- Constraints may be any combination of domain knowledge and data.
- Constraint sets may be nonconvex.
- Generalization of Bayesian inference that can incorporate additional structural constraints.

Main Contributions

Applications

- Constrained multitask learning and parameter estimation:
  - Applied to recommender systems and fMRI.
  - Rank constraints on the postdata mean matrix.
  - Kronecker constraints on the postdata covariance matrix.
  - Sparsity constraints on prior precision matrix.
- Nonparametric multitask learning:
  - Applied to predictive modeling of transposable data.
  - Nuclear norm constraints on the mean function.
- Multitask bipartite ranking:
  - Applied to disease-gene prioritization.
  - Ordering constraints on ranking variables.
  - Nuclear norm constraints on mean function of regression variables.

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Gaussian Process (GP)

- Collection of random variables $\{X(i),\ i \in \mathbb{I}\}$ completely described by:

$$\mu(i) = \mathrm{E}\left[\, X(i) \,\right],$$
$$\mathcal{C}(i,i') = \mathrm{E}\left[\, (X(i) - \mu(i))\big(X(i') - \mu(i')\big) \,\right].$$

- The collection $\mathbf{x} = \{x(i),\ \forall i \in \mathsf{J}\}$ is jointly Gaussian for any finite index set $\mathsf{J} \subset \mathbb{I}$.

- Matrix-variate Gaussian process (MV-GP) $\mathcal{MGP}\left(\phi, \mathcal{C}_{\mathsf{N}}, \mathcal{C}_{\mathsf{M}}\right)$ is a special case:
    - Double index $(m,n) \in \mathbb{M} \times \mathbb{N} = \mathbb{J}$.

$$\mathcal{C}((m,n),(m',n')) = \mathcal{C}_{\mathsf{M}}(m,m')\mathcal{C}_{\mathsf{N}}(n,n').$$

Relative Entropy (Kullback-Leibler divergence)

For probability measures $P, \ Q$

Let P be absolutely continuous with respect to Q, there exist probability density functions $p, \ q$ so that:

$$\mathrm{KL}(p\|q) = \int_{\mathbb{X}} p(x) \log \frac{p(x)}{q(x)} dx$$

Some useful optimization-theoretic properties:

- Strictly convex wrt p.
- $\mathrm{KL}(p\|q) \geq 0$.
- $\mathrm{KL}(p\|q) = 0$ iff. $p = q$.

Exponential families

$$p_{\boldsymbol{\theta}}(x) = h(x)e^{\langle \boldsymbol{\eta}(\boldsymbol{\theta}), \mathbf{t}(x)\rangle - A(\boldsymbol{\theta})}$$

- $\boldsymbol{\eta}(\boldsymbol{\theta})$ natural parameter
- $\mathbf{t}(x)$ sufficient statistics
- $h(x)$ base measure
- $A(\boldsymbol{\theta})$ log-partition function

The domain of the parameter $\boldsymbol{\theta}$ is a convex set defined as:

$$\boldsymbol{\Theta} = \left\{ \boldsymbol{\theta} \;\middle|\; \int_{\mathbb{X}} h(x)e^{\langle \boldsymbol{\eta}(\boldsymbol{\theta}), \mathbf{t}(x)\rangle} dx < \infty \right\}.$$

Constraints

We study constraints of the form $\mathrm{E}\left[\,\boldsymbol{\beta}(x)\,\right] \in \mathsf{C}$.

- $\boldsymbol{\beta}$ is called the *feature function*.
- C is a constraint set.

Examples:

- Empirical average (Jaynes, 1957): $\mathrm{E}\left[\,\boldsymbol{\beta}(x)\,\right] = \frac{1}{N}\sum_n \boldsymbol{\beta}(\hat{x}_n)$.
- Structural constraints (this dissertation):

$$\mathrm{E}\left[\,\boldsymbol{\beta}(x)\,\right] \geq 0, \quad \left\|\mathrm{E}\left[\,\boldsymbol{\beta}(x)\,\right]\right\|_0 \leq \epsilon.$$

Constrained Relative Entropy Minimization

Problem Statement

$$\inf_{q \in \mathcal{P}} \mathrm{KL}(q \| p) \text{ s.t. } \mathrm{E}_q \left[\boldsymbol{\beta} \right] \in \mathsf{C}$$

Assumptions:

- $\mathsf{C} \subset \mathcal{B}$ is closed.
- if q_* is a solution, then $\mathrm{E}_{q_*} \left[\boldsymbol{\beta} \right] = \mathbf{a}_*$ is bounded.

Representation result

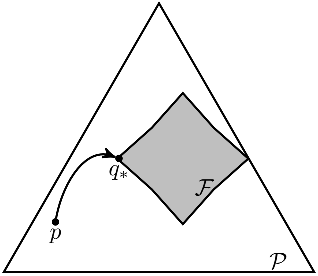
Every q_* can be represented as:

$$q_*(x) = p(x) e^{\langle \boldsymbol{\lambda}_*, \boldsymbol{\beta}(x) \rangle - G(\boldsymbol{\lambda}_*)}$$

where $\boldsymbol{\lambda}_*$ is a function of $\mathbf{a}_*$.

Main Idea

Find solution using exponential family representation



$$\min_{\mathbf{c} \in \mathsf{A}} \left[\min_{q \in \mathcal{P}} \mathrm{KL}(q \| p) \text{ s.t. } \mathrm{E}_q \left[\boldsymbol{\beta} \right] = \mathbf{c} \right]$$

- Inner problem is "easy" to solve.
- Find compact $\mathsf{A} \subset \mathsf{C}$ so that $\mathbf{a}_* \in \mathsf{A}$.
- Define $\mathcal{F} = \{ q_{\mathbf{c}} \; \forall \; \mathbf{c} \in \mathsf{A} \} \subset \mathcal{P}$.
- Show that $q_* \in \mathcal{F}$.

Generalize to any $\mathcal{Q} \subset \mathcal{P}$ iff. $q_* \in \mathcal{Q}$.

Conjugate Priors for Relative Entropy

Motivation

- Exponential family representation requires normalization constant $G(\boldsymbol{\lambda})$.
- In many cases, computing $G(\boldsymbol{\lambda})$ is a challenging high dimensional problem.

Definition

The distribution $p \in \mathcal{Q}$ is a relative entropy conjugate prior distribution if any solution $q_* \in \mathcal{Q}$.

Conjugate Priors for Relative Entropy

Some properties

No need to compute $G(\boldsymbol{\lambda})$ explicitly if $p \in \mathcal{Q}$ is conjugate:

$$f_* = \operatorname*{arg\,min}_{f \in \mathcal{Q}} \mathrm{KL}(f \| p) \text{ s.t. } \mathrm{E}_f \left[\boldsymbol{\beta} \right] \in \mathsf{C}$$

and $f_* \equiv q_*$.

Proposition

Let

$$\mathcal{Q} = \left\{ p \;\middle|\; p_{\boldsymbol{\eta},\nu}(x) = h(x,\nu) e^{\langle \boldsymbol{\eta}, \boldsymbol{\beta}(x) \rangle - D(\boldsymbol{\eta},\nu)} \right\},$$

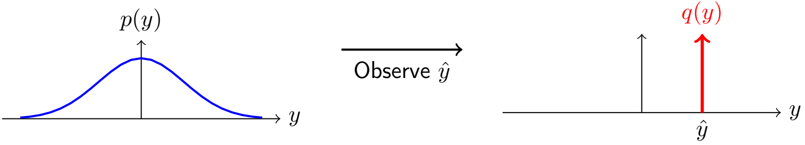
$\mathcal{Q}$ are a family of relative entropy conjugate priors i.e. any $q_* \in \mathcal{Q}$.

Constrained Bayesian Inference

Bayesian Inference $\subset$ Constrained Relative Entropy

Sample space: $\mathbb{X}$ latent variables and $\mathbb{Y}$ observations.

- Once you observe $y = \hat{y}$, there is no longer any uncertainty! Williams (1980)



- Hence $q(y) = \delta_{\hat{y}}$
- Equivalent constraint set $\mathrm{E}_q\left[\,\delta_{\hat{y}}\,\right] = 1$

Bayesian Inference ⊂ Constrained Relative Entropy

Solve:

$$\min_{q \in \mathcal{P}} \left[\mathrm{KL}(q(x,y) \| p(x,y)) \, \text{s.t.} \, \mathrm{E}_q \left[\, \delta_{\hat{y}} \, \right] = 1 \right]$$

Solution is the Bayesian posterior!

$$q_*(x,y) = q_*(x|y=\hat{y})\delta_{\hat{y}} = p(x|y=\hat{y})\delta_{\hat{y}}$$

In other words:

$$q(x|y=\hat{y}) \equiv p(x|y=\hat{y})$$

Bayesian Inference with Additional Constraints

Our approach - incorporate further constraints on $q(x)$.

Constrained Bayesian inference

Solve:

$$\min_{q(y),\ q(x|y)\in\mathcal{P}} \left[\mathrm{KL}(q(x|y)q(y)\|p(x,y)) \text{ s.t. } \substack{\mathrm{E}_q[\,\delta_{\hat{y}}\,]=1 \\ \mathrm{E}_q[\,\boldsymbol{\beta}(x)\,]\in\mathsf{C}} \right]$$

or the equivalent problem:

$$\min_{q\in\mathcal{P}} \left[\mathrm{KL}(q(x)\|p(x|y)) \text{ s.t. } \mathrm{E}_q\left[\,\boldsymbol{\beta}(x)\,\right] \in \mathsf{C} \right]$$

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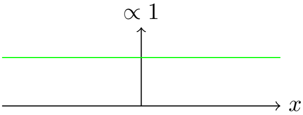
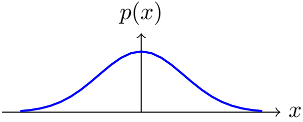
Overview of the Approach

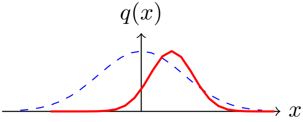


Domain $\mathbb{X}$
Complete ignorance



Maximize entropy given constraints

$$\min_p \left[\mathrm{H}(p) \ \textsf{s.t.}\ \mathrm{E}_q \left[\, \gamma(x) \,\right] \in \mathsf{D} \right]$$



Minimize relative entropy
given data and constraints

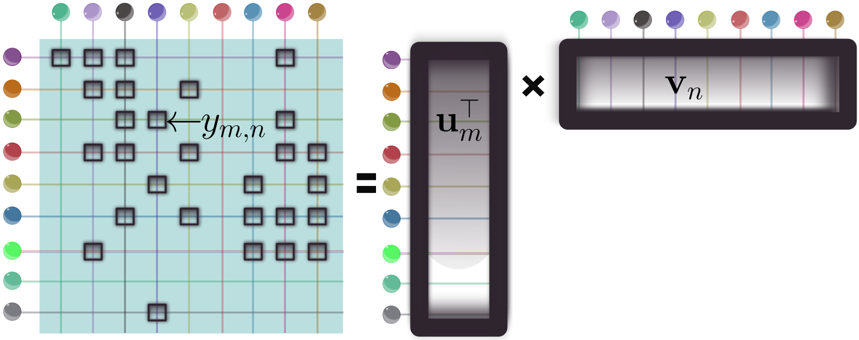
$$\min_q \left[\mathrm{KL}(q \| p) \ \textsf{s.t.}\ \mathrm{E}_q \left[\, \beta(x) \,\right] \in \mathsf{C} \right]$$

Illustrative Example

Low Rank Expectation Constraints

Matrix Factorization

- Estimate rank R factors $\mathbf{u}_m \in \mathbb{R}^R$ and $\mathbf{v}_n \in \mathbb{R}^R$ so that $y_{m,n} \approx \mathbf{u}_m^\top \mathbf{v}_n$.



Initial constraints and Prior Distribution

Domain:

- $\mathbf{y} \in \mathbb{R}^K$ with $(m, n) \in \mathsf{K}$
- $\mathbf{W} \in \mathbb{R}^{M \times N}$, $\mathbf{w} = \mathsf{vec}(\mathbf{W})$, let $\mathbf{P} : \mathsf{M} \times \mathsf{N} \mapsto \mathsf{K}$.

Initial information:

- $\mathrm{E}\left[\,\mathbf{y}|\mathbf{w}\,\right] = \mathbf{P}\mathbf{w}$, $\mathrm{E}\left[\,\mathbf{y}\mathbf{y}^\top\,\right] = \sigma^2\mathbf{I}$.
- $\mathrm{E}\left[\,\mathbf{w}\,\right] = \mathbf{0}$, $\mathrm{E}\left[\,\mathbf{w}\mathbf{w}^\top\,\right] = \mathbf{C} \otimes \mathbf{R}$.

Prior distribution

- Solve for maximum entropy distribution given constraints.
- Unique solution:

$$p(\mathbf{y}|\mathbf{w}) = \mathcal{N}\left(\mathbf{P}\mathbf{w}, \sigma^2\right), \quad p(\mathbf{w}) = \mathcal{N}\left(\mathbf{0}, \mathbf{C} \otimes \mathbf{R}\right).$$

Constrained Relative Entropy Approach

- Observe $\mathbf{y} = \widehat{\mathbf{y}}$
- Additional constraints $\mathrm{rank}(\mathrm{E}\left[\,\mathbf{W}\,\right]) \leq R$.

Solution

- Let $\mathsf{C} = \{\mathbf{B} \,|\, \mathrm{rank}(\mathbf{B}) \leq R\}$
- $p(\mathbf{W}|\mathcal{D}) = \mathcal{N}\left(\mathbf{A}, \mathbf{\Sigma}\right)$ is the Bayesian posterior.
- p is a relative entropy conjugate prior for $\boldsymbol{\beta}(\mathbf{W}) = \mathbf{W}$.
- Hence q is Gaussian $q(\mathbf{W}) = \mathcal{N}\left(\mathbf{M}_*, \mathbf{S}_*\right)$ and:

$$\mathbf{M}_*, \mathbf{S}_* = \operatorname*{arg\,min}_{\mathbf{M},\mathbf{S}} \Big[\mathrm{KL}(\mathcal{N}\left(\mathbf{M}, \mathbf{S}\right) \| \mathcal{N}\left(\mathbf{A}, \mathbf{\Sigma}\right)) \text{ s.t. } \mathbf{M} \in \mathsf{C} \Big]$$

Bayesian Approach

Factor Model

Prior Distribution:

$$\mathbf{y}|\mathbf{w} \sim \mathcal{N}\left(\mathbf{P}\mathbf{w}, \sigma^2\right),$$
$$\mathbf{W} = \mathbf{U}\mathbf{V}^\top, \;\; \mathbf{u}_m = \mathcal{N}\left(\mathbf{0}, \mathbf{R}\right), \;\; \mathbf{v}_n = \mathcal{N}\left(\mathbf{0}, \mathbf{C}\right).$$

Inference:

- Easy to compute some marginals e.g. $p(\mathbf{y}|\mathbf{U})$ (Lawrence and Urtasun, 2009),
- but $p(\mathbf{U}, \mathbf{V}|\mathbf{y})$ is analytically intractable!

In practice:

- Compute MAP estimate (equivalent to matrix factorization)
- Variational approximation.
- Sampling: $\mathrm{E}_{p(\mathbf{U},\mathbf{V}|\mathbf{y})}\left[\,\mathbf{W}\,\right]$ is unlikely to be low rank.

Application to Multitask Learning

- Constrained multitask learning and parameter estimation:
  - Applied to recommender systems and fMRI.
  - Rank constraints on the postdata mean matrix.
  - Kronecker constraints on the postdata covariance matrix.
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- Nonparametric multitask learning:
  - Applied to predictive modeling of transposable data.
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- Multitask bipartite ranking:
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  - Ordering constraints on ranking variables.
  - Nuclear norm constraints on mean function of regression variables.

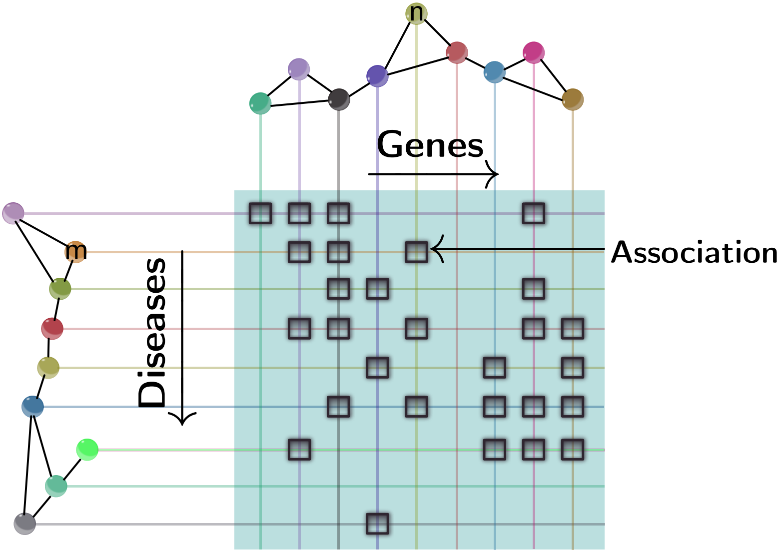
Multitask Bipartite Ranking

for Disease-Gene Prioritization

Genetic Diseases

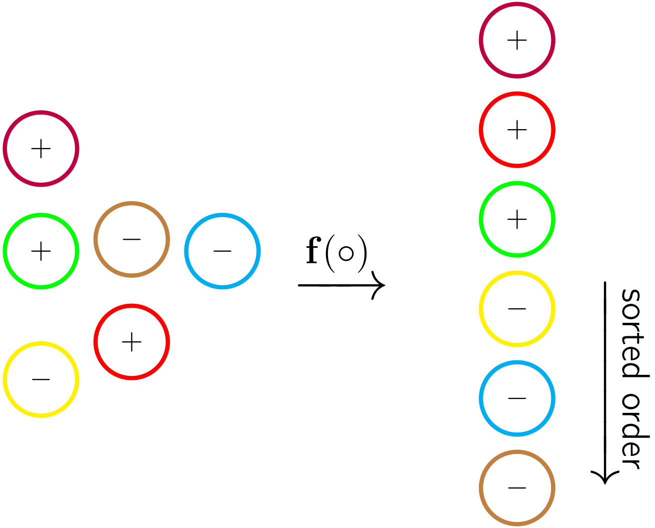
- Asthma, Cancer, Alzheimer's and many other diseases are associated with genetic mutations.
- Medical interest in unknown disease gene associations for targeted treatment, gene research, etc.
- $20,000 - 25,000$ human genes and thousands of diseases so enumerative search is computationally intractable.
- Computational models can be used to suggest most likely genetic associations.

Gene Disease Data



Bipartite Ranking

Inferring order from binary examples



Problem Setup

Sample Space:

- Associate $x_{m,n}$ to each observation $y_{m,n}$ (*ranking variable*).
- Associate $z_{m,n}$ to each $x_{m,n}$ (*regression variable*).

Prior Distribution

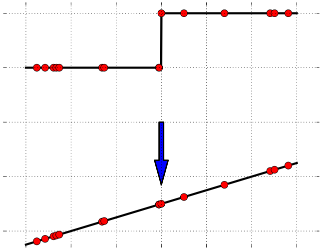
$$x_{m,n} \sim \mathcal{N}\left(z_{m,n}, \sigma^2\right), \quad Z \sim \mathcal{MGP}\left(0, \mathcal{C}_{\mathsf{M}}, \mathcal{C}_{\mathsf{N}}\right).$$

Regression variable constraint

Nuclear norm constraints for parsimony and performance:

$$\mathrm{E}\left[\,Z\,\right] \in \mathsf{T}_\epsilon = \{\Phi \mid \|\|\Phi\|\|_{1\text{-}\mathcal{H}_\mathcal{C}} \leq \epsilon\}$$

Ranking Variable Constraint



- Adapted from monotone retargeting (Acharyya et al., 2012)
- Key idea: Match ordering in $\mathbf{x}_m$ with ordering in $\mathbf{y}_m$
- Encoded as $\mathrm{E}\left[\,\mathbf{x}\,\right] \in \mathsf{R}_{\mathbf{y}}$

Inference

The resulting problem is given by:

$$q(\mathbf{x}, Z) = \arg\min_{q \in \mathcal{P}} \begin{bmatrix} & \mathrm{KL}(q(\mathbf{x}, Z) \| p(\mathbf{x}, Z)) \\ \text{s.t.} & \mathrm{E}_q\left[\,\mathbf{x}\,\right] \in \mathsf{R}_{\mathbf{y}},\ \mathrm{E}_q\left[\,Z\,\right] \in \mathsf{T}_\epsilon \end{bmatrix}$$

Solution

- $q(\mathbf{x}, Z)$ is a Gaussian process.
- Solution is unique!
- The marginal distribution $q(Z)$ is a matrix-varite GP with constrained (usually low rank) mean function.

Key Steps

- $q(\mathbf{x}, Z)$ is Gaussian for any finite index set via conjugacy.
- $\mathrm{KL}(q(\mathbf{x}, Z) \| p(\mathbf{x}, Z))$ reduces to $\mathrm{KL}(q(\mathbf{x}, \mathbf{Z}) \| p(\mathbf{x}, \mathbf{Z}))$
    - Proof uses representation theorem for spectral regularization (Abernethy et al., 2009).
    - $\mathbf{Z}$ is the finite "hidden" matrix corresponding to observations.
- Solve for $q(\mathbf{x}, \mathbf{Z})$.
- "Expand" finite $q(\mathbf{x}, \mathbf{Z})$ to random process $q(\mathbf{x}, Z)$
    - Using Kolmogorov's extension theorem (Kolmogorov, 1933).

Experiments

Datasets:

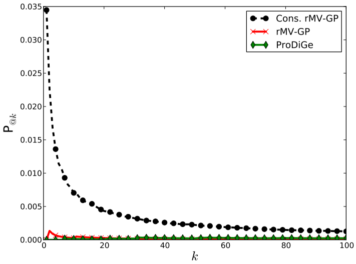
- **OMIM**: Set of manually-generated review articles linking inheritable diseases to one or a few genes ($M = 3,210,\ N = 13,614,\ J = 3,636,\ d = 0.0083\%$).
- **Medline**: Set of disease gene associations generated by processing annotations in the NIH PubMed/Medline literature ($M = 4,496,\ N = 21,243,\ J = 250,190,\ d = 0.36\%$).

Experimental Setup:

- "Known" diseases: randomly hidden associations.
- "New" diseases: randomly hidden diseases (*cold start*).

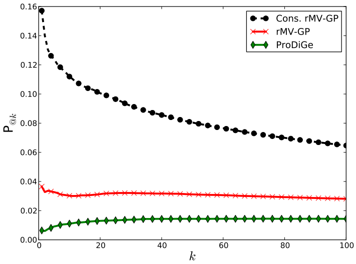
Results

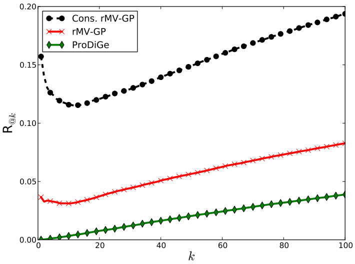
OMIM



Results

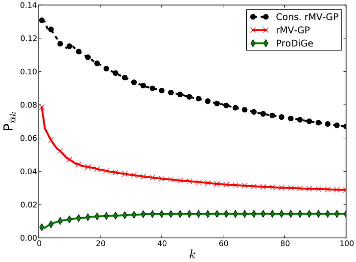
Medline "Known" Diseases

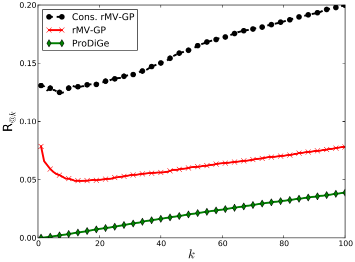




Results

Medline "New" Diseases





Predicted Candidate Genes

Alzheimer's Disease

Rank	Gene	Description
3	IGF1	Insulin-signaling protein linked to aging
9	MTHFR	Enzyme linked to cognitive impairments
15	IL1RN	Inflammatory marker linked to AD
16	APOE	Lipoprotein component linked to AD

Prostate Cancer

Rank	Gene	Description
2	CRP	Marker linked to onset age and survival
7	AGT	Downstream products linked to metastasis
9	VEGFA	Promotes blood vessel growth in tumors
13	MMP9	Protein linked to metastatic process

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Conclusion

Developed a framework for probabilistic inference subject to expectation constraints:

- constraints may be any combination of domain knowledge and data.
- constraint set may be nonconvex.

Applied the results to multitask learning:

- Constrained multitask learning and parameter estimation.
- Nonparametric multitask learning for transposable data.
- Multitask bipartite ranking for disease gene prioritization.

Future Work

- Constrained relative entropy inference is difficult to optimize using sampling techniques. These may be necessary for complicated problems.
- The presented inference approach can be extended to other divergence metrics such as Csiszár divergences and Bregman divergences.
- Hyperparameter optimization is the most challenging aspect of the current approach. More research is required to improve available methods for large scale problems.
- Further investigation is required to fully understand the biological implications of the multitask bipartite ranking model.

Thank You

Related Publications

- Oluwasanmi Koyejo and Joydeep Ghosh. Constrained Bayesian inference for low rank multitask learning. In *Proceedings of the 29th conference on Uncertainty in artificial intelligence (UAI)*, 2013b. (Oral)
- Oluwasanmi Koyejo and Joydeep Ghosh. A representation approach for relative entropy minimization with expectation constraints. In *Workshop on Divergences and Divergence Learning (WDDL)*, 2013a
- Cheng Lee, Oluwasanmi Koyejo, and Joydeep Ghosh. Identifying candidate disease genes using a trace norm constrained bipartite raking model. In *Engineering in Medicine and Biology Society (EMBC)*, 2013
- Sreangsu Acharyya*, Oluwasanmi Koyejo*, and Joydeep Ghosh. Learning to rank with Bregman divergences and monotone retargeting. In *Proceedings of the 28th conference on Uncertainty in artificial intelligence (UAI)*, 2012
- Oluwasanmi Koyejo and Joydeep Ghosh. A kernel-based approach to exploiting interaction-networks in heterogeneous information sources for improved recommender systems. In *HetRec '11*, pages 9–16, 2011

Related Publications

Submitted Publications

- Oluwasanmi Koyejo, Cheng Lee, and Joydeep Ghosh. Constrained relative entropy minimization with application to disease gene prioritization. 2013d. Under review
- Oluwasanmi Koyejo, Cheng Lee, and Joydeep Ghosh. A constrained matrix-variate Gaussian process for transposable data. 2013c. Under review
- Sreangsu Acharyya, Oluwasanmi Koyejo, and Joydeep Ghosh. Learning to rank with Bregman divergences and monotone retargeting. 2013. Under review

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- Mijung Park*, Oluwasanmi Koyejo*, Joydeep Ghosh, Russell R. Poldrack, and Jonathan W. Pillow. Bayesian structure learning for functional neuroimaging. In *International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2013
- O. Koyejo, P. Patel, J. Ghosh, and R. A. Poldrack. Learning predictive cognitive structure from fMRI using supervised topic models. In *International Workshop on Pattern Recognition in NeuroImaging (PRNI)*, 2013a
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- Richard Souvenir and Oluwasanmi Koyejo. Manifold learning and its applications: Reports of the AAAI 2009 fall symposia. *AI Magazine*, 31 (1):88–94, 2010

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Submitted Publications

- R. A. Poldrack, D. M. Barch, J. P. Mitchell, T. D. Wager, A. D. Wagner, J. T. Devlin, C. Cumba, O. Koyejo, and M. P. Milham. Towards open sharing of task-based fMRI data: The OpenfMRI project. 2013. Under review
- Oluwasanmi Koyejo, Sreangsu Acharyya, and Joydeep Ghosh. Retargeted matrix factorization. 2013b. Under review

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Miroslav Dudík, Steven J. Phillips, and Robert E. Schapire. Maximum entropy density estimation with generalized regularization and an application to species distribution modeling. *J. Mach. Learn. Res.*, 8:1217–1260, December 2007. ISSN 1532-4435.

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